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Multiscale transport concept for nanoporous materials incorporating microstructure and interface properties at nanoconfinement ARTURAS ZIEMYS, Houston Methodist Research Institute, MILJAN MILOSEVIC, Belgrade Metropolitan University, MILOS KOJIC, Houston Methodist Research Institute, MULTISCALE TRANSPORT TEAM — Transport theories based on the continuum hypothesis may not be appropriate, especially in case of diffusion, due to surface effects at nanoscale. Our computational and experimental findings, supported by studies elsewhere, revealed the necessity to account for interface and confinement effects. Thermodynamic aspects were established that might be responsible for reduced diffusivity at interface; more specifically – due to entropy-enthalpy compensation and cage-breaking processes. The thickness of liquid with altered diffusivity at solid-liquid interface depends on material and diffusing molecule nature and properties. We have developed a concept and computational model to bridge those molecular effects within nanoconfinement with transport at macro scale for systems where interface dominates over other properties (e.g. nanochannels, nanopores, polymers). The concept was validated against molecular transport through nanochannels and polymers. Novel parameters are introduced that determine diffusion regime and kinetics within the nanoscale confined fluids. New diffusion transport characteristics are established when nanochannel confining dimension approaches sizes of diffusing molecules, determining bounds of the non-Fickian transport regimes. The developed multiscale method could be used to study material transport and optimize nanoporous materials for biomedical and industrial applications.

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