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Concentration-Dependent Transport in Finite Sized Composites:

Modified Effective Medium Theory

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Abstract

Current models for transport in dispersions, while grounded in well-established effective medium theory (EMT), rely on the assumption of uniformity of the driving force. As consequence, theoretical approaches cannot accommodate driving force inhomogeneities as well as variations over the space occupied by the dispersed phase particles, and existing EMT-based models therefore fail to represent finite particle size effects. Moreover, because transport coefficients are generally considered uniform, such models largely pertain to the Henry's law region. Here, using the context of permeation in mixed-matrix membranes (MMMs), we introduce a self-consistent theory for transport in dispersion-based composites, which captures effects of isotherm nonlinearity and dispersant size without introducing fitting parameters, and accurately predicts concentration-dependent permeabilities. The model is validated against rigorous 3d simulations of transport in filler-polymer composite MMMs, with excellent agreement between theoretical results and those from simulation. Both model and simulations confirm isotherm nonlinearities to

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