Posudek práce

předložené na Matematicko-fyzikální fakultě Univerzity Karlovy v Praze

□ posudek oponenta□ diplomové práce
Autor: Mikulas Peksa Název práce: Investigation of matter transport by means of PFG NMR Studijní program a obor: Physics/ Biophyiscs Rok odevzdání: 2011
Jméno a tituly vedoucího/oponenta: Prof. Martin Hof Pracoviště: J. Heyrovský Institute of Physical Chemistry, Academy of Sciences of the Czech Republic Kontaktní e-mail: hof@jh-inst.cas.cz
Odborná úroveň práce: □ vynikající
Věcné chyby: ☐ téměř žádné
Výsledky: □ původní i převzaté
Rozsah práce: □ veliký
Grafická, jazyková a formální úroveň: □ velmi dobrá (graphics, of course, language, I cannot judge)
Tiskové chyby: I cannot judge
Celková úroveň práce: □ velmi dobrá

Slovní vyjádření, komentáře a připomínky oponenta:

The thesis deals with a topical issue consisting in description and measurement of species self-diffusion in heterogeneous (in particular porous) media. The application of this fundamental research can be found in many fields of human activity such as civil and mining engineering, chemical industry, hydrogeology and with a progressive tendency also in biophysics, biomedicine and related regions.

Although the NMR spectroscopy with pulsed gradients of magnetic field has been used for measurement of self-diffusion coefficients since long this is by no means any routine technique to investigate mass transport in porous or composite media. The applicability of the technique is dependent on spatial arrangement of material constituents e.g. pore size, pore shape and pore connectivity on one side and material properties (e.g. magnetic susceptibility of solid and fluid and transport and sorption properties of the fluid) on the other.

The author decided to follow in description of mass transport in porous media the approach based on transport-related structure parameters which separates the effect of pore structure from that of material properties of fluid. In contrast to macroscopic measurements of transport-related structure parameters which provides pore tortuosity and porosity of transport pores combined into a single non-separable quantity, NMR spectroscopy allowed a direct evaluation of material tortuosity. Due to the above strong dependence of NMR applicability on specific features of the porous materials the author selected for the study three substantially different types of porous media (i) model systems represented by assemblies of non-consolidated glass microspheres of various size, (ii) well characterised consolidated porous materials - alpha alumina ceramics and also porous glass and (iii) a material with a labyrinthic structure (high tortuosity factor) – geopolymer. As fluids the author used hydrocarbons (n-hexane), water and water solution of LiCl and similar salts.

The measurements of torutosity factors for all investigated types of porous materials was successful. The author managed the measurement and analysis of the dependence of apparent self-diffusion coefficient for long observation times. I understand that in the region of short observation times there are still some open problems and the present study is a good starting position for a future investigation. To this direction there are pointing my questions given below.

As to my best knowledge this study on self-diffusion of liquid fluids in porous media is the first of this kind accomplished in this country and I appreciate very much management of series experimental problems encountered by the author during this work. The author showed a deep theoretical knowledge of this rather complex subject.

Případné otázky při obhajobě a náměty do diskuze:

- 1. I know that the concept of *transport-related structure parameters* is well applicable to describe the transport of non-sorbing gaseous species in porous solids. My questions are: "Is it also the case for liquid fluids? What would happen if you use instead of n-hexane another tracer? Would be a tortuosity value measured with a particular liquid tracer applicable to describe e.g. the self-diffusion of the corresponding species in vapour state?
- 2. In conclusion presented on page 88 of the thesis, 2^{nd} item there is a statement that the parameter S_V (defined as ratio of porous system surface to porous system volume) is underestimated for pore size less than 50 µm. It is also reported that this discrepancy was established by comparison of porosity values. I could not find any such comparison in the text. I could find only the Figure 6.9 (page 68) with porosity values estimated using the parameter S_V obtained from NMR measurements. I would expect to find at this place a comparison with porosity data obtained from independent measurements based on measurement of sample volume, sample mass and density of glass microspheres. Can you comment on it.
- 3. I understand that the above discrepancy is due to some problems with accuracy of the measured dependence of apparent self-diffusion coefficient on observation time in the region of short observation times. Is there any idea how to improve the accuracy of NMR data in this region?

Práci □ doporučuji uznat jako diplomovou/bakalářskou.
Navrhuji hodnocení stupněm: □ výborně

Místo, datum a podpis oponenta: