Simulation of gas diffusion in highly porous nanostructures by direct simulation Monte Carlo

A Direct Simulation Monte Carlo (DSMC) method is utilized to simulate gas diffusion in nanoscaled highly porous layers. An open source solver has been extended with the variable soft sphere (VSS) binary collision model and the inflow boundary model was adjusted for small numbers of DSMC particle initialization. Comparison with the analytical diffusion equation illustrate the improvement of the VSS model compared to the variable hard sphere model (VHS). Subsequently, several highly porous particle layers (gas sensors synthesized by flame spray pyrolysis and isotropic layers) build up by 10 nm particles have been investigated. Results for DSMC gas diffusion in the porous structures are in agreement with the well established dusty gas model (DGM). However, while DGM requires measurements or estimations of pore sizes, porosity, and tortuosity and furthermore is limited to homogenous layers, the present contribution shows significant advantages of DSMC in describing gas diffusion in non-isotropic porous structures.

General information
State: Published
Organisations: City University of Hong Kong, University of Bremen, Technical University of Denmark
Pages: 69–76
Publication date: 2014
Peer-reviewed: Yes

Publication information
Journal: Chemical Engineering Science
Volume: 105
ISSN (Print): 0009-2509
Ratings:
BFI (2019): BFI-level 2
Web of Science (2019): Indexed yes
BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Scopus rating (2017): CiteScore 3.44 SJR 1.043 SNIP 1.516
Web of Science (2017): Impact factor 3.306
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 3.05 SJR 1.039 SNIP 1.464
Web of Science (2016): Impact factor 2.895
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): CiteScore 2.96 SJR 1.022 SNIP 1.589
Web of Science (2015): Impact factor 2.75
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): CiteScore 2.81 SJR 1.104 SNIP 1.629
Web of Science (2014): Impact factor 2.337
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): CiteScore 2.95 SJR 1.145 SNIP 1.843
Web of Science (2013): Impact factor 2.613
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): CiteScore 2.77 SJR 1.172 SNIP 1.828
Web of Science (2012): Impact factor 2.386
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 2