A CFD Analysis of the Operating Conditions of a Multitube Pd Membrane for H2 Purification

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Abstract

The production of hydrogen is an important process for the chemical and energy fields due to its application on ammonia and methanol production, and as a green fuel. Currently, the production of hydrogen is achieved by steam reforming; hence, the purification of H2 from syngas is required. The purification of hydrogen using palladium membranes is encouraged due to their capacity to produce pure hydrogen inexpensively. Nevertheless, the behavior of multitube membrane modules is not predictable due to the vast variety of operational conditions and physics involved during the separation. Consequently, a CFD model using COMSOL Multiphysics® Software of a multitube palladium membrane module was developed using experimental data as the base of the model.

In this module, hydrogen enriched syngas is introduced as feed on the shell side, while the pure hydrogen is removed on the tube side. The simulation solved the continuity and Navier-Stokes equations for the given geometry. The physics involved were "Laminar Flow" and "Transport of Diluted Species". In order to simulate the hydrogen flux across the membrane boundaries, Sieverts' law was defined. In contrast with previous models which applied source and sink terms to simulate transport across the membrane, our model used a flux expression on the shell side which described the mechanism more accurately.

The model was used to understand the behavior of the module at different Reynolds numbers and residence times which affect the mass transfer resistances and Péclet numbers. The results of the simulation depicted hydrogen concentration profiles throughout the shell of the membrane module. It represented accurately, the concentration polarization formed by mass transfer resistances. These resistances are caused by the slow hydrogen diffusion through a hydrogen depleted gas layer adjacent to the membrane's surface as shown in Figure 1.

In addition, it was found that at high Reynolds number, the membranes were utilized more uniformly and more effectively (Figure 2). This phenomenon occurs since the depletion of hydrogen in the shell is reduced and the concentration polarization layer is reduced. The reduction of the polarization layer is caused by maximizing the effect of the advective forces of the flow and minimizing the effect of diffusion. The hydrogen recovery, which is defined as the percentage of hydrogen removed from the feed, decreased since more hydrogen was introduced to the membrane module.

Furthermore, the model showed that at higher residence times, better hydrogen recovery was achieved. This was the result of allowing diffusion to take place for a longer time. Although higher recovery was achieved, the utilization of the membrane was reduced. The membrane was not used effectively since hydrogen was separated at the beginning of the membrane as shown in Figure 3, and so there was no driving force for the rest of the membrane. The velocity of the feed was optimized by maximizing recovery and reducing concentration polarization.

Reference

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Figures used in the abstract

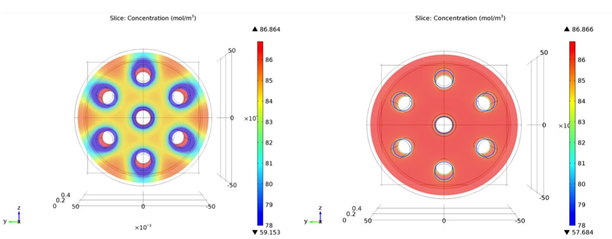

Figure 1: Cross-sectional concentration profiles at different Reynolds number. Left: Low Reynolds number; Right: High Reynolds number.

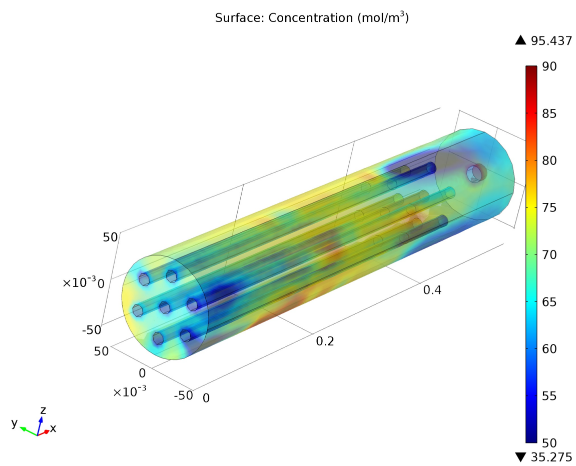

Figure 2: Concentration profile on the axial direction at a high Reynolds number.

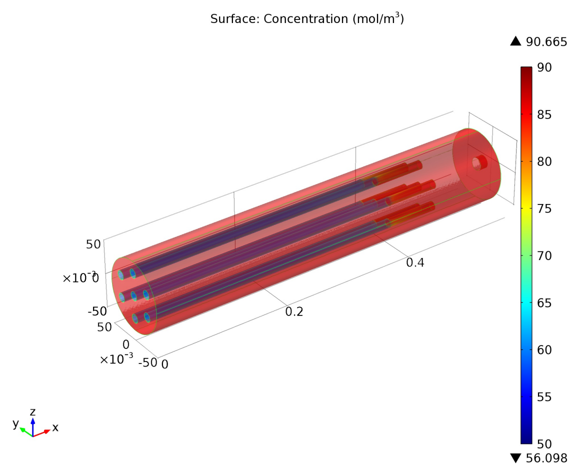

Figure 3: Concentration profile on the axial direction at a low Reynolds number.