

## Measurement of Permeation Parameters of Hydrogen in HDPE

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### Introduction

When high-density polyethylene (HDPE) is used to contain the H<sub>2</sub> gas under high pressure, a certain amount of H<sub>2</sub> gas permeates through the HDPE. To understand the mass transport behavior, we need to estimate the permeation parameters of the system. In the experiment, a HDPE sample is undergoing a suddenly applied pressure maintained for several hours followed by a low pressure maintained for several hours at constant temperature. Pressure, time, and flow rate were measured and used to estimate the parameters. Some techniques previously used to estimate these parameters which described in [1] which used some portion of data or only the pressurization process. We, however, introduce a new approach to estimate the pressure dependence permeation parameters under a pressurization-depressurization cycle which uses both transient data and steady state data.

### Theory and Model

The theory of diffusion in a plane sheet of one-dimensional isotropic matrix is well known. Diffusion of a low molecular weight gas permeating through rubbery polymers is Fickian, for which the diffusivity coefficient is independent of the gas concentration in the polymer and the solubility follows Henry's law [2]. By these assumptions, a one-dimensional diffusion model was developed with the method of Green's functions. Then the mathematical model was used to estimate the parameters. The parameters were varied, through the use of a curve-fitting technique, to obtain the best fit between the model and the experimental flow rate in both transient and steady state phases.

### Results and Discussion

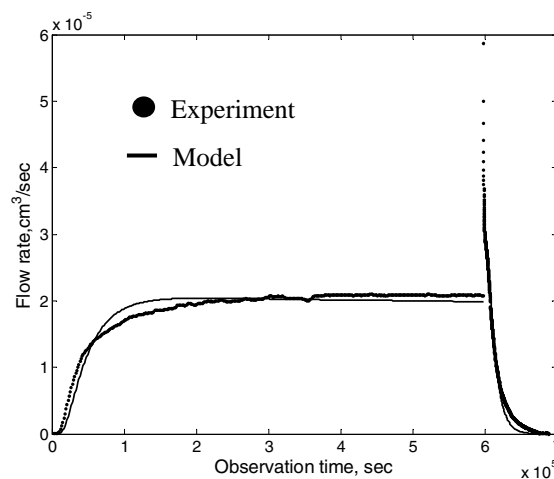
The H<sub>2</sub> gas flow rate from the experiment and model were plot against time as shown in Figure 1. The model flow rate is calculated using permeation parameters which are diffusivity coefficient and solubility from the best fit.

For the pressurization process, the pressure dependent flow rate was calculated from the solution given by the method of Green's function [3]. The model gave a best fit in the early time and late time portion of the flow rate profile. The early time portion is strongly influenced by the diffusivity coefficient while the late time portion is influenced by the solubility. The diffusivity coefficient

and the solubility are  $4.156 \text{ e-}07 \text{ cm}^2/\text{s}$  and  $6.838 \text{ e-}14 \text{ kmol/Pa/cm}^3$ , respectively.

In the depressurization process, the permeation rate is not a function of pressure. The best fit occurs in the early time and late time region. However, the permeation parameters were found to be different compared to pressurization. The diffusivity coefficient and the solubility are  $1.320 \text{ e-}06 \text{ cm}^2/\text{s}$  and  $2.188 \text{ e-}14 \text{ kmol/Pa/cm}^3$ , respectively.

This measurement method can be used to study H<sub>2</sub> gas and HDPE under repeating pressure cycles such as in components associated with fuel cells and gas pipes.



**Figure 1. Experimental and the model (using the best fit parameters) gas flow rate in a high pressure and low pressure cycle.**

### References

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- [2] M. H. Klopffer, B. Flaconeche, and P. Odru, "Transport properties of gas mixtures through polyethylene", *Plastics, Rubber and Composites*, 36 (2007), 184-189.
- [3] J.V. Beck, K.D. Cole, A. Haji-Sheikh, and B. Litkouhi, *Heat Conduction Using Green's Functions*, Hemisphere Publishing Corp., New York, 1992.