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Fluid Dynamic Modeling of Hydrogen Permeation through Membrane

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Abstract*--In this investigation, computational fluid dynamics were used to simulate the diffusion of gases through membrane base on finite element analysis.The permeation of hydrogen transport through membranes has been modeled due to solving conservation equations for gas component in the feed/retentate and permeate sides of the membrane. COMSOL Multiphysics 3.5 software used to implement the mesh and solve the diffusion equations.The simulation results indicated that the removal of H_2 increased with decreasing the gas velocity in the membrane, the concentration gradients are of great interest to determine the local diffusion coefficient of hydrogen through the membrane The highest hydrogen permeation flux and the lowest hydrogen concentration on the membrane surface were obtained for ahigh gas flow rate in feeding section.

***Index Terms*-CFD, hydrogen permeation, hydrogen transport membrane, gas separation, molecular diffusion;**

I. INTRODUCTION

Diffusion is a process that allows ions or molecules to move from where they are more concentrated to where they are less concentrated. This process accounts for the movement of many small molecules across a cell membrane. Diffusion is the process by which cells acquire food and exchange waste products Diffusion is one of the main transport mechanisms in chemical systems. Molecular diffusion is in many cases the only transport mechanism in micro porous catalysts and in some types of membranes. Membrane gas separation is a dynamic and rapidly growing field due to the high selectivity and fluxes achievable by membranes, low energy requirements, and simple, easy to operate modules. As a result, membranes have the potential of acquiring a significant industrial role in the gas separation area, particularly if they can compete economically with traditional separation methods such as cryogenic distillation and pressure-swing absorption. The vast majority of commercial membrane systems are polymeric because of processing feasibility and cost. Today, membrane processes are used in a wide range of applications and the number of such applications is still growing. The technology inherits certain advantages over other methods. These advantages include compactness and light weight, low labor intensity, modular design that allows for easy expansion or operation at partial capacity, low maintenance, low energy requirements, low cost, and environmentally friendly operations [1]. Membrane materials currently used in gas separation application are understood to permeate and separate small molecules based on this mechanism [2]. For gas separation, the selectivity and permeability of the membrane determines the efficiency of the gas separation process and porosity is an important characteristic of such membranes The polymeric membranes used for gas separation can be classified into two classes based on flux density and selectivity: porous and non-porous. A porous membrane has highly voided structure with randomly distributed interconnected pores through out the polymer matrix. The gas separation process in porous membranes is mainly a function of the permeate and polymer membrane properties such as the permeate molecular size, pore size and pore-size distribution of polymer. Porous membranes used for gas separation can exhibit high fluxes but still provide low selectivity [3]. Nonporous membranes have been mainly used in gas separation. This type of membrane provides high selectivity or separation of gases from gas mixtures but the permeate flux is usually low. An important property of a nonporous membrane is that even gases of similar size may be separated if their solubility in the polymer differs significantly [4], Pandey and Chauhan In the 1990's, Generon, Praxair, and Medal had released new polymeric membrane with oxygen/nitrogen selectivity's of 6 –8. Thesemembranes could gas separation has grown into a $150million/year industry and the future membrane market has-been anticipated to reach $760 million/year by 2020 [5].The majority of the gas separations involve the separation of non condensable gases, such as N_2 from air, CO_2 from CH_4, and H_2 from N_2, Ar or CH_4. The concentration gradients through the membrane obtained by simulation are of great interest to determine the local diffusion coefficient of hydrogen through the membrane. In the present work, modeling of time dependent concentration profiles of H_2 through membrane was performed using commercial CFD Comsol multi physics based on finite element analysis. Delivered liquid nitrogen for nitrogen purity and offered a application has grown to many small users. This account for 2001, one-third of new nitrogen production, and currently, there are 5000 – 10,000nitrogen systems operating worldwide [5].Since hydrogen-separating membranes have been launched in 1980, membrane based cost-competitive alternative top reduce more than 99 %.

II. GEOMETRY OF MODEL

Three different coupled domains were considered in this investigation: permeate compartment, membrane and feed compartment. The geometry of the three domains is axis-symmetric and flow is introduced in axial position; as a consequence, the solution for the velocity has axial symmetry and can be solved in a two-coordinate system, The dimensions of the membrane contactor used for the numerical simulation are each compartments has area of $5x10^{-7}$ m^2 that are divided by the membrane of $1x10^{-6}$ m^2 and the membrane

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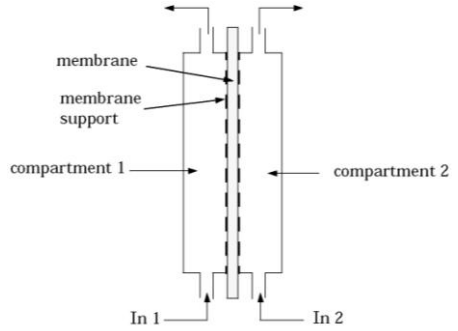
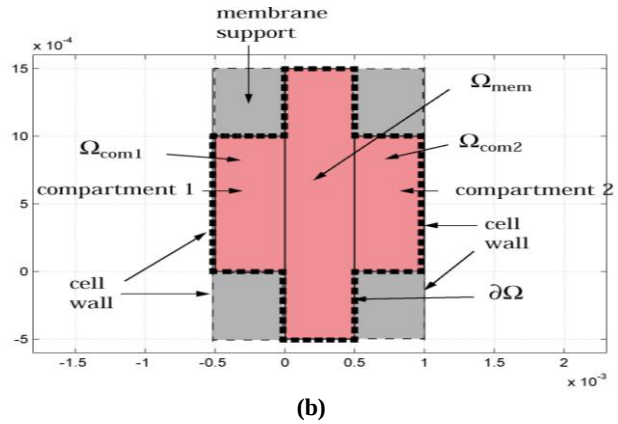
support, assume that the membrane support makes perfect contact to the membrane and constitutes an obstacle for the diffusion process. Further assume that the compartment between the support and the wall of the cell is closed. This implies that the compartments on each side of the membrane are confined by the membrane support at the top and bottom by the walls of the measuring cell on the sides. The schematic representation of a simple gas membrane process and boundaries of domain is shown in Figs. 1a and 1b. The mentioned system could be used to measure the hydrogen permeability through a membrane. In feed compartment introduce nitrogen with a low concentration of hydrogen. Only nitrogen would be present in permeate compartment at the beginning of the experiment. The model of our system is obtained by making a mass balance, as a function of time, for hydrogen diluted in nitrogen. Use the diffusion equation with neglect the transport of nitrogen through the membrane and the change in pressure due to the transport of hydrogen from one compartment to the other. Furthermore, neglect convection in the compartments and assume that the membrane contains the same amount of hydrogen per unit volume as the compartment.



(a)



(b)

Fig 1. (a) Cell unit. (b) Boundary of separation system

III. GOVERNING EQUATIONS

The gas flow in the permeate and feed compartments was modeled using the implementation of the Navier-Stokes and continuity equations in 2D. As there are not significant pressure gradients, the flow could be modeled considering a constant gas density in each compartment. For all the studied cases, the value of the Reynolds number in the inlet tubes was less than 35, therefore, laminar flow conditions could be assumed for the flow calculation in the compartments. For the permeate compartment, as the hydrogen concentration was low, conventional convection and diffusion were used to model the hydrogen transport [6]. The assumptions mentioned above make it possible to describe the system with the following equations:

A. Continuity equation

The unsteady-state continuity equation for the transport of H_2 inside the membrane, which is considered to be due to diffusion alone, may be written as:

$$\frac{\partial c}{\partial t} - D\nabla^2 c = 0 \quad (1)$$ For compartments

$$\frac{\partial c}{\partial t} - D_m \nabla^2 c = 0 \quad (2)$$ For membrane

Where c denotes concentration (mole m^{-3}), t time (s), D and D_m the diffusion coefficients in the compartments and in the membrane, respectively (m^2 s^{-1}).

Equations, 1 and 2 are solved with initial condition $c(0,x) = c_0$ in Ω_{com1} and $c(0,x) = 0$ in Ω_{mem} Ω_{com2}.

When the membrane is filled with gas phase, there are two mass transfer resistances for transport. These mass transfer resistances include transfer of hydrogen from the bulk gas to the membrane wall and diffusion across the pores of the membrane to the membrane–absorbent interface, where a chemical/physical change takes place.

B. PDE model

In Comsolmultiphysics the velocity profile through the separation cell due to following PDE mode

$$e_a \frac{\partial^2 u}{\partial t^2} + d_a \frac{\partial u}{\partial t} + \nabla.(-c\nabla u + \alpha u + \gamma) + \alpha u + \beta \nabla u = f \quad (3)$$

For simplicity, assume that the coefficients are $\alpha = \beta = \gamma = 0$ and $c = f = da = 1$ in present model

IV. MODELING

The concentration gradients through the membrane obtained by simulation are of great interest to determine the local diffusion coefficient of hydrogen through the membrane. An FEM model was proposed using Comsol Multi physics software to determine the repercussion of the coating layer on the hydrogen diffusion and on the effective diffusion coefficient, the software used to implement the mesh and solve the equations. Which is an efficient tool for modeling complex systems for which fluid dynamics and mass and heat transfer are relevant.

A. Domain definition

The permeability of the membrane is measured by introducing the species of interest in a carrier gas on one side of the membrane and the pure carrier gas on the other side of the membrane. The composition in the two compartments, on

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each side of the membrane, is measured as a function of time in order to estimate the permeability of the species diluted in the carrier gas. The system that will be treating is similar to the one used to measure the permeability of gases in membranes three different coupled domains was considered: permeate compartment, membrane and feed compartment. The geometry of the three domains is axis-symmetric and flow is introduced in axial position; as a consequence, the solution for the velocity has axial symmetry and can be solved in a two-coordinate system using Cartesian coordinates. This fact reduces the computing effort to solve the problem without loss of precision.

B. Meshing

Figure 2 shows a detail of the meshes used for the geometry of the simulated cell dimensions, in order to ensure that the solution obtained was grid independent, the necessary level of the refining mesh was studied for the reference case. The mesh was gradually refined starting from a coarse mesh (250 elements). For a total number of cell elements greater than 4000, we observed that the modulus of the relative error of the hydrogen balance for the entire rig was less than 0.1%. The meshes were refined at the interfaces between domains and the areas with changes of flow direction that were detected in the preliminary calculations. For the reference case, the final numbers of mesh elements was 2656 for the membrane geometry and 1376 for the permeate and feed compartment, respectively.

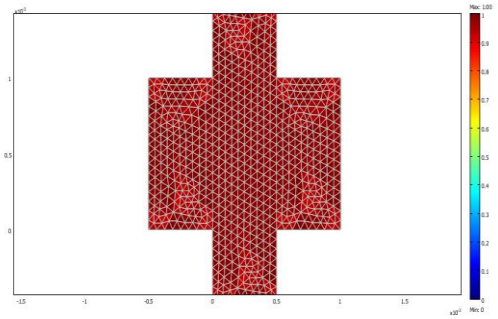

Fig. 2 meshing of simulated model.

V. RESULTS AND DISCUSSION

A permeability of hydrogen through membrane has been simulated using Comsol multi physics 3.5, the simulated results have been presented graphically. The CFD simulation of the concentration profile through membrane as shown in Fig.3. It's clear that the surface of diffusing species, hydrogen, is introduced in compartment 1 at the beginning with initial concentration of 0.3mol/m^3. The ceramic membrane used in the simulations is porous and is the most important part of the membrane contactor. The ceramic membranes for gas separation are very tortuous and can provide high concentration difference across the membrane. As the hydrogen flows through the feed side, it is transferred towards the membrane pores due to the concentration gradient. Significant concentration change across the ceramic membrane shows that the main concentration change occurs in the membrane side, i.e. main mass transfer resistance is located in this part. It is due to high tortuosity of the applied membrane which provides a long path for transport of H_2 through the membrane pores.

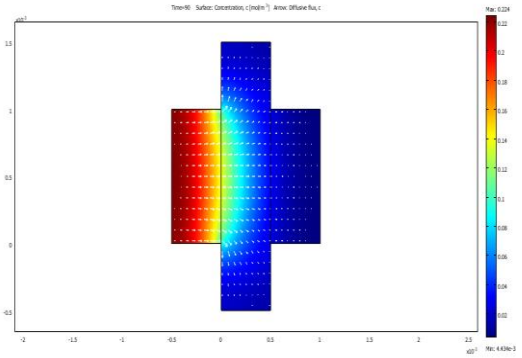

Fig.3 Concentration profile of H_2 in the menmbrane, surface is distribution of hydrogen and arrow is concentration profile.

The diffusion flux against arc length was plotted in Fig. 4, for time intervals of (0-300 sec) with increment of 30 sec at the membrane interface, It's observed that the flux has a shape of parabolic function with maximum values at a center of distance in feed compartment, the diffusive flux will be decrease with increase of diffusion time it has a value of 0.149 mole/m^3through the first 30 sec and becomes0.099 after 300sec.

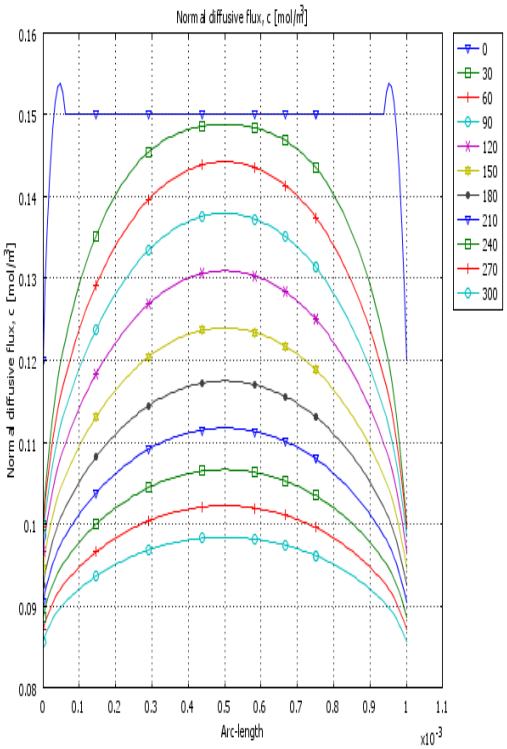

Fig.4 Diffusion flux profiles against arc length in feed compartment for different time period.

The velocity distribution and concentration gradient as shown in Fig. 5.

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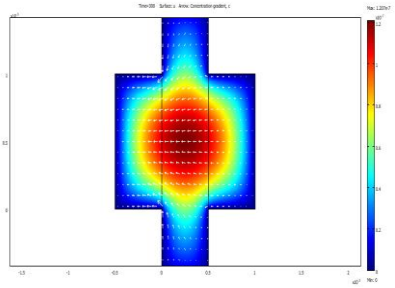

Fig.5 velocity distribution through cell, surface: velocity profile of hydrogen and arrow: concentration gradient.

VI. CONCLUSION

Computational Fluid Dynamic approach was used to simulate the diffusion of gases through membrane and continuum flows on the feed/retentate and permeate sides of membrane. In this approach, model the membrane by creating a bounded region separating the feed/retentate side from the permeate side in which only the phenomenological equations of the activated gas transport model apply. COMSOL multi physics was employed to solve the model equations, continuity equations for H_2 in the feed/retentate and permeate sides of the membrane. The simulation results indicated that the removal of H_2 increased with decreasing the gas velocity in the membrane. The model predictions also reveal that the main mass transfer resistances for transport of H_2 are located in the membrane and gas phase. Ceramic membrane has the highest resistance because of its high tortuosity.

VII. ACKNOWLEDGMENT

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