Finite Element Analysis Used to Model VIP Barrier Film Performance

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Introduction

- Barrier film most critical component of VIP
- Some VIP applications require 10 to 50 year life
- Oxygen Transmission Rates (OTR)
  - ASTM D3985 23ºC 50% RH
  - Films are at or below the test limit of 0.0005 cc/m^2 day
  - 2 metallized layer film OTR < 0.0005
  - 3 metallized layer film OTR < 0.0005

Introduction Cont.

- Barrier film developer has no feed back for improvement
- VIP manufacturer not able to accurately predict real performance for further advanced barrier films
- This presentation proposes
  - Use computer Finite Element Analysis (FEA) to predict OTR when below test limit

Atmospheric Gases

- VIP barriers reduce transmission of
  - Oxygen
  - Nitrogen
  - Water vapor
  - And other atmospheric gases

Water Vapor

- Water vapor transmission (MVTR)
  - Test ASTM F1249-90
    - Performance is not at limit of test
  - Mechanism of transmission different from other atmospheric gases
  - Very detrimental to VIP performance
  - Desiccant very effective and inexpensive in adsorbing water vapor
- The proposed model does NOT include water vapor transmission

Theory

- Oxygen diffusion approximated by Fick's 1st law
  - J = D dc/dx
    - J is diffusion rate
    - D is diffusion coefficient
    - dc/dx is concentration gradient
- Fick's law is analogous to Fourier's law governing conduction heat transfer
  - Fourier's law
    - q = -kdT/dx
      - q = heat transfer
      - k is thermal conductivity
      - dT/dx is temperature gradient

FEA Computer Model

- FEA Thermal conductivity model can be used to model diffusion
  - Can be 3 dimensional
  - Can have multiple layers
  - Can have multiple materials
  - Can have local defects
  - Diffusion rate can change with temperature

FEA Model Assumptions

- [Decker 2002] PET at 12 µm is 100 cm^3O_2/m^2
- A commercial single metallized barrier is 0.055 OTR
- The same manufacturer two layer metallized barrier is < 0.0005
- If homogenous diffusion, two layer should be 0.0275
- However, there is a110 times reduction not a factor of 2.

FEA Model Assumptions Cont.

- [Decker 2002] suggested that metallized layers may have “pinholes” in the metallization
  - Suggests metallized layers be modeled as “pinholes” where almost all the diffusion occurs with very little going through the continuous metallization area
  - In a single layer barrier the O_2 diffuses straight though the polymer “pinhole”
  - In a two layer barrier the O_2 diffuses through the 1^{st} layer “pinhole” and then must diffuse horizontally through the polymer until it reaches a “pinhole” in the 2^{nd} layer
- This multi-layer “pinhole” theory could account for the huge difference between a single layer and 2 layer metallized barrier

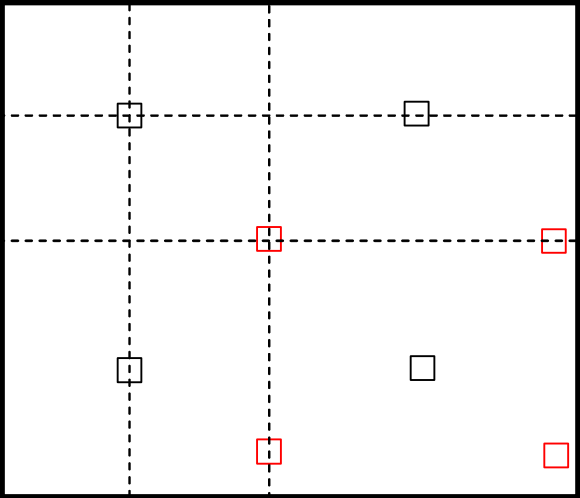
FEA Model Construction

- We can assume a polymer thickness but there are still two more variables
  - “Pinhole” area
  - Distance between “pinholes”
- The single metallized layer OTR and OTR through the base polymer allows us to calculate the “pinhole” area assuming the OTR through the continuous metallization area is very, very small compared to the “pinhole”

FEA Model Construction

- Build the two layer FEA model and adjusting the “pinhole” distance until the OTR for the two metallized layer is met
- Note: the OTR for the one and two metallized layer came from one manufacturer.
- OTR for other metallized layers from other manufacturer’s may be very different.
  - OTR depends on many product and process variables

FEA Model Construction

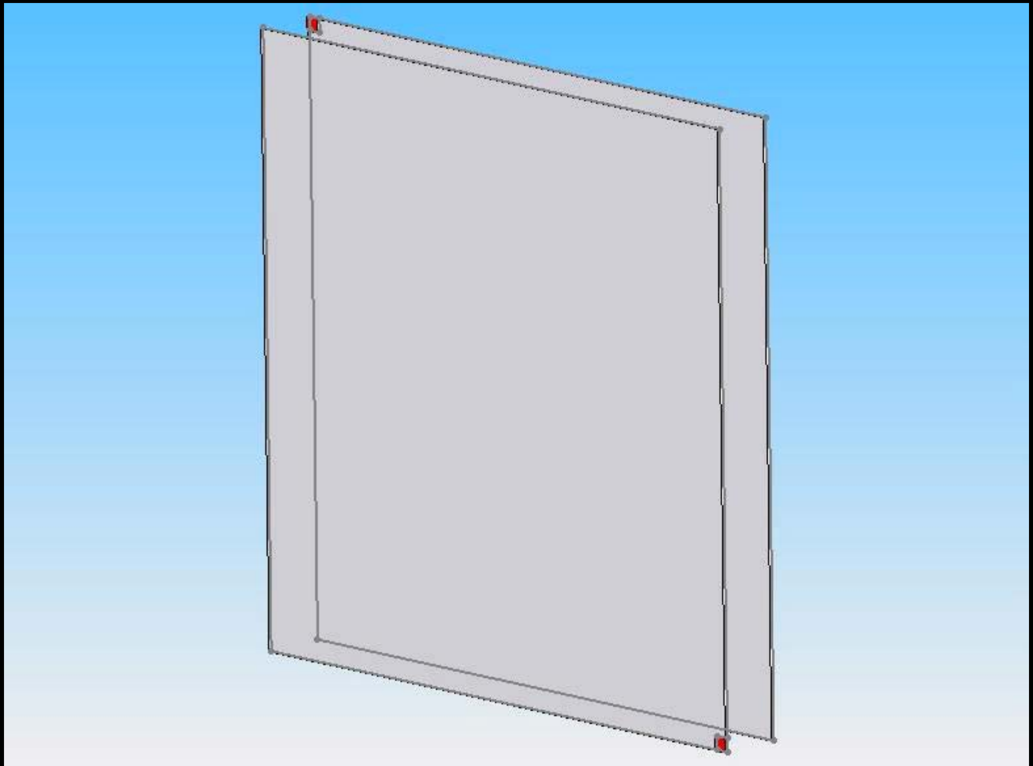


Represent Planes of Symmetry

Represent Holes on Layer 1

Represent Holes on Layer 2

FEA Model Construction



- Nothing beyond a plane of symmetry needs to be in an FEA model
- Two layer FEA model reduced to above

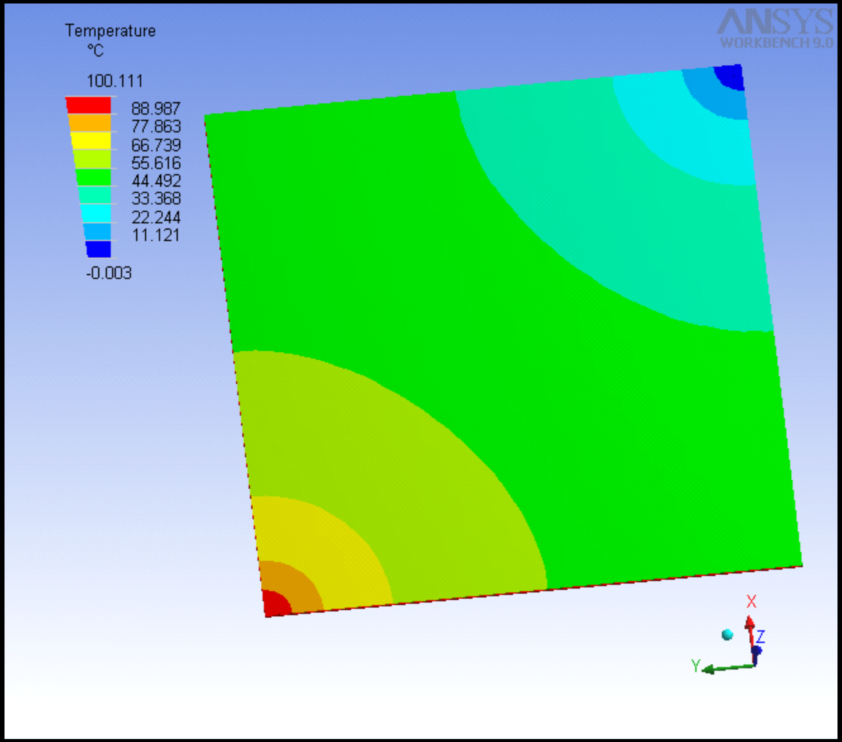
FEA Model Construction

- Red squares are holes in metallization
  - Polymer assumed to still be present
- Red squares are actually ¼ "pinhole" area because of cuts at planes of symmetry
- Assuming OTR of 12 micron PET is 100 and OTR of single metallized layer is 0.055
  - Red "pinhole" area is 1/2000 of model area
- The dimensions of the Red "pinholes" and total model area are adjusted to obtain the two metallized layer OTR of 0.0005

FEA Model Construction

- Final model dimensions for these particular barrier films are
  - Model dimensions are 2.5 mm x 2.5 mm
  - Red “pinhole” is 0.0559 mm x 0.0559 mm
  - 12 micron PET film per layer
- Multiple layer models are constructed as
  - 12 micron PET then metallization the Red pinhole in one corner
  - 12 micron PET then metallization the Red pinhole in opposite corner
  - Etc.
- None of the models had a seal layer since it does not represent a significant diffusion barrier

Analysis Results



- Diffusion pattern from one “pinhole” to “pinhole” in opposite corner
- The 100º C temperature difference represents the partial pressure driving force

Analysis 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

- 1 and 2 layer systems agree since they were used to build the model
- 3 and 4 layer systems are forecasts
  - Further real world data would help build confidence in the modeling

Model Validation

- VIP were constructed with 3 and 4 metallized layer barriers
- VIP were very thin (1.65 mm) and 559 mm x 914 mm
  - One corner 203mm x 279 mm was 8.25 mm thick
    - This allows thermal conductivity testing of the one corner

Model Validation

- This very large surface area to volume accelerates aging by about 10 to 1 compared to some of our normal panel dimensions
- A far excess amount of desiccant was used in each panel to eliminate the effect of water vapor in the results
- All panels were aged at 93.3ºC for 2 weeks

Model Validation Results

- The four metallized layer barrier VIP took about 30% longer to reach the same conductivity increase
- The FEA model predicted a 35% lower OTR for the 4 metallized layer barrier compared to the 3 metallized layer barrier
- This is a start in building confidence in the modeling technique

Alternate Barrier Design

- A benefit of the modeling is the ability to better understand why the results occur
- Also the modeling allows rapid evaluation of possible barrier design options
- Reviewing the model results led to two possibilities
  - Increase the average distance between “pinholes”
    - Not necessarily an easy thing to do
  - Decrease the cross-sectional area of the polymer between the metallization layers

Alternate Barrier Design

- A new configuration was selected
  - PET/metallization/adhesive (3 micron)/metallization/PET/seal layer
  - Diffusion cross-section reduced from 12 microns to 3 microns
- Model results for the new configuration were OTR of 0.0001
  - This new 2 metallization layer design is a 500% improvement over the previous 2 metallization design
  - It is also a 60% improvement over the 4 metallization layer design
- Designing an improved barrier involves more design concerns but the model does point a potential direction for improvement

Conclusions

- The similarity of Fick's law of diffusion and Fourier's law of conduction allows the use of Finite Element Thermal Analysis software to model 3 dimensional diffusion problems
- Diffusion through metallized VIP barrier films can be approximated as "pinhole" defects in the metallization
- The FEA model can be used to approximate the OTR of barriers below the limit of testing
- Large surface area to volume VIP aged at high temperatures can be used to help validate the FEA modeling
- An alternate barrier design may provide a barrier design direction for lower OTR of the VIP barrier