WESTERN SYDNEY UNIVERSITY

Nanoscale Organisation and Dynamics Group

# Langevin dynamics as a tool for the modelling of restricted diffusion

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**Abstract**
Restricted diffusion within a pore space is commonly described in terms of the apparent diffusion coefficient, $D_{app}$, which can be measured experimentally using NMR. The time dependence of $D_{app}/D_0$ can be used to infer certain features of the pore-space morphology, making NMR diffusion measurements an invaluable tool for structural characterisation of porous media.

Calculation of $D_{app}$ from known pore-space geometry has traditionally been based on "geometric" considerations, whereby the diffusion propagator is found by solving the diffusion equation subject to the appropriate boundary conditions, and then translated into $D_{app}(\Delta)$. This is technically challenging for all but the simplest geometries, and no general analytic solution is known for a pore space with arbitrary boundaries. Short-Δ asymptotic analysis yields an analytic relationship between $D_{app}/D_0$ and the surface-to-volume ratio of the pore space. In the long-Δ limit, a similar relationship exists between $D_{app}/D_0$ and tortuosity. The latter is typically represented as an expansion in terms of $1/\Delta$ and $1/\Delta^{3/2}$; however, no comprehensive justification exists for the form of this expansion.

We present a novel method for the calculation of $D_{app}(\Delta)$ based on replacing geometric boundary conditions with an analytic potential representing the interaction between diffusing particles and the pore-space walls, and applying Langevin dynamics (LD) to model the diffusion of the particles under the assumption of local Boltzmann equilibrium. For proof-of-principle, we considered a classic model system, a stack of parallel semipermeable barriers. We obtained an analytic solution for $D_{app}(\Delta)$ in the long-Δ limit and compared it with the results of numerical LD simulations. The analytic solution was consistent with the numerical LD results, demonstrating the viability of the LD-based approach for semi-analytic evaluation of $D_{app}$ in the long-Δ limit for a pore-space with a periodic but otherwise arbitrary geometry. We discuss possible generalisations of the LD approach using *q*-space analysis, as well as the prospects of extending it to 2D and 3D pore spaces.

**Profile**
Dr Konstantin Momot is a Senior Lecturer in Experimental Physics at Queensland University of Technology. His research interests are centred around magnetic resonance spectroscopy and imaging and include experimental MR, molecular simulations and MR theory. His contributions to diffusion MR include the CONVEX and DQDiff experiments, diffusion NMR spectroscopy of model drug delivery systems, as well as applications of diffusion micro-MRI to a range of biological tissues and biomaterials.

**Staff and students at all levels are welcome to attend.**

**Venue and Time:**
This talk will be held on 9th March at 2:00 pm on the Campbelltown Campus in Building 21, Lecture Theatre 6 (CA. 21.G.18).

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