FMRI RET 2016- Rate of Sorption of Chloroform into Polymers using a Quartz Crystal Microbalance

Robert Herzog[1], Dr. Scott Campbell[2], Jonathan Samuelson[2], Greg Barone[3]

1. Strawberry Crest High School; 2. Chemical and Biomedical Engineering, University of South Florida; 3. King High School

Abstract

The sorption rate of chloroform into Polyethylene glycol (PEG) and Polystyrene (PS) was determined using a quartz crystal microbalance[1]. A diffusion coefficient was calculated for several levels of exposure of chloroform for each polymer using finite and infinite slab analyses for comparison.

Background

The full apparatus housing for organic vapors and polymer coated quartz crystal

Due to long time scales being necessary in order to measure sorption of organic vapors into polymers, one approach is to use very thin layers of polymers in solubility measurements. This can be achieved by taking advantage of the high sensitivity of a quartz crystal microbalance to small changes in mass as measured by frequency (f) shifts that result from changes in mass.

Mounted Quartz crystal ready to be placed in temperature controlled cell.

Objectives

The diffusion rates of several organic vapors into different polymers were first examined to find a system that presented a good opportunity to examine diffusion rates. Upon selecting a suitable system different methods of analysis were explored to find a method of determining sorption rates at different levels of exposure.

Approach

Two methods of analysis were employed for comparison; the infinite slab analysis, which is more accurate at short time durations and the finite slab analysis, which is more accurate at longer time durations. Both analyses are based on the relationship as described by Fick's Law:

$$\partial C / \partial t = D \partial^2 C / \partial x^2$$

Where C is the concentration of the organic vapor, t is the time of exposure of the polymer to the organic vapor. X is the distance the organic vapor has diffused into the polymer and D is the diffusion coefficient of diffusion

For the finite slab analysis the following is assumed and the equation for deriving the diffusion coefficient is as follows:

at $t = 0$ $C = C_0$ for all x
at $x = 0$ $C = C_{eq}$ for all t
at $x = L$ $\partial C / \partial x = 0$ for all t

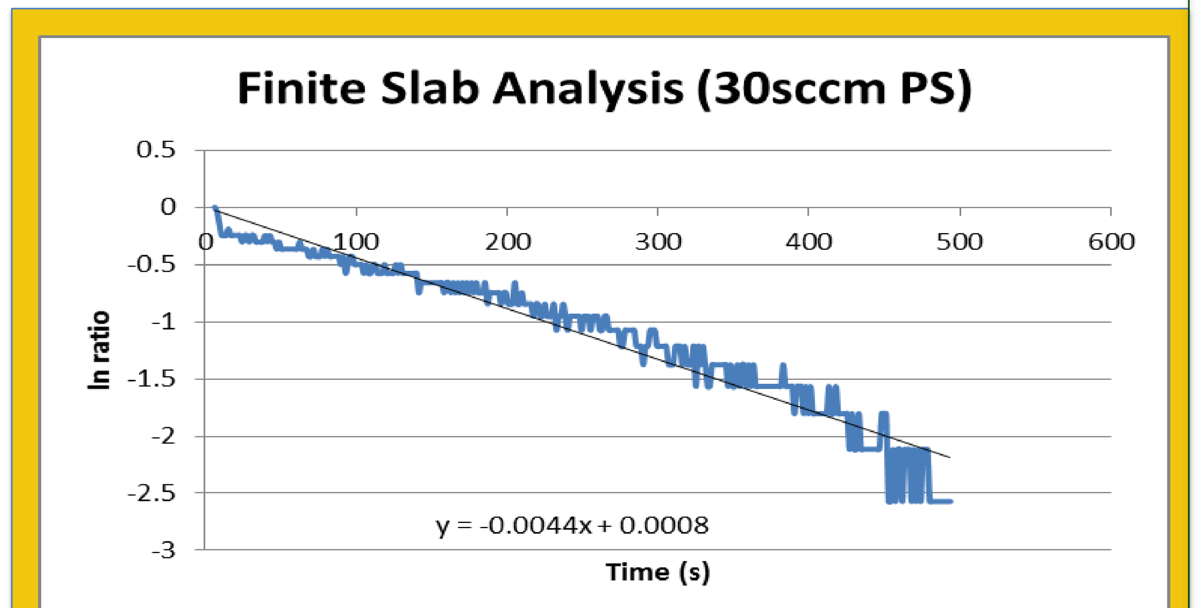
The mathematical solution of Fick's law with these conditions results in the equation below:

$$\ln R = \ln 8/\pi^2 - \pi^2 Dt/4L^2$$

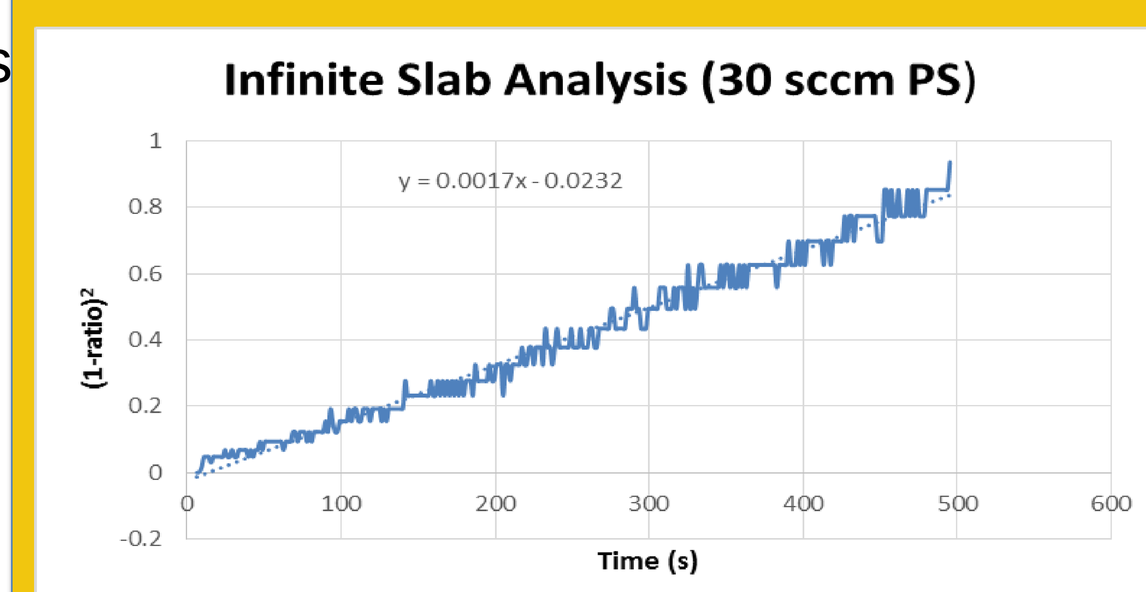
For the infinite slab analysis the following is assumed:
at $t = 0$ $C = C_0$ for all x
at $x = 0$ $C = C_{eq}$ for all t
At $x = \infty$ $C = C_0$ for all t

Under these conditions the mathematical solution of Fick's law results in the equation below:

$$(1-R)^2 = 4Dt/L^2\pi$$



Above: Infinite slab analysis of PS at 30sccm
Below: Finite slab analysis of PS at 30 sccm



Where L is the maximum thickness of the polymer coating and $R = f - f_{eq} / f_0 - f_{eq}$

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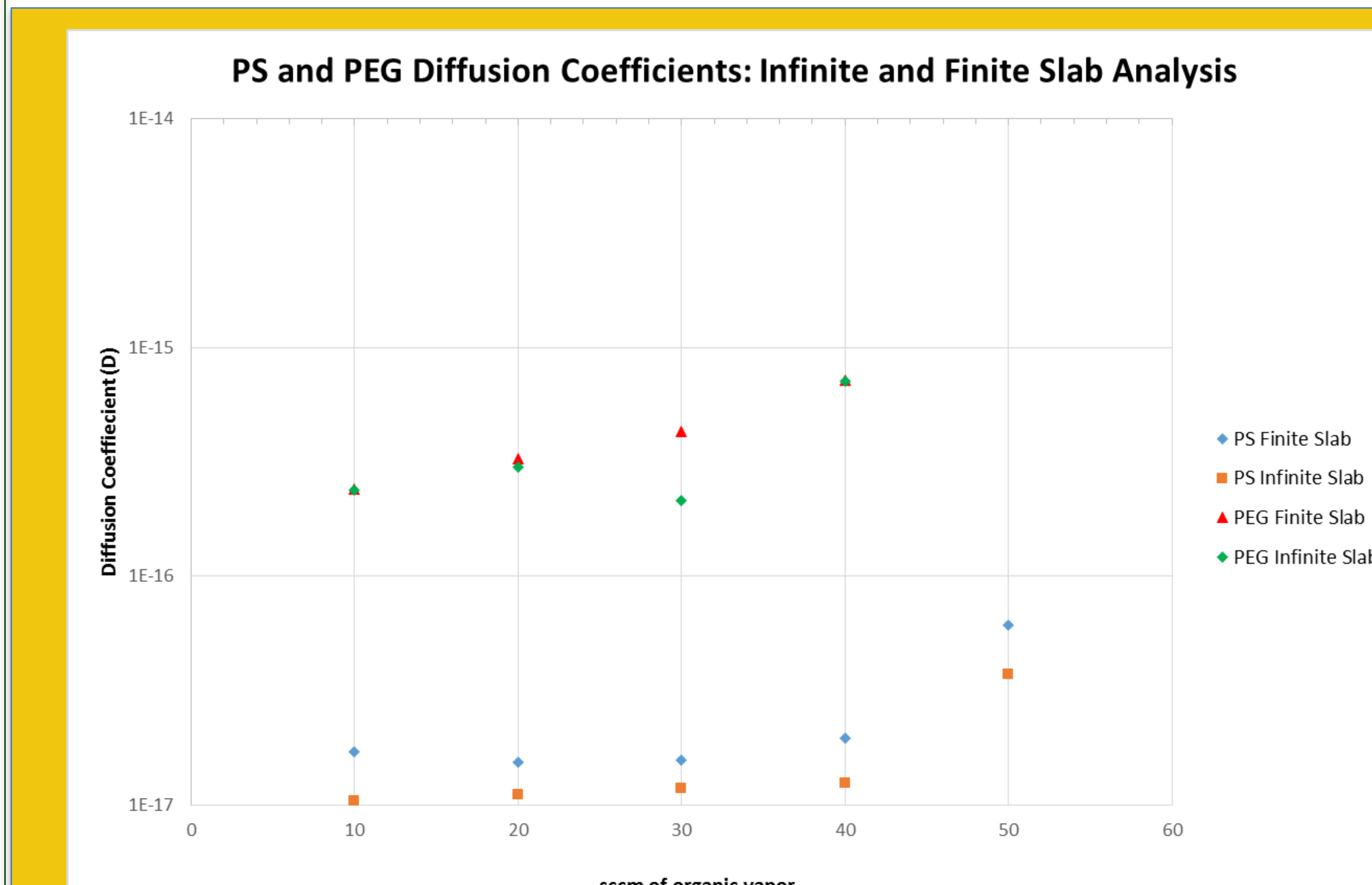
Conclusions

Both the infinite slab and finite slab analyses yielded diffusion coefficients that were not significantly different for a given polymer when exposed to chloroform. This suggests that either analysis might alone be suitable for future experiments on an individual polymer although due to the ease of use both analyses are recommended.

The results showed that PS had a significantly lower diffusion coefficient than PEG at 10 to 40sccm exposures of chloroform vapor when analyzed with both the infinite and finite slab analysis.



Diffusion coefficients for PS and PEG as determined by the infinite slab and finite slab analyses. Within each analysis type and polymer no significant differences were observed (error bars not shown).

Referenced Resources

1. Wong, Howard C., Scott W. Campbell, and Venkat R. Bhethanabotla. "Sorption of benzene, toluene and chloroform by poly (styrene) at 298.15 K and 323.15 K using a quartz crystal balance." Fluid phase equilibria 139.1 (1997): 371-389.

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