

Assessing the Coupled Heat and Mass Transport of Hydrogen through a Palladium Membrane

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As the energy prices increases and the supply of oil is limited, it becomes important to improve the efficiency of the most common industrial processes. The water-gas-shift reaction is one such process where one wishes to extract hydrogen from the reaction. For this purpose the membrane reactors are an interesting alternative to the more traditional reactors. This is mainly due to the opportunity for an *in situ* removal of the products (or of unwanted by-products from the chemical reaction), as well as the possibility of a high yield from equilibrium limited reactions. A thin palladium membrane separating two gas phases of hydrogen was used as a model system. The palladium membrane was chosen as it is purely selective towards transport of H₂. The coupled transport of hydrogen and heat through the membrane, including the dissociative adsorption and desorption of hydrogen at the surface, was studied as a one dimensional problem. This was done using the systematic approach of non-equilibrium thermodynamics. The membrane was considered to be a homogeneous system and the surface of the membrane was defined as the region between the gas phase and the palladium. In the system under consideration there are two such planar layers of molecular thickness; one at each side of the membrane. We show that with this approach, which deviates from Sievert's law, we are able to calculate the direct impact that a temperature gradient, or a heat flux, has on the hydrogen flux. Vice versa, we show how the dissociative adsorption reaction leads to heat sinks and sources at the surface.