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PFG NMR Study of Liquid n-Hexane Self-Diffusion in the Bed of Porous Glass Beads

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1. Introduction

Prediction of transport behaviour of liquid species in porous materials with hierarchical porous structure is of primary importance for many branches of science and engineering. It concerns first of all chemical technology and biotechnology. It has also application in civil engineering, hydrogeology, oil production and many other spheres of action. The diversity and complexity of material with porous structure requires elaboration of concepts and approaches to predict transport behaviour on the basis of efficient measurement of appropriate characteristics, so called transport related structure characteristics. In the present study PFG NMR technique is applied to measure effective self-diffusion coefficients of liquid n-hexane in a set of model porous materials represented by (i) beds of compact glass beads of various size and size distribution and (ii) beds of porous glass beads containing pore systems of different size with relatively narrow size distribution.

2. Experimental and results

Samples of glass beads of two kinds were used to prepare unconsolidated beds of particles: (i) Compact glass beads were purchased from Glass spheres s.r.o. Jablonec nad Nisou. (ii) Glass granules CPG (controlled pore glasss) purchased from BDH chemicals Ltd. The properties of the samples used are summarized in Table I.

Table I Samples of glass beads

Sample number	Bead size [μm]	Pore size [Å]	Supplier
1	1-50	-	Glass spheres s.r.o. Jablonec nad Nisou
2	70-110	-	Glass spheres s.r.o. Jablonec nad Nisou
3	100-200	-	Glass spheres s.r.o. Jablonec nad Nisou
4	325-430	-	Glass spheres s.r.o. Jablonec nad Nisou
5	120-200	240	BDH chemicals Ltd.
6	120-200	370	BDH chemicals Ltd.
7	120-200	700	BDH chemicals Ltd.
8	120-200	1250	BDH chemicals Ltd.

Self-diffusion of n-hexane was measured in beds of beads ≈ 4.2 mm × 30 mm. The NMR tubes were randomly packed with beads and n-hexane was introduced by distilling upon glass sample outgassing.

Self-diffusion was measured using pulsed field gradient stimulated-echo technique. Measurements were carried out using spectrometer Bruker Avance 500 working at magnetic field of 11.7 T. All the measurements were carried out via observation of ^{1}H spins. The temperature dependence of diffusion coefficients was observed in the temperature region between 200 and 335 K. Another experimental parameter adjusted was diffusion time Δ which was varied in the region between 30 and 450 ms. The temperature dependences of n-hexane effective self-diffusion coefficients in porous media were compared with that for liquid n-hexane free of glass beads and the ratio of D_{eff} /D_0 were evaluated for situations where the porous medium appears to be pseudohomogeneous (e.g. Arrhenius plots of D_{eff} for porous medium is parallel with that for pure liquid n-hexane).

3. Examples of the results of PFG NMR measurements of self/diffusion coefficients

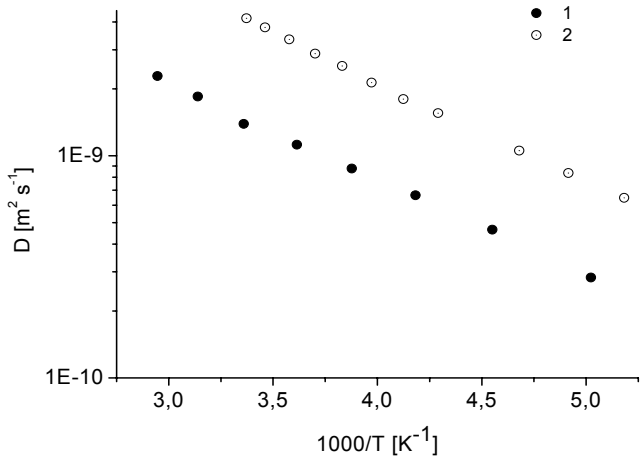

Fig. 1: **Temperature dependence of effective diffusion coefficient** 1 – diffusion coefficient in glass bed of sample 3; 2 – diffusion coefficient of pure liquid n-hexane

4. Conclusion

The ratio D_{eff}/D_0 was evaluated for a set of particle beds both with simple and hierarchical porous structure. The parameters D_{eff} /D_0 were related to quantity S/V where S and V stands for pore surface and volume, respectively.

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