

## Spectrally Resolved Turbulent Flow in Porous Structures Using Modulated Gradient Diffusion NMR

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Introduction: Turbulent flow is relevant to fields such as meteorology, medicine, and chemical engineering. Turbulence has been quantified using pulsed field gradient NMR over the last 35 years. Despite widespread use, these measurements lack specificity, returning only the mean squared fluctuating velocity. Analogous to restricted diffusion, modulated gradient methods [1] have been proposed to measure the turbulent energy spectrum [2] thereby gaining more information on the microscale characteristics of the flow.

Methods: We simulated the NMR signal from computational fluid dynamics simulations. We consider two cases: (1) direct numerical simulation (DNS) of homogeneous turbulence [3] that resolves eddies at all scales. (2) large eddy simulation (LES) of a periodic Schwarz Diamond network [4]. Trajectories (Fig. 1) were generated from the velocity fields for use in the NMR simulations. The modulated gradients were designed using the workflow in [5].

Results and Discussion: The diffusion spectrum tensor for the homogeneous DNS obtained using simulated NMR was in excellent agreement with the ground truth. Because NMR operates in a Lagrangian frame (following nuclei along their trajectories), the power-law scaling of the diffusion spectrum is -2 and not -5/3 observed by optical and probe techniques. Simulated experiments on the LES were in poor agreement with the ground truth because the assumption of a Gaussian phase distribution was not satisfied. Instead, the phase follows a Laplace distribution (Fig. 2), illustrating the need for an appropriate theoretical formulation, or gradient waveforms that can produce a Gaussian phase distribution.

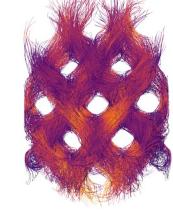


Fig. 1: Trajectories for turbulent flow in a Schwarz Diamond network used to simulate modulated gradient NMR experiments.

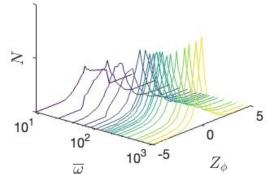


Fig. 2: Distribution of phase for simulated modulated gradient NMR experiments showing a Laplace distribution.

<u>Conclusions:</u> Modulated gradient diffusion NMR can accurately measure the turbulent diffusion spectrum provided that the assumption of a Gaussian phase distribution is met. This method allows for more detailed study of turbulence features such as isotropy, energy cascading, and dissipation in various systems. Experiment design for microimaging and preclinical systems is the subject of ongoing work.

References: [1] Callaghan & Stepišnik, J. Magn. Reson. (1995). [2] Dillinger, et al., Magn. Reson. Med. (2022). [3] Biferale, et al., TURB-Lagr Database (2024). [4] Clarke, et al., Chem. Eng. J. (Submitted) [5] Jiang, et al., Magn. Reson. (2023).