

Transverse relaxation rate as a function of physiological parameters: Empirical modelling of Monte-Carlo data

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Introduction

As experimenters investigate ever more detailed questions using BOLD fMRI, interpretation of BOLD data will require increasingly sophisticated analysis techniques. Key to these analyses is a model of the dependence of BOLD signal on various physiological and physical properties. At present such models are constrained to asymptotic limits ('static diffusion regime' [1], 'motional narrowing regime' [2]) or are specific to low field strengths [3, 4]. In the current study we used Monte-Carlo modelling to estimate R_2' decay across a wide range of input parameters, and then modelled this data set empirically.

Methods

Monte-Carlo methods were similar to those used by Boxerman et al. [5]. Vasculature was modelled as networks of infinite cylinders, with a susceptibility difference between the intra- and extra- vascular spaces. Baseline blood volume fraction was varied between 1 and 4%. Protons diffused through these networks ($D = 0.7 \times 10^{-9} \text{ m}^2 \text{ s}^{-1}$, $1.45 \times 10^{-9} \text{ m}^2 \text{ s}^{-1}$ for extra- and intra-vascular spaces respectively) according to a 3-d Gaussian distribution (1-d Gaussian distributions across three orthogonal directions). A scaling factor applied to the diffusion co-efficient allowed re-use of the vessel networks for modelling of vessel radii from $1 \mu\text{m}$ to $50 \mu\text{m}$. At each time step ($dt = 0.1 \text{ ms}$) local field strength was calculated using the standard infinite cylinder equations (MKS units).

$$\Delta B_z = \begin{cases} B_0 \frac{\Delta\chi}{2} \left(\frac{R}{r}\right)^2 \cos(2\phi) \sin^2(\theta), & \text{outside cylinder} \\ B_0 \frac{\Delta\chi}{6} (3\cos^2\theta - 1), & \text{inside cylinder} \end{cases} \quad \text{Eq. 1}$$

(ΔB_z = change from B_0 . $\Delta\chi$ = susceptibility difference. R = vessel radius. \mathbf{r} = perpendicular from cylinder axis to proton. $r = |\mathbf{r}|$. θ = angle between the B_0 and cylinder axis. ϕ = angle between \mathbf{r} and projection of B_0 in plane orthogonal to the cylinder axis). The sum of ΔB_z across vessels was used to calculate precession frequency and thus phase shift at each time point for each proton. Phase shift was summed across proton path and averaged across protons to give a macroscopic Gradient-Echo signal decay. This decay was modelled as an exponential with decay rate R_2' .

Results

The resulting data sets were fitted empirically as a function of the baseline blood volume fraction (v), field strength (B_0), susceptibility difference ($\Delta\chi$), radius dependent term (p) and gyromagnetic ratio (γ).

$$R_2' = v \cdot \frac{\gamma}{3} \cdot B_0 \cdot \Delta\chi \cdot (1 - \exp(-p \cdot B_0 \cdot \Delta\chi)) \quad \text{Eq. 2}$$

The vessel radius dependent term p was found to be well modelled by,

$$p = K \cdot (1 - \exp(-a \cdot r^b)) \quad \text{Eq. 3}$$

where K , a and b are constants and r is the vessel radius expressed in microns (i.e. 1-50). Non-linear optimisation across the analytic Monte-Carlo data set yielded values of $K=4.88 \times 10^6$, $a=0.025$ and $b=1.73$. Equation 2 provided an excellent fit to the Monte-Carlo data (fig. 1).

Discussion

Data from the Monte-Carlo modelling formed a multi-parametric data set which was the subject of empirical modelling. A relatively simple model (eq. 2) was found to accurately and completely model the multi-parametric data space. This model has the advantages of explicitly including vessel radius, susceptibility difference, baseline blood volume and field strength effects while having only three free parameters. In its small asymptotic limit, the model was found to predict a quadratic dependence on susceptibility difference, in line with the literature [6]. In its large asymptotic limit, the model was found to be identical to a previous analytic model [1]. Although the Monte-Carlo simulations used in this paper still make use of several simplifying assumptions, they offer promise of much more realistic modelling efforts in the future.

References

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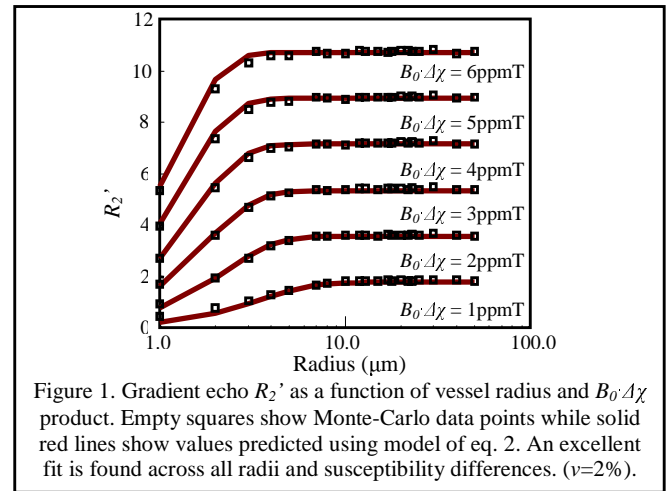


Figure 1. Gradient echo R_2' as a function of vessel radius and $B_0 \Delta\chi$ product. Empty squares show Monte-Carlo data points while solid red lines show values predicted using model of eq. 2. An excellent fit is found across all radii and susceptibility differences. ($v=2\%$).