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The synthesis of functionalized silica materials using the flow microreactor

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Back in the early 90s of last century, hybrid organic-inorganic materials which include functionalized organosilicon materials have received serious attention from many scientists due to the potential of properties combination for creating the novel structures [1]. In general, functionalized silica materials are widely used as absorbents, catalysts, preservatives for live vaccines, fillers and rippers. The scope of application can be significantly enhanced by a deeper study of the surface layer and technological conditions of its formation. Consequently, it is possible to receive materials for various purposes by varying the nature of functional groups. The laboratory synthesis of such compounds has already been realized in the O.O. Chuiko Institute of Surface Chemistry [1]. But the experiment requires precise control of process conditions and considerable expenditure of time and reagents. Moreover, the sample does not give complete information about the structure of synthesized materials. These and other problems of an empirical investigation are successfully solved by modeling of reaction transformation in the special technological equipment. Nowadays, the most promising devices for chemical synthesis are flow microreactors [2, 3]. This fact is motivated by fundamental advantages of miniaturized reaction systems compared to conventional chemical equipment, namely: process intensification; inherent reactor safety; broader reaction conditions including up-to the explosion regime; distributed production; faster process development; easier scale-up of production capacity; lower costs for materials, energy and transportation; more flexible response to market demands; et al [3, 4, 5]. Moreover, practical experiments of different processes based on microreaction technology have proved that flow microreactors can be applied to green and sustainable production of chemical substances on industrial scales [3].

The benefits of microdevices described above give the grounds to assume that miniaturized reaction systems can be used to perform a synthesis of functionalized silica materials. On the other hand, by means of modeling of the functionalization process it is possible to provide clear guidance for sustainable chemical synthesis of substances with useful properties in chemical industry and technology, biochemistry, pharmaceutics and medicine [3, 6, 7].

By virtue of these arguments, carrying out the process of silica functionalization in the flow microreactor has the potential to optimize the entire process, while previous modeling allows considering different scenarios of materials synthesis.

So we divided our investigation into two major parts:

First, theoretical computer calculations are aimed to determine the most probable space restructuring of the silica surface layer functionalized with different groups (phosphinoxide, amine and thiourea groups).

The second stage is exploring of approaches to the modeling of different reactions and processes in the microreactor. The finite purpose of this step is to simulate the process of silica surface functionalization in the flow microreactor.

Construction and previous optimization of structures was performed with a help of molecular mechanics approximation methods using MM+ force field. For the quantum chemical calculations we used the method of density functional theory (DFT) B3LYP approximation with a local approximation of exchange-correlation potential (basis set 6-31 G(d, p)) [8].

In the following, we are going to develop the computational flow dynamic (CFD) model for the study of all microreactor hydrodynamic effects, heat transfer, mass transfer and parameters of the process with the help of suitable computer programs and methods. At present, there are a lot of successful commercial software packages for modeling complex chemical processes. The most popular of them are Aspen HYSYS, Aspen Plus, ANSYS, CHEMCAD, Pro II, Mathcad, COMSOL Multiphysics.

As a result of quantum chemical modeling of functionalized silica materials, the exact parameters of the structures were found. The adequacy of the results of quantum chemical modeling was confirmed by comparing the calculated values of IR (infrared) and NMR (nuclear magnetic resonance) spectra against the similar data of practical experience.

In accordance with the complexity of the functionalized materials synthesis has been proved the expediency of the flow microreactor implementation to carry out the process of silica surface functionalization. The next step of this investigation will be the development of a mathematical model of the functionalized silica materials synthesis in the flow microreactor and its realization in the appropriate software environment. Ultimately, a clear guidance for sustainable chemical synthesis and large-scale production of functionalized sorbents will be provided.

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