



Permeation Basics

MOCON Web Seminar Series

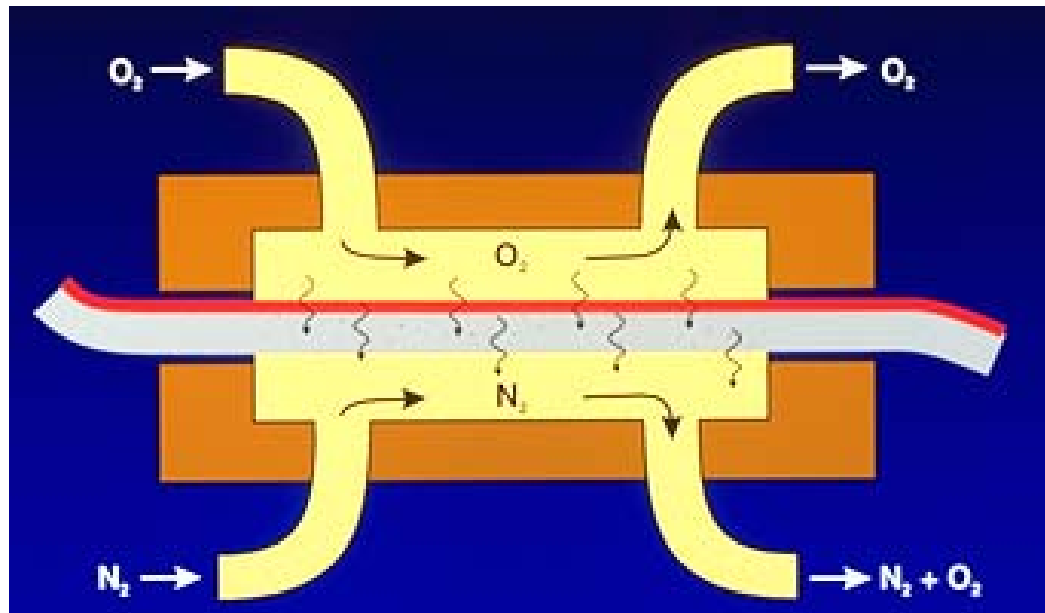
Presenter: Michelle Stevens

[The perfect package...]

- Contains and encloses the product
- Provides an inert, perfect barrier between the product and the environment
- DOES NOT EXIST!

[Permeation]

The movement of gases or vapors across a packaging material



Driving force

■ CHEMICAL POTENTIAL

- Fundamental driving force that prompts a molecule to diffuse within a polymer
- Analogous to the electrical potential of a battery
- Substances will naturally tend to move from a higher chemical potential to a lower one
- FOR MOST PACKAGING APPLICATIONS, THE ACTIVITY CAN BE REDUCED TO CONCENTRATION OR PARTIAL PRESSURE

[Solubility]

- Process by which a gas compound is molecularly mixed with a solid is called a solution.
- SOLUBILITY provides a relationship between the concentration in the solid and the concentration (or partial pressure) in the gas.
- Henry's Law constant is also called the solubility constant, S , and is a function of temperature.

[Diffusion]

- Introduces the rate aspect of mass transfer.
- Process by which matter is transported from one part of a system to another as a result of random molecular motions.
- Fick's First Law

$$F = -D \frac{\partial c}{\partial x}$$

[Permeability]

$$P = DS = \frac{qL}{At\Delta p}$$

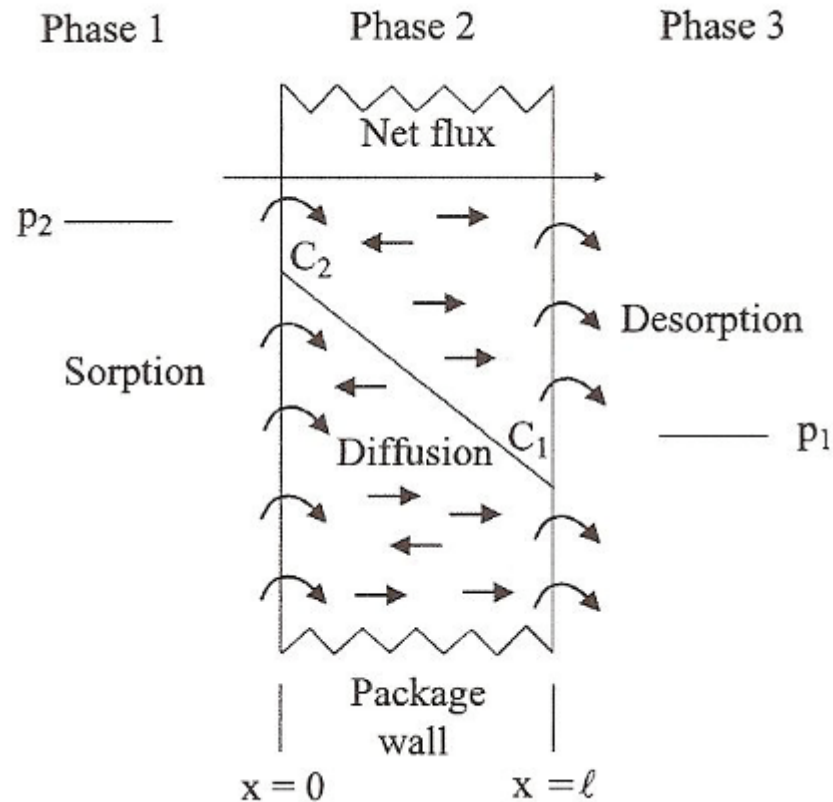
Where P is the permeability coefficient, D is the diffusion coefficient, S is the solubility coefficient, q is the quantity of permeant transferred by a unit of area, A, in a time t, l is the thickness of material and Dp is the partial pressure difference.

Permeation mechanism

1. Permeant dissolves at the polymer interface
2. The permeant diffuses within the polymer from the side of high concentration toward the low concentration side
3. The permeant diffuses out from the opposite polymer interface.

[Permeation]

The movement of gases or vapors across a packaging material



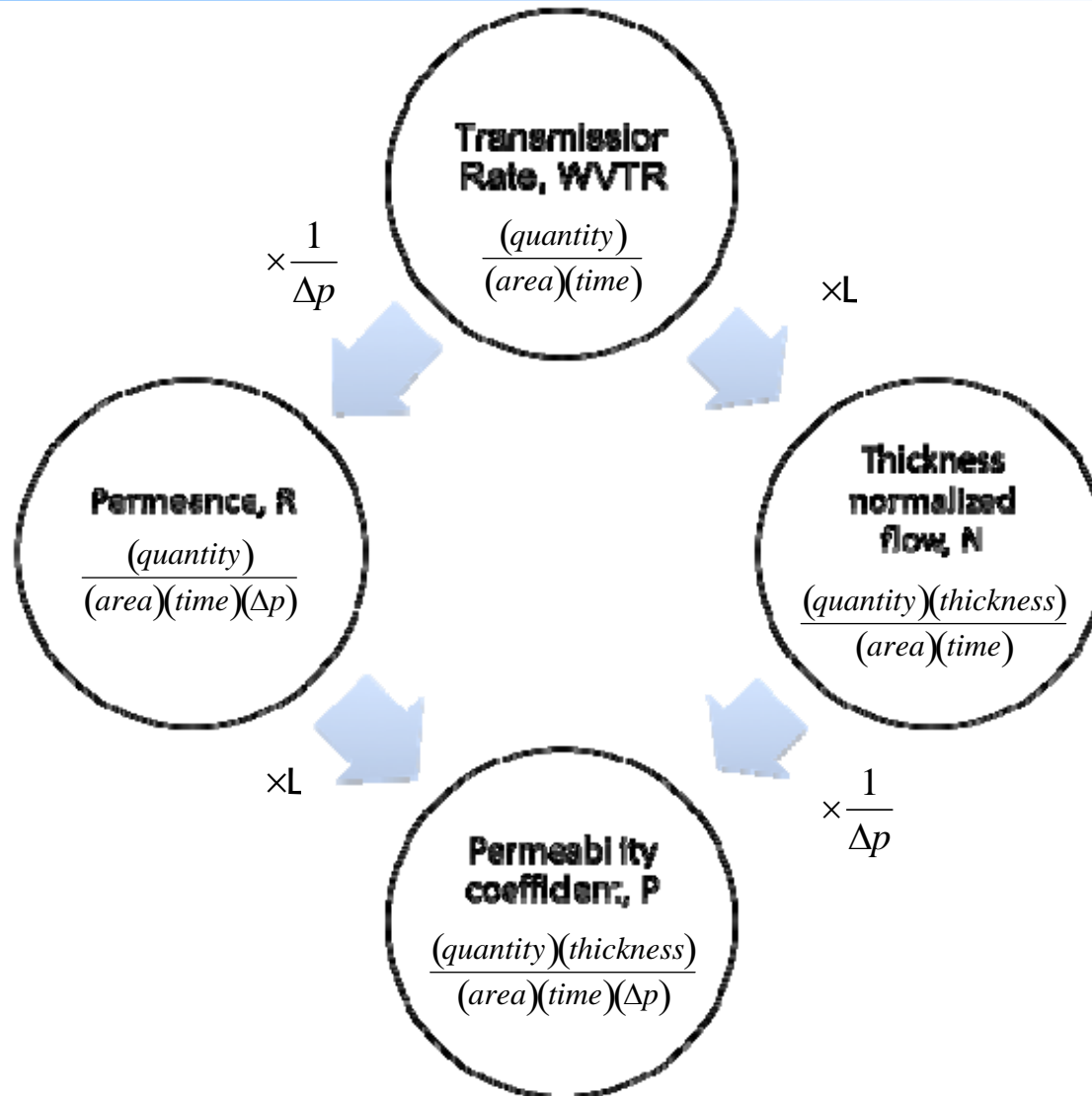
[Polyethylene example]

- A material that is a good barrier has a low value of the combined S and D values for a particular penetrant.
- Polyethylene is an excellent barrier to water because water has low S and D values in PE.
- However, PE is not an excellent barrier to O₂ because O₂ has higher S than water.

Variables Affecting Permeability

- Chemical structure of the polymer
- Chemical structure of the permeant
- Temperature
- Humidity
- Physical structure of the polymer
- Permeant concentration

Commonly used terms



Units

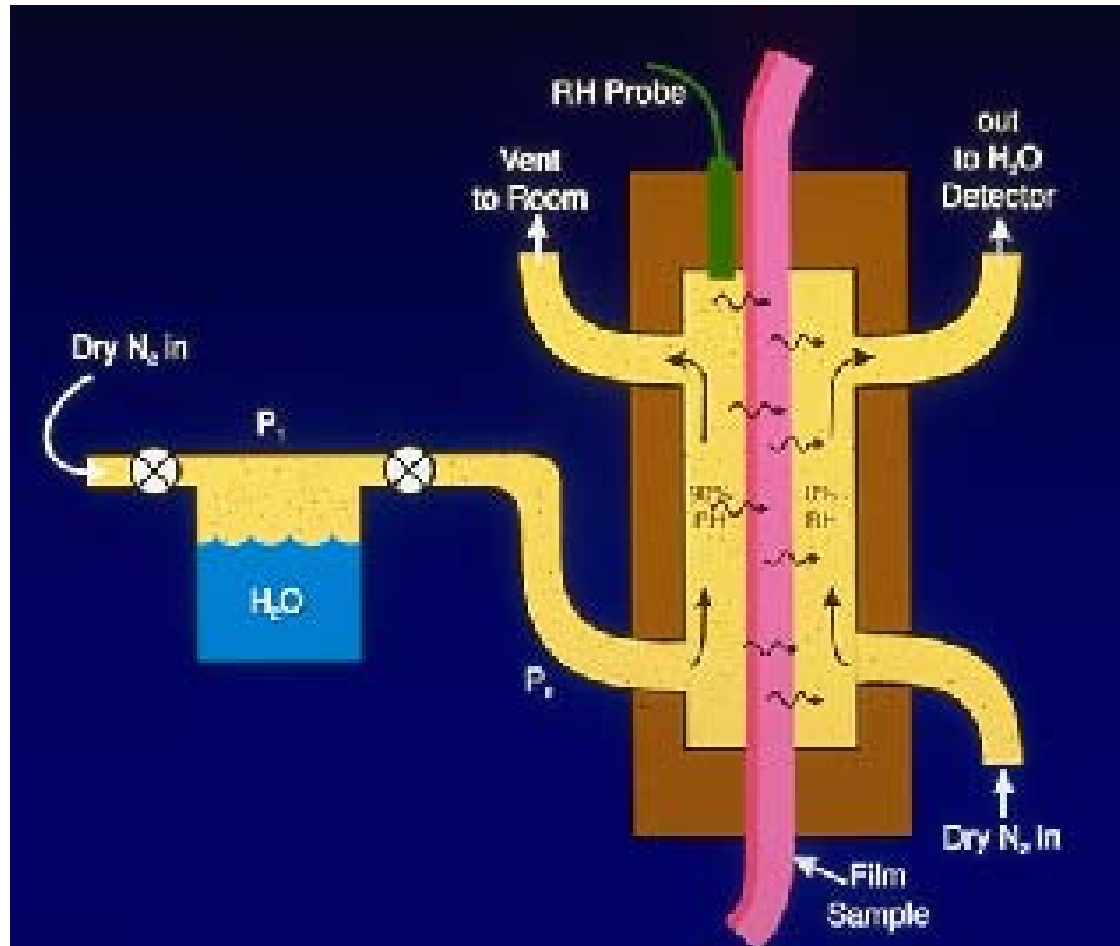
Variable	Common Units	SI units
q, quantity	g, cm ³ (STP), mol	kg
l, thickness	cm, mil	m
t, time	hour, day	sec
A, area	cm ² , in ² , 100 in ²	m ²
p, partial pressure	atm, psi, cm Hg, mm Hg	Pa

The permeability coefficient, P, is expressed in a combination of the above units:

$$\frac{\text{cm}^3 \text{ (STP) mil}}{\text{m}^2 \text{ day atm}}$$

$$\frac{\text{kg m}}{\text{m}^2 \text{ sec Pa}}$$

Measuring Transmission Rate



[Example]

- Calculate the minimum thickness of PET of a product that has an end of shelf life when it has reacted with 0.005% oxygen. The package is a 500 ml container with 400cm² area. Storage conditions are 25C and 60%RH and the desired shelf life is 6 months.

Example, continued

$$L = \frac{PtA\Delta p}{q}$$

Measured P at 25C is 22 cm³ mm/(m² day kPa)

t = 6 months = 180 days

A = 400 cm² = 0.04 m²

Dp = 0.21 atm = 21.27 kPa

$$q = 500 \text{ ml} \times \frac{0.005}{100} \times \frac{\text{mol}}{32 \text{ g}} \times 22,412 \frac{\text{cm}^3}{\text{mol}} = 17.5 \text{ cm}^3 (\text{STP})$$

$$L = \frac{\frac{22 \text{ cm}^3 (\text{STP}) \mu\text{m}}{(\text{m}^2)(\text{day})(\text{kPa})} \times 180 \text{ days} \times 0.04 \text{ m}^2 \times 21.27 \text{ kPa}}{17.5 \text{ cm}^3 (\text{STP})} = 193 \mu\text{m} = 7.6 \text{ mil}$$



Thank you!!

Questions, please

**For a copy of today's seminar
or to ask further questions, email:
webinars@mocon.com**

Next Month's Seminar

Title: Permeation Basics II

Date: *November 10, 2010*

Time: *10:00 AM - 11:00 AM CST*