Numerical Analysis of NMR Diffusion Experiments in Complex Systems

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1. Introduction

The pulsed gradient spin-echo (PGSE) nuclear magnetic resonance experiment is now a formidable tool for probing porous media through geometry-dependent diffusive diffraction effects. However, for anything but relatively simple geometries numerical approaches must be used to model and interpret the experimental results. Here a simple, powerful, flexible and computationally efficient finite element method approach is developed and demonstrated. The results show that this new approach has great potential for modelling the results of PGSE experiments on real porous systems.

The study of porous media is vital to our continued understanding of physical systems, and further development of analysis techniques. Porous media can be on the nanometre scale, such as liquid crystal aggregates [1], to the 10-100 μm scale for systems such as human brain cells [2] and porous rock [3].

When diffusion is measured in a restricted system over a sufficiently long time period, the diffusion coefficient will become a function of the dimensions and shape of the restricting geometry [4]. This may lead to the appearance of diffraction-like effects in the echo attenuation profile at regular intervals that depend on the geometry and the magnetic gradient wave vector. Diffusion-diffraction peaks allow molecular motion to be used as a probe to characterise the porosity of the system. However, for diffusing systems more complex than unbounded free diffusion there are significant computational barriers to finding exact molecular models describing this effect [5]. For these complex geometries, numerical methods become necessary.

Numerical methods suitable for studying diffusion include Brownian dynamics simulations [6; 7], which are a subset of Monte Carlo simulations [8; 9; 10], and finite element differencing and analysis [11; 12]. Numerical simulations of both gas and fluid diffusion are common and these methods have been used to simulate PGSE experiments. Hagslätt *et al.* [13; 14] simulated a diffusion propagator and echo attenuation profile through finite element analysis. Similarly, Harkins *et al.* [15] employed finite element analysis in diffusion calculations, but only to calculate apparent diffusion coefficients. Direct simulations of the Bloch-Torrey equations are less common. Blees examined the effect of finite gradient pulses on the diffusion-diffraction profile of a planar pore using a finite differencing approach to solve the Bloch-Torrey equations that describe nuclear magnetism in the presence of diffusion [12], and it is this approach that has been extended to higher-dimensional geometries using finite element analysis.

2. Finite Element Analysis

Finite Element Analysis divides the domain to be analysed into a mesh of connected nodes called "elements," and converts the operating equation of the system into a series of simple numerical expressions. These simple expressions ("degrees of freedom") are computationally intensive by hand, but their iterative nature makes them suitable to be solved by a computer.

The restricting domains are created using CAD software, and the transverse magnetisation of the spin system at each element stored as a complex value, with second order or higher polynomials interpolating between these points. Integrating the equations with time dependence is performed using the Backwards Differentiation Formula, and analysis of the PGSE echo attenuation is performed by integrating across the entire boundary and normalising to the echo signal with zero magnetic gradient.

3. Conclusion

Preliminary results comparing analytical results calculated using the Short Gradient Pulse approximation to finite element simulations show excellent correlation. A numerical scheme for simulating diffusion during gradient pulses is presented, extensible to real-world problems such as the presence of background gradients in porous media. Finite Element simulation of the Bloch-Torrey equations is a very promising tool for the study of porous systems, and this technique should open up research into solutions to a variety of real-world problems.

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