

Water Transport: Diffusion and Reaction

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Abstract

Porous media is known to greatly affect the diffusion behavior. Both effects have been explored to study the porous structure in order to understand the fluid flow. In addition to reduced diffusion constant, the diffusion propagator can be significantly different from bulk diffusion such as its Gaussian form. This behavior is reflected in diffusion behavior (such as kurtosis) as well as relaxation. For example, slow diffusion could cause multiple relaxation peaks in NMR relaxation spectrum for a single pore size. However, in real porous materials, pore size distribution also results in multiple or broad relaxation times. As a result, it is often difficult to differentiate the intrinsic complex diffusion behavior from the presence of pore size distributions.

We have studied several two-dimensional NMR methods in order to distinguish the presence of complex diffusion and the pore size distributions. For example, we have found unique features in the T1-T2 correlation experiment that unambiguously identify the slow diffusion behavior irrespective of the pore sizes. Also we design a 3-pulse-gradient echo (a version of the Double-Pulsed-Field-Gradient) experiment that could quantify the non-Gaussian diffusion behavior (such as kurtosis). Using analytical and numerical solutions of the diffusion dynamics and numerical simulation we have demonstrated these effects and found them consistent with experimental results. These new methods allow the investigation of porous media to extend beyond the language of average SVR.

Water transport is also important for chemical reactions in porous materials. An example is discussed on the degradation of polylactic acid. Poly(lactic acid) (PLA) is a bio-based, degradable polymer widely used in consumer products as well as industrial applications. After fulfilling its desired functions, PLA degrades into environmentally benign water soluble lactic acid. To accelerate this degradation at low temperatures, we developed a zinc oxide NP-PLA composition for oil and gas industry. Different water pools are identified using ^1H NMR T_2 spectrum and their evolution during the degradation process is measured in order to determine directly the rate of PLA hydrolysis. The NMR method allows a direct measurement of water imbibition and movement between different pools in the solid, heterogeneous/composite systems.