

Designing of the membrane's morphology with prescribed structure and diffusion properties

Preparation of a membrane with prescribed properties, which can provide a chance to control mass transport and decide about the time and number of particles released from the membrane is nowadays one of great importance scientific problems. In our previous papers it was shown that at intermediate and long time-scale the diffusion type depends on the membrane structure but not on the specific process that causes the movement. The effective diffusion exponent seems to depend on an average size of domains that are penetrated by randomly moving tracers and density of obstacles [1-3]. This work describes an attempt to create an accurate computer model of a particular morphology of membrane i.e. polymeric matrix with dispersed nanoparticles. In particular to develop a computer program to design the structure of membrane with prescribed the size and shape distribution of obstacles (nanoparticles, aggregates of nanoparticles). Good qualitative and quantitative agreement can be seen between graphical output of the models and microscopy images. The presented results may be used in the design and preparation of polymeric membrane with nanofillers for separation and pervaporation process.

[1] M. Krasowska, A. Strzelewicz, A. Rybak, G. Dudek, M. Cieřła, *Structure and transport properties of ethylcellulose membranes with different types and granulation of magnetic powder*, Physica A: Statistical Mechanics and its Applications, **452** 241 (2016)

[2] M. Cieřła, E. Gudowska-Nowak, F. Sagues, I.M. Sokolov, *Tracer diffusion inside fibrinogen layers*, Journal of Chemical Physics, **144** 044706 (2014)

[3] M. Krasowska, A. Strzelewicz, G. Dudek, M. Cieřła, *Structure-diffusion relationship of polymer membranes with different texture*, Physical Review E **95**, 012155 (2017)

Primary authors: STRZELEWICZ, Anna (Department of Physical Chemistry and Technology of Polymers, Silesian University of Technology, Gliwice, Poland); DUDEK, Gabriela (Department of Physical Chemistry and Technology of Polymers, Silesian University of Technology, Gliwice, Poland); CIEřŁA, Michał (M. Smoluchowski Institute of Physics, Jagiellonian University, Kraków, Poland); KRASOWSKA, Monika (Department of Physical Chemistry and Technology of Polymers, Silesian University of Technology, Gliwice, Poland)

Presenter: CIEřŁA, Michał (M. Smoluchowski Institute of Physics, Jagiellonian University, Kraków, Poland)