Finite Element Analysis Used to Model VIP Barrier Film Performance

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1 Introduction

The barrier film is the most critical component in vacuum insulation panels (VIP). It is required to maintain the low pressure in the panel. Many applications of VIP require a life of 10 to 50 years or more. Through the last about 5 years a great deal of improvement has occurred in barrier film performance. Often barrier oxygen transmission rates (OTR) are lower than what can be measured in laboratory tests. As developers try to further improve barrier performance the improvement can not be quantified through testing. An example is a two metallized layer barrier could have an OTR less than 0.0005 cc/m²day by ASTM D3985 23 ºC 50%RH testing. The 0.0005 OTR is the lowest value that can be measured in laboratory testing. A three metallized layer barrier would also have stated performance of less than 0.0005 OTR. This situation results in not being able to provide feed back to the barrier film developer and not allowing the VIP manufacturer and user to be able to predict performance versus time benefit from the improved barrier.

This paper describes the use of Finite Element Analysis (FEA) computer models to estimate the impact of barrier film design changes when the actual transmission rate is lower than the current ability to measure through testing.

2 Theory

VIP barrier films reduce the transmission of oxygen, nitrogen, and other atmospheric gases such as water vapour. The mechanism of transmission for water vapour can be different from oxygen transmission. The modelling technique described in this paper does not apply to water vapour transmission (MVTR). MVTR is tested by ASTM F1249-90 and currently barrier performance in MVTR is not at the limit of the ability to test. Also although water vapour can be very detrimental to VIP performance, desiccant can be used inexpensively and very effectively to reduce or eliminate the water vapour effect on VIP.

Oxygen diffusion through a barrier can be approximated by Fick's 1st law, which states:

$$j_i = D_{ij} \frac{dc_i}{dx}$$

Where the variables are rate of diffusion (j) of matter (i) where D_{ij} is diffusion coefficient of the matter i in a medium j, and $\frac{dc_i}{dx}$ describes the concentration gradient in the diffusion direction. Fick's law is very analogous to Fourier's law governing conductive heat transfer which states:

$$q = -kA\frac{dT}{dx}$$

Where q is the heat transfer in the x direction, $\frac{dT}{dx}$ is the temperature gradient in the x direction, A is the area normal to the temperature gradient, and k is the thermal conductivity. The above similarity in the equations allows us to use a FEA computer program running a thermal conductivity analysis to model a diffusion problem. The diffusion model can be three dimensional with multiple layers and multiple material properties and local defects. If the data were available, it could even include the change in diffusion rate with temperature.

FEA Model assumptions

[Decker 2002] report typical values of permeation for basic polymers such as PET are 100 $cm^3 O_2/m^2$ day atmosphere at 12 µm. A commercial single metallized layer barrier has an OTR of 0.055 and a two metallized layer barrier from the same company has an OTR of less than 0.0005. If the metallized layer represents a homogenous diffusion resistance then the two layer design should have an OTR of 0.0275 or half the single layer. Clearly something has caused the more than 110 times reduction in OTR. As suggested by [Decker 2002], it is more realistic to assume the metallization layers have pinhole defects. In the single layer O_2 diffuses through the pinhole with very little going through the metallized polymer film that does not have a pinhole. In the two layer barrier the O_2 diffuses through the pinhole in the first layer and then must diffuse out from the pinhole through the polymer supporting the second metallization layer until a pinhole is found in the second layer. This multi-layer pinhole theory could account for the observed huge increase in performance between a single layer and two layer designs and will be the basis of our FEA model.

3 Construction of the FEA model

To construct a barrier film model we have the thickness of each layer but we need to know what size to make the pinhole and how far apart the pinholes should be. The area of the pinhole and the distance between the pinhole in one layer to a pinhole in the next layer will represent the average of real world values specific to a particular metallized film. These are two big unknowns. We will use the two real world data points for a single metallized layer and two metallized layer barrier designs that came from one manufacturer to determine the average pinhole area and average spacing. This gives us our two equations for our two unknowns. At this point it should be mentioned that all metallization layers are not the same. They can vary widely based on polymer surface conditions, process conditions, etc. Thus, the general modelling approach can be used for many applications but the exact pinhole area and diffusion distance between pinholes will vary widely from product to product. Figure 1 below is a diagram of the pinhole model.

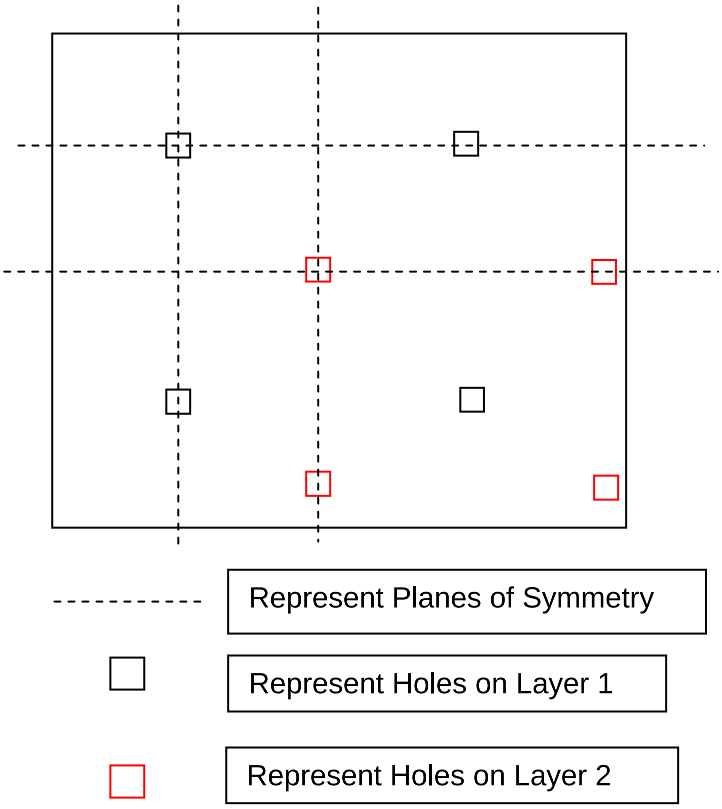

Figure 1: Pinhole model with planes of symmetry.

Nothing beyond a plane of symmetry needs to be included in an FEA model. Thus the FEA 2 layer model is reduced to the representation below.

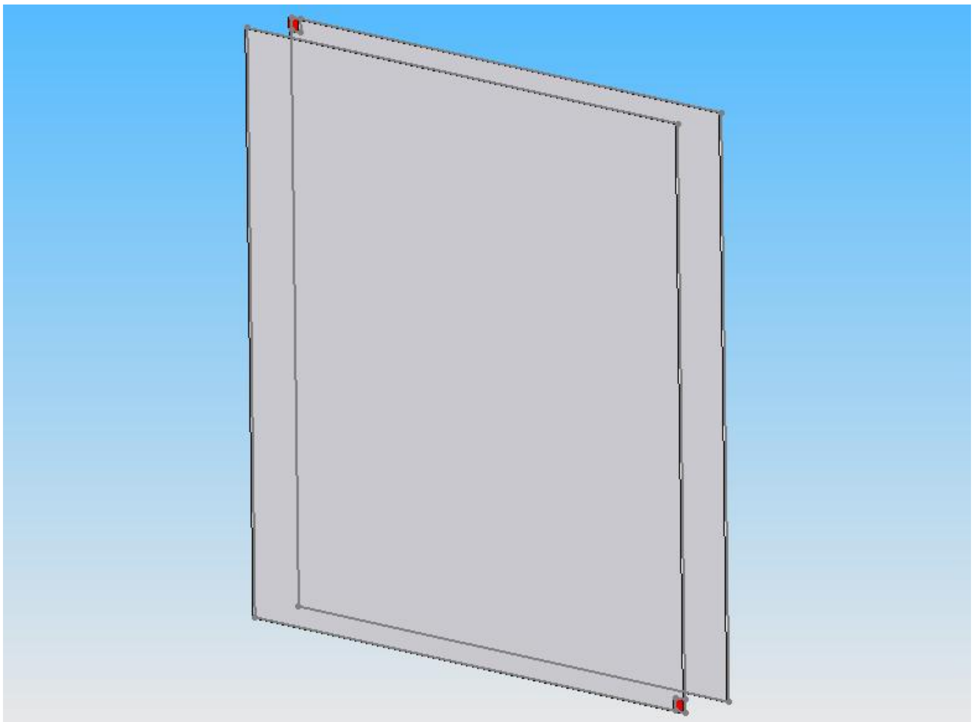

Figure 2: Two layer FEA model.

The small red squares are the holes in the metallization (actually modelled as PET polymer). Note the red squares are actually ¼ the actual pinhole since the pinholes are cut at two planes of symmetry. The pinhole area to the total model area is based on the OTR for a single layer and the assumption that a metallized layer with no defects has virtually 0.0 OTR. If a PET 12 micron thick has an OTR of 100 and the single metallized layer barrier has an OTR of 0.055 then the ratio of areas of the pinhole to the model total area is about 1/2000 of the total model area. Now if we model a two metallized layer barrier and vary the distance between holes in the first to second layers (total model size) until we satisfy both the pinhole area and the two layer OTR of less than 0.0005 (we will assume it is actually at 0.0005), we can arrive at the actual model configuration for this particular metallized layer. It should be noted that it has been assumed that the PET of the metallized layer is 12 micron thick.

The final model is 2.5 x 2.5 mm with 12 micron thick PET for each layer and the model pinhole (1/4 the area of the pinhole without planes of symmetry) is 0.0559 x 0.0559 mm. The multiple metallized layer models are constructed with a 12 micron PET layer then metallized layer with a pinhole in one corner then 12 micron PET then metallized layer with a pinhole in the opposite corner then PET then metallized layer with a pinhole, etc. Note none of the models had a seal layer since it does not represent a significant diffusion barrier.

4 Model Results

Configuration	Model OTR	Mfg. Stated OTR
1 layer – PET/MET w pinhole	0.055	0.055
2 layer – PET/MET w pinhole/PET/MET w pinhole	0.0005	< 0.0005
3 layer – PET/MET w pinhole/PET/MET w pinhole/ PET/MET w pinhole	0.00026	< 0.0005
4 layer – PET/MET w pinhole/PET/MET w pinhole/ PET/MET w pinhole/PET/MET w pinhole	0.00017	< 0.0005

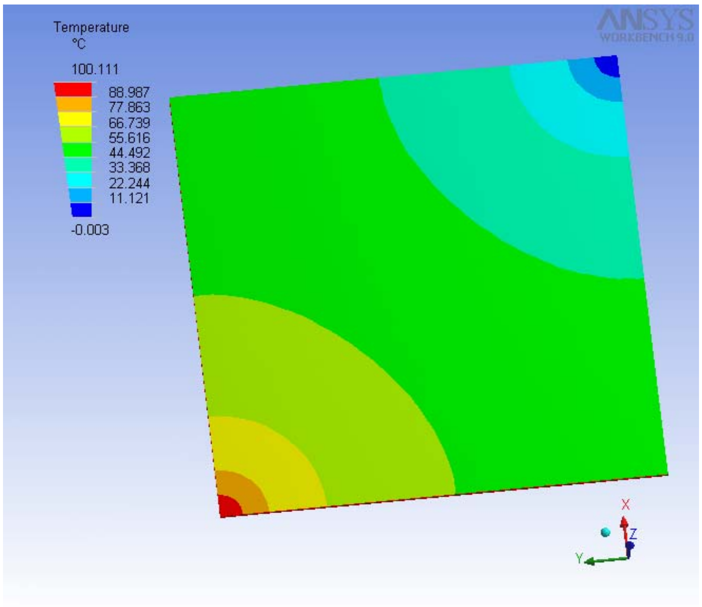

Figure 3: Diffusion pattern from one pinhole to pinhole in opposite corner

The computer model above used a 100º C temperature difference to represent the atmospheric pressure driving force.

The 1 layer and 2 layer model results should agree perfectly since we used them to define the model parameters. Layers 3 and 4 are forecasts based on the model. It would build confidence in the model if we had some real world data that was not used in building the model.

5 Model validation

Because the OTR of the three and four layer configurations is below the values that can be determined in testing, an alternate approach was developed. VIP were constructed using the three layer and four layer barriers. The VIP were very thin (1.65 mm thick) and 559 x 914 mm with a 203 x 279 mm area in one corner that was 8.25 mm thick. This configuration produces a lot of surface area to volume and gives an aging "acceleration" factor of about 10 to 1 compared to our normal panel configuration. Thus one month of aging the above panels is equivalent to 10 months of aging our normal panels. The test panels included far excessive amount of desiccant to eliminate the effect of water vapour permeation. The panels were aged at 93.3º C for 2 weeks. Thermal Conductivity measurements were made a several time points in the two weeks. The four layer barrier took approximately 30% longer to reach the same level of conductivity. This agrees very well with the model prediction of 35% lower OTR for the 4 layer barrier. This testing is one small step in building confidence in the FEA model.

6 Alternate barrier configuration

One of the benefits of using a computer model is it can provide insight as to why a particular performance occurs. In reviewing the results from the above models it became clear that the barrier could be improved by either increasing the average distance from one pinhole to another or by decreasing the cross-sectional area of the polymer layer (current model is PET) that is between the metallized layers. Changing the average distance between pinholes may be a difficult task. However, changing the cross-sectional area of the layer between the metallized layers may be fairly easily done. A new barrier configuration that would accomplish the reduction in cross-sectional area is:

- PET/metallization/adhesive (3 micron)/metallization/PET/seal layer
- This configuration takes the diffusion cross-sectional area from 12 microns down to 3 microns.
- OTR model results are 0.0001

This two metallized layer configuration is about a 500% improvement compared to the previous 2 layer configuration and even a 60% improvement compared to the four layer configuration. Designing a new improved barrier involves many variables such as processing without damaging the barrier. However, the above shows the potential to use a computer model to identify design directions that might be beneficial.

7 Conclusions

- The similarity of Fick's 1st law of diffusion and Fourier's law of thermal conduction allows the use of standard Finite Element Analysis software to model a 3 dimensional diffusion problem as an analogous thermal model.
- Diffusion through VIP barrier films involving metallized layers can be approximated as pinhole defects in the metallization.
- The FEA model provides an approximate OTR for barriers that have an OTR below the current limits of testing.
- VIP aging at high temperature provides some validation of the FEA modelling technique.
- An alternate barrier construction investigated using the FEA model may provide a barrier design direction that substantially reduces the OTR of the VIP barrier.

8 Reference

[Decker 2002] ***Basic Principles of Thin Film Barrier Coatings***, W. Decker, Toray Plastics (America), Inc., North Kingstown, RI; and B. Henry, University of Oxford, Oxford, United Kingdom; Society of Vacuum Coaters 2002 45th Technical Conference Proceedings