Understanding Facilitated Transport

While many separation processes can be carried out through the use of membranes, large units in the chemical process industry still are rare[1]. There are many reasons for this that include both technological and economic factors. Often, small fluxes of the solute through the barrier make membrane separations slow, inefficient and sometimes undesirable as compared to alternative technologies. There have been a large number of studies published in the literature that attempt to remedy this problem. One possible solution to increase fluxes in membrane separations is known as facilitated transport, which is a process whereby the permeation of a solute across a membrane is chemically augmented[2]. The concept of facilitated transport is deeply rooted in biology. For example, the transport of molecules from the bloodstream into cells is thought to be due to facilitated transport processes. Specialized membrane proteins have been developed that transport specific molecules across the cell walls; these species would otherwise have difficulty passing through[3]. Furthermore, molecules which can bind and solubilize an otherwise sparingly soluble species for transport purposes have been developed in biological systems. Not surprisingly, the first laboratory experiments which attempted to duplicate this phenomena focused on the steady state diffusion of oxygen across thin films of aqueous hemoglobin solutions[4].

Facilitated transport in synthetic membranes still is not well understood at a molecular level. Experimental studies of facilitated transport continue today, especially in liquid membranes. An example of a facilitated transport experimental apparatus is shown in Figure 1.

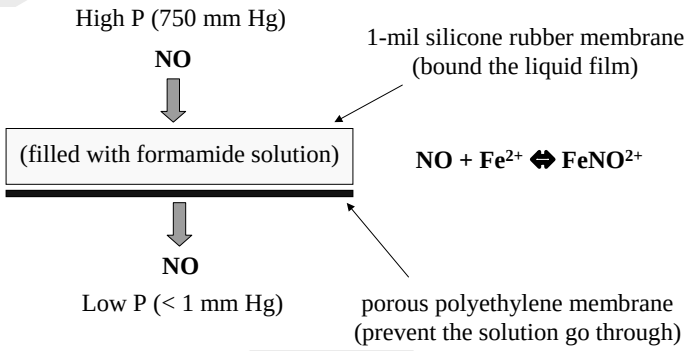

Figure 1: An example of an experimental apparatus to study facilitated transport, adapted from Reference 2.

The goal of this study is to use non-equilibrium lattice density functional theory to gain an understanding of the enhancement in transport rates through membranes. It has been postulated by many researchers that facilitated transport is due to the presence of an extra component, a carrier molecule, within the membranes[5]. The carrier has a high affinity for the solute; it can bind the solute and carry it across the membrane. The solute is released upon reaching the other side. Although the carrier-mediated diffusion process is almost certainly slower than pure Fickian diffusion (due to the larger mass of the complex), there is a sizeable increase in the solubility of the carrier-solute complex in the membrane over the unbound solute. This large increase in solubility is probably responsible for the enhancement of transport rates. Enhancement factors of between 2 and 20 (or even larger) have been observed in experiments.

In this study, the membrane is modelled to have a certain concentration of fixed (membrane) sites, carrier molecules, and holes. A large concentration of the solute is maintained on one side of the membrane, and a vacuum is held on the other. Diffusion is allowed by movement of the

Professor Marc Donohue
Department of Chemical Engineering
Johns Hopkins University

solute into the holes, a process by which it can move through the membrane to the other side. At any time within the membrane, solute also can bind to a carrier molecule to form a new chemical species, a complex. The solubility of the compounds in the membrane is controlled by adjusting the intermolecular interactions between all of the components in the membrane.

Our results to date suggest that facilitated transport does not occur if the carrier molecules have isotropic interactions. Hence, we currently are changing the model so these molecules have directional interactions. We believe this modification is necessary for facilitated transport to occur. Once proof of concept is demonstrated, future studies will involve the use of molecules with more realistic interactions, making comparisons with experimental data possible.

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Professor Marc Donohue
Department of Chemical Engineering
Johns Hopkins University