DIFFUSION OF N-HEXANE AND ITS OXIDATION PRODUCTS IN POROUS MEDIA OF ACTIVATED CARBON

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Introduction

Wood is often used as a raw material for activated carbon . The product has an intricated capillary structure originating from the capillary structure of wood. Dispersed activated carbon is notable for high specific surface as well as for anisotropy of the volume inside micro-particles (in capillaries) and in the space between them. Process of n-hexane oxidation (by means of air oxygen) in the volume of activated carbon was investigated and dependence on topology of microstructure was discussed there.

Experimental

The study is based on previous works of investigation of reaction kinetics [1] and identification of reaction products [2]. Using activated carbon sample described in [1] reaction products consists of (mol fraction is shown in brackets): acetone (trace amount), propionic acid (0.25), methyl ethyl ketone (0.14),valeric acid (0.02) heptanone (0.13), heptyl aldehide (0.02), octanone (0.05), nonanone-2 (0.22) and nonanone-3 (0.16).

Microstructure of activated carbon was evaluated by means of scanning electron microscope JEOL 820 SEM in secondary electron mode. With the object operating additional information about spatial structure, bulk, particle and pycnometric densities of activated carbon sample were determined [3, 4]. Electron micrographs were scanned into computer's memory.

Results and Discussion

Using information mentioned above, the model consisting from topological units and reflecting microstructure of activated carbon was built. The whole dispersed bulk of carbon was divided into 3 different topological units: (a) the particles (consisting of capillaries and solid phase); (b) inter-particle space; (c) transition layer (Fig. 1).

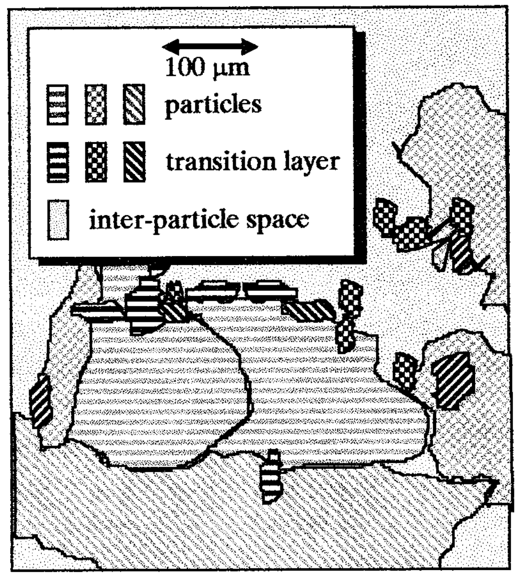

Figure 1. Computer developed model of activated carbon electron micrograph. Shading lines represent spatial arrangement of capillaries.

On the basis of discussed model spatial parameters of those topological units were determined. Results are presented in Tab. 1.

Table 1. Reconstruction of the spatial structure of activated carbon using electron micrographs and density measurement data.

Topological unit	Sp. volume; vol/cm^3	Sp. surface; sq/cm^2
Capillaries	0.30	0.068
Transition layer	0.41	0.200
Inter-particle space	0.13	0.130
Solid phase	0.11	0.602

Using data about spatial topology of activated carbon volume diffusion currents of n-hexane and its oxidation products in porous media were determined. Results are presented in form of weighed graph in Fig. 2.

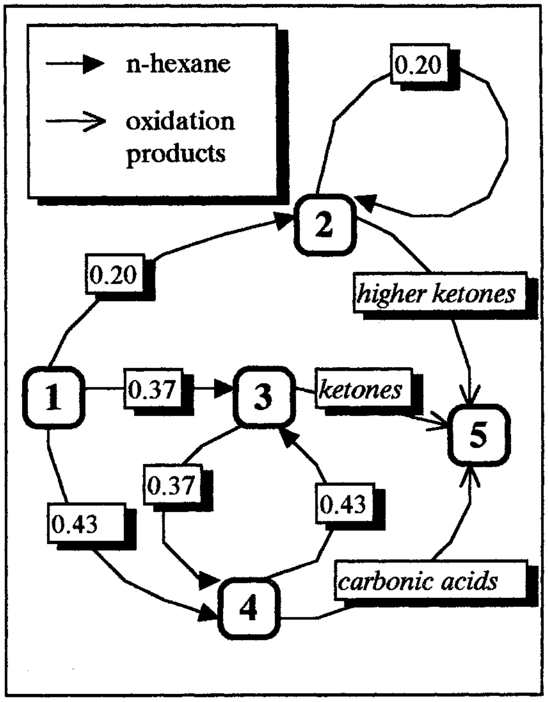

Figure 2. Graph model of diffusion of n-hexane and its oxidation products in porous media of activated carbon. Nodes: 1 - n-hexane in volume of non-porous reaction chamber; 2, 3, 4 - n-hexane in activated carbon volume (2 - capillaries; 3 - transition layer; 4 - inter-particle volume); 5 - products of n-hexane oxidation in the reaction chamber. Mol fraction of n-hexane in different topological units of activated carbon is also presented there.

Diffusion of n-hexane in bulk of activated carbon is determined taking into account specific volume and specific surface of topological units. During the process of intrusion one can see the domination of few weighed links in this graph. Mass transport into topologically inhomogeneous media (that exists in the volume of activated carbon) is divided between two currents. The diffusion between capillaries and inter-particle space is quite limited. Therefore, the part of n-hexane being intruded into capillaries should be isolated there. Another part of gaseous phase (in transitional zone and inter-particle volume) should be allowed to flow from one topological unit to another with fast equal probability.

Amount of those present products of n-hexane oxidation varies in large scale. Main part of them consists of carbonic acids and higher ketones. Search for correlation between amount of n-hexane intruded into topological units of carbon and amount of its oxidation products was done. Tests show being evident correlation there. Tendency towards formation of different oxidation products in different topological units is also seen. In capillaries and transition layer occurs formation of ketones, while inter-particle space favors production of carbonic acids. At the same time in capillaries occurs formation of products of higher molar mass.

Conclusions

Diffusion of n-hexane and its oxidation products in porous media of activated carbon was investigated. Products of oxidation were identified. Computer model of activated carbon microstructure based on electron micrographs and density measurements was built. Using this model process of intrusion of gaseous n-hexane into pores and inter-particle space of carbon was analyzed. There was ascertained that mass transport into topologically inhomogeneous media (that exists in the volume of activated carbon) is divided between two currents: into capillaries and inter-particle space/transition layer. Tendency towards formation of different oxidation products in capillaries and inter-particle space is also seen. In capillaries occurs formation of ketones with higher molar mass, while inter-particle space favors production of carbonic acids.

References

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