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Generation of prototype membranes with prescribed structure and diffusion properties comparable to real hybrid polymer membranes

This work aims to create prototype structures of hybrid polymeric membranes with the desired quantity, size and distribution of obstacles, which corresponds to the given amount of magnetite in the hybrid alginate membrane. The membrane is represented by a black and white image where the black regions corresponds to polymer matrix and are available for diffusive particles and the white ones are obstacles, which cannot be penetrated by tracer particle. The work describes two algorithms used to generate prototype membranes. The first method (algorithm A) subdivides the whole membrane into multiple square blocks, each of size z by z pixels. Each block can independently become an obstacle with probability equal to the given ratio of obstacles. The second method (algorithm B) accounts for the possibility of irregular, differently shaped obstacles. They are grown around randomly distributed seeds until desired amount of polymer matrix is reached. The membranes are characterized by the following characteristics: the amount of polymer matrix, the fractal dimension of polymer matrix, the average size of polymer matrix domains, the average number of obstacles in the proximity of each polymer matrix pixel. For both presented algorithms, generated membranes possessing specific parameters are comparable to the real hybrid alginate membranes filled with magnetite.

[1] G. Dudek, M. Krasowska, R. Turczyn, M. Gnus, A. Strzelewicz, Structure, morphology and separation efficiency of hybrid Alg/Fe₃O₄ membranes in pervaporative dehydration of ethanol, Separation and Purification Technology 182 (2017) 101–109.

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

Summary

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

Presenter: CIESLA, Michal (M. Smoluchowski Institute of Physics, Jagiellonian University, Kraków, Poland)

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