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# Multicomponent Transport in Nanoporous Networks: Theory and Simulation

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**Abstract**

We present a new theory to estimate fluxes and effective transport conductances of binary mixtures through a membrane comprising a nonuniform porous medium with both pore size and pore length distributions, using the Onsager formulation at the single pore level. The theory defines a conductance of each species that is dependent on the concentration gradients of the various species, and on using effective medium theory determines the fluxes and concentration profiles self-consistently in the porous medium. The transport of $CH_4/H_2$ mixtures in a silica membrane having a known pore size distribution is examined using this theory, and the results compared with those from rigorous simulations, showing good agreement. It is found that an optimal network coordination number exists at which species fluxes are a maximum, due to the opposing effects of increasing porosity and mean pore length with increase in coordination number. Further, network fluxes decrease with increase in pore dispersion, indicating that uniform pore size is optimal. A species and pressure-dependent optimal temperature is also predicted, due to the competing effects of increase in diffusivity and decrease in adsorption on increasing temperature. It is seen that the $CH_4$ selectivity is very sensitive to temperature, and undergoes a cross-over, with the membrane being more selective to $CH_4$ at low temperature and to $H_2$ at high temperature. In general, the selectivity is very sensitive to the distribution of pore volume, and for bimodal pore networks, undergoes a sharp transition at the percolation threshold, when the smaller pore size is impermeable to the larger species, $CH_4$. The approach offers a convenient adaption of effective medium theory to multicomponent systems with nonlinear isotherms, overcoming drawbacks of existing theory.

**Keywords:** porous network, binary mixture transport, effective medium theory, oscillator model, Maxwell-Stefan equation

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