Transmission Rate of PET Bottles: Part 1

Question:

Is there a (simple) method for shelf life oxygen transmission based on a permeation factor of the resin/preform of a PET container for ice tea.

Recommendation:

Recommendation from Joel Fischer MOCON's lab manager in our corporate office in Minneapolis, Minnesota.

Establishing a shelf life model based upon resin or preform information, can be difficult. The reason is that the final bottle structure will have its own surface area, thickness and crustallinity. The resin and preform are fairly amorphous and lack the crystallinity and orientation that impact the diffucsion of oxygen in the formed bottle. Therefor a lot of the gas barries is due to the processing of the bottle (stretch ratios and such) and could be difficult to predict.

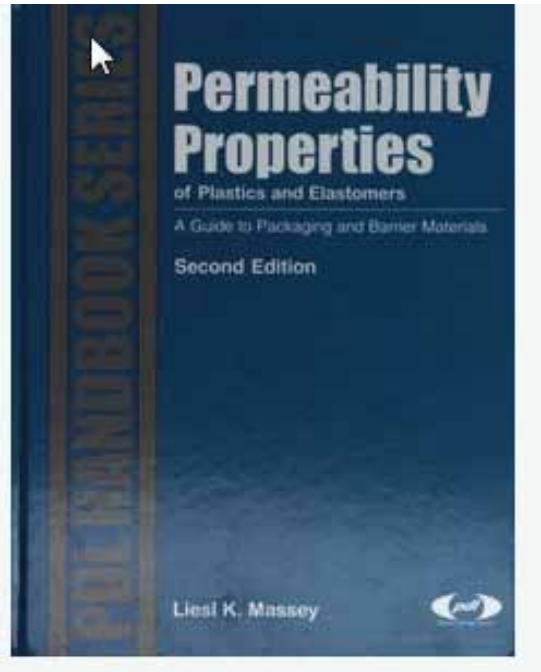
I have two generic recommendations:

1. You can utilize the generic information that's listed in the book we referenced (Permeability Properties of Plastics and Elastomers) and normalize the values within that book to your material choice and beverage bottle size.

2. There is a commerical model program called the MRule. It was prodcued by former carbonated soft drink material engineer (Mark Rule) and has a lot of inputs for variability of polymer type, size, crystallinity ... etc. My perspective is that the model is a good "ball park" estimate for gaugin materials. However, when companies are engineering the heck our of polymers and trying to minimize the packaging costs via lighteighing bottles, the acutal OTR data from such bottles is best for gauging shelf life.

If you're looking for a very good generic source of innate transmission rate / permeability data, we recommend a book that is published by the Plastics Design Library.

http://www.ebook3000.com/Permeability-Properties-of-Plastics--and-Elastomers--A-Guide-to-Packaging-and-Barrier-Materials-by-Liesl-K--Massey_127495.html



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Transmission Rate of PET Bottles: Part 2

Question:

We have looked into the MRule software and it remains to be one of interest but what I am trying to do at the moment is possibly combine measurements for total package oxygen (TPO) and an oxygen permeation coefficient to produce some kind of simplified model to represent the real amount of oxygen in the bottle at any time. Do you think this is reasonable?

Recommendation:

Recommendation from Joel Fischer MOCON's lab manager in our corporate office in Minneapolis, Minnesota.

Your approach does make sense to me.

You'll have an initial oxygen concentration in your bottle and more oxygen from room air will permeate in over time, until the bottle is at equilibrium with the air around it.

This may be a nuance to your thoughts, but I wouldn't focus upon permeation coefficients, but actual measured oxygen transmission rate into your bottle in terms of cc/day. Bottles have closures and sometimes there's more ingress due to a closure and potential permeation/leakage around the threads into the bottle. That's why a "whole bottle test" with a closure produces the best results for understanding the bottles barrier capabilities.

The "worse case" model would have a starting amount of oxygen (choose your unit, but I'd start with cc's) and then add cc's of oxygen using the OTR value for each day.

I say this is "worse case", because a true ingress model will need to account for the driving force (partial pressure) differential change between the oxygen inside the bottle and the oxygen outside the bottle. Simply stated, as oxygen accumulates inside the bottle, the gradient changes and the OTR proportionally drops. Once the oxygen inside the bottle reaches equilibrium to the outside oxygen level (i.e. both sides 20.9%), the net OTR = 0.

The math isn't too bad. Two things to be aware of:

1. If you're set on utilizing permeation coefficient numbers, you'll need to normalize them to the average surface area and sidewall thickness of a bottle.

2. Most data you'll see for OTR is for 100% oxygen. Permeation units (if not normalized to mmHg or some pressure unit) will need to be adjusted for room air pressure (I'd assume 760mmHg as full pressure or 100% oxygen and then take 20.9% of that for my OTR).

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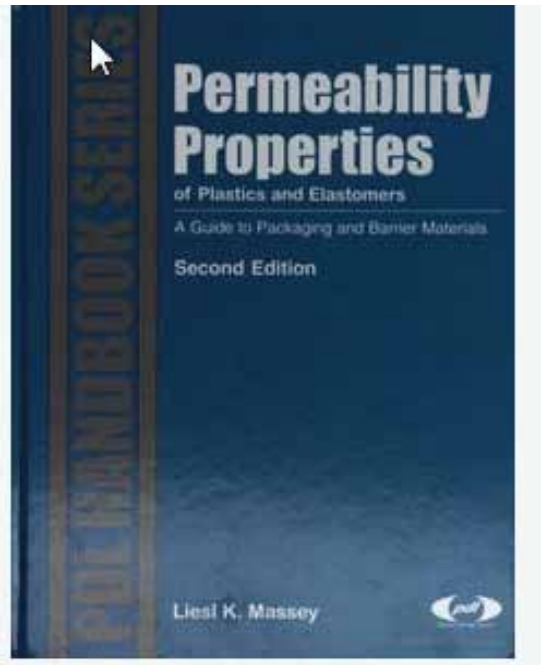
http://www.ebook3000.com/Permeability-Properties-of-Plastics--and-Elastomers--A-Guide-to-Packaging-and-Barrier-Materials-by-Liesl-K--Massey_127495.html



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