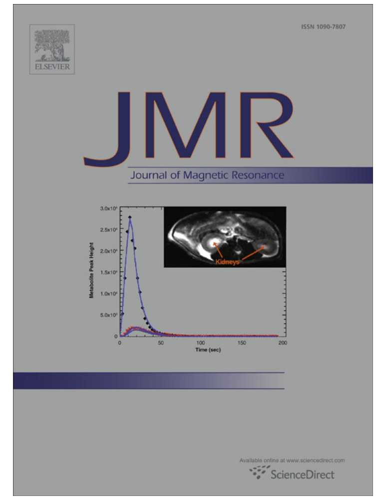
Accepted Manuscript



Exploring diffusion across permeable barriers at high gradients. II. Localization regime

Denis S. Grebenkov

PII: S1090-7807(14)00236-5
DOI: http://dx.doi.org/10.1016/j.jmr.2014.08.016
Reference: YJMRE 5500

To appear in: *Journal of Magnetic Resonance*

Received Date: 12 April 2014
Revised Date: 27 August 2014

Please cite this article as: D.S. Grebenkov, Exploring diffusion across permeable barriers at high gradients. II. Localization regime, *Journal of Magnetic Resonance* (2014), doi: http://dx.doi.org/10.1016/j.jmr.2014.08.016

Exploring diffusion across permeable barriers at high gradients. II. Localization regime

Denis S. Grebenkov

Laboratoire de Physique de la Matière Condensée,
CNRS – Ecole Polytechnique, F-91128 Palaiseau, France

Abstract

We present an analytical solution of the one-dimensional Bloch-Torrey equation for diffusion across multiple semi-permeable barrier. This solution generalizes the seminal work by Stoller, Happer, and Dyson, in which the non-Gaussian stretched-exponential behavior of the pulsed-gradient spin-echo (PGSE) signal was first predicted at high gradients in the so-called localization regime. We investigate how the diffusive exchange across a semi-permeable barrier modifies this asymptotic behavior, and explore the transition between the localization regime at low permeability and the Gaussian regime at high permeability. High gradients are suitable to spatially localize the contribution of the nuclei near the barrier and to enhance the sensitivity of the PGSE signal to the barrier permeability. The emergence of the localization regime for three-dimensional domains is discussed.

Keywords: Bloch-Torrey equation, permeability, diffusion, exchange, localization
PACS: 76.60.-k, 82.56.Lz, 87.61.-c, 76.60.Lz, 82.56.Ub

1. Introduction

Diffusion magnetic resonance imaging (dMRI) is a broadly applied non-invasive technique to study anatomical, physiological, and functional properties of biological tissues such as brain, skin, lungs, bones [1–6]. Since cells are separated from the extra-cellular space by semi-permeable cellular membranes, a reliable interpretation of dMRI signals requires accounting for water exchange across these barriers. Numerous works have been devoted to water exchange and aimed to estimate the permeability of cellular membranes [7–39] (see an overview and extended bibliography in [40]).

In most approaches, the dMRI signal is measured (or computed) at relatively small diffusion-encoding gradients g or b-values ($b \propto g^2$) at which the cumulant expansion of the signal can be truncated after the second-order term in the gradient: $S \simeq \exp(-bD_{\mathrm{a}})$. The estimated effective (or apparent) diffusion coefficient D_{a} can in turn be related to the permeability. This second-order approximation (known also as the Gaussian phase approximation), fails at high gradients [3, 41, 42]. Many models have been proposed to remedy this failure and to get a simple fitting formula for the dMRI signal in an extended range of applied gradients: kurtosis model based on the cumulant expansion [43, 44] and phenomenological models such as bi-exponential model [45–49], stretched-exponential model [50, 51], distributed models [52, 53], etc. These models start from the Gaussian dMRI signal and modify it in a convenient way. For instance, two Gaussian signals are superimposed in the bi-exponential model, while the next-order term of the cumulant expansion is included in the kurtosis model. Although these models are often successful in fitting experimental data on a broader range of gradients, none of them has addressed the theoretical question how the dMRI signal is indeed modified at high gradients.

In the seminal paper, Stoller, Happer, and Dyson predicted the emergence of the so-called localization regime at high gradients [54]. Since the motion of the nuclei near an impermeable boundary is more restricted, their local transverse magnetization is less attenuated, as compared to the bulk magnetization. This effect, known as diffusive edge enhancement, has been observed experimentally [55] (see also [56]). Stoller *et al.* provided a *non-perturbative* analysis of the one-dimensional Bloch-Torrey equation and obtained non-Gaussian asymptotic behavior of the dMRI signal at high gradients: $\ln S(g) \propto g^{2/3}$, in sharp contrast to the usual Gaussian form $\ln S(g) \propto g^2$ [54]. Moreover, de Swiet and Sen extended this non-Gaussian behavior to generic geometrical restrictions [57] while Hürlimann and co-workers have confirmed these theoretical predictions experimentally [58] (see reviews [3, 59] for details).

In the present work, we extend the concept of the transverse magnetization localization to *semi-permeable* barriers. Applying high gradients, one can eliminate the contribution from bulk diffusion in order to enhance the relative contribution of the signal coming uniquely from the nu-

Email address: denis.grebenkov@polytechnique.edu (Denis S. Grebenkov)