SHELF LIFE MODELING

Definition

- No universal definition (depends on person, product, and application)
- Packaging

  Time between when the product is put in the package until the product is unacceptable
- Term project:
  - Shelf life based on moisture content
  - Time between when the product is put in the package and the product is at its final moisture content
  - Final moisture content (M_f)
    - Moisture content that the product reaches at the end of the experiment
    - Moisture content that is equilibrium with the storage relative humidity
    - Moisture content or water activity that product is in unacceptable condition
      - Internet
      - PIRA
      - FSTA

How to determine shelf life

- Actual experiment
  - Real data
  - Time consuming & costly
- Accelerated experiment
  - Reduced time
  - Correlation between shelf life at accelerated & normal condition must be valid
- Modeling

Factor affecting shelf life

1. Products
   a. Product dry weight (W_d)
   b. Initial moisture content (M_i)
   c. Critical moisture content (M_f)
   d. Product ingredient/processing
2. Package
   a. Permeability coefficient (P)
   b. Surface area of package (A)
   c. Thickness (ℓ)
3. Distribution environment
   a. Temperature (T)
   b. Relative humidity (RH)

Shelf life modeling

Moisture gain in the product = Moisture permeate through pkg

1. Moisture gain in the product (Q) = $W_d.dM$

Where W_d is product dry weight

dM is change in moisture content $(M_f - M_i)$

2. Moisture permeate through pkg (Q) $= \dfrac{P.A.\Delta p}{\ell} \cdot dt$

Where P is permeability coefficient

A is area

ℓ is thicknes

dt is time

p is water vapor partial pressure = p_s(RH/100) = $p_s . a_w$

Δp is partial pressure difference = $(p_{out} - p_{in})$

$= p_s(a_{w\,out} - a_{w\,in})$

$a_{w\,in} = f(M)$

$$Q = \frac{P.A.p_s}{\ell}\left(a_{w_{out}} - a_{w_{in}}(M)\right) \cdot dt$$

$$\boxed{\int_0^t dt = \frac{W_d \cdot \ell}{P.A.p_s} \int_{M_i}^{M_f} \frac{dM}{\left(a_{w_{out}} - a_{w_{in}}(M)\right)}}$$

Shelf life modeling

1. Analytical model
   a. Integrated linear model
   b. Integrated GAB model
2. Numerical method
   a. Log method
   b. Middle point method

<u>Integrated Linear Model</u>

- Although sorption isotherm is S-shape, it is common that it contains a straight line portion.
- Linear isotherm:

$$M = \beta . a_w + \alpha \longrightarrow a_w = \frac{(M - \alpha)}{\beta}$$

- Shelf life model based on linear isotherm

$$t = \frac{\ell\, W_d \beta}{P\, A\, p_s} \cdot \ln\left[\frac{a_{w\,outside} - a_{w\,t=0}}{a_{w\,outside} - a_{w\,t=t}}\right]$$

- Two ways to obtain slope of isotherm (β)
  - o Linear regression of many data points
  - o Calculated from two data points

Integrated GAB Model

- GAB provides the best fit to sorption isotherm for a wider range of moisture activity
- GAB equation

$$\frac{M}{W_m} = \frac{C\,k\,a_w}{(1-ka_w)(1-ka_w+Cka_w)}$$

$$\downarrow$$

$$a_w = \frac{2+\left(\frac{W_m}{M}-1\right)C-\left[\left(2+\frac{CW_m}{M}-C\right)^2-4+4C\right]^{1/2}}{2k(1-C)}$$

- Shelf life model based on GAB model

$$t = \frac{H}{\varepsilon\,\varphi}$$

$$H = \left[M_f - M_i + \frac{2W_mC}{\varepsilon}\ln\left(\frac{\varepsilon M_f - 2W_mC}{\varepsilon M_i - 2W_mC}\right)\right]$$

$$\varepsilon = (1-C)[(2ka_{w\,o})-2]$$

$$\varphi = \frac{A\,P\,p_s}{2k(1-C)\,\ell\,W_d}$$

- Limitation

  C must be a lot larger than 2. Usually, must be greater than 20. If it is less than 20, numerical model should be used.

Log Method

- Numerical method based on integrated linear isotherm
- Assumed linear relationship between each point on moisture sorption isotherm
- Shelf life (t_i) is calculated between each experimental point on the moisture sorption isotherm within the range of initial and final moisture content using the following equation:

$$t_i = \frac{\ell\,W_d\beta}{P\,A\,p_s}\cdot\ln\left[\frac{a_{w\,outside}-a_{w\,t=0}}{a_{w\,outside}-a_{w\,t=t_i}}\right]$$

- Total shelf life = summation of t_i

Middle Point Method

- Numerical method based on constant pressure model
- Shelf life is calculated in the same manner as the log method but using different equation:

$$t_i = \frac{\ell\,W_d}{P\,A\,p_s}\cdot\frac{\Delta M}{a_{w\,outside} - a^*_{w\,i\,inside}}$$

- Constant partial pressure different: $a_{w\ outside} - a^*_{w\,i\ inside}$ where

$$a^*_{wi\ inside} = \frac{(a_{w1}+a_{w2})}{2}$$

Example to use with shelf life calculation

1. Products
   - Product dry weight (W_d) = 20 g
   - Initial moisture content (M_i) = 2.5 %
   - Critical moisture content (M_f) = 4 %
   - Isotherm information

Relative humidity, %	Moisture content, %
0	0
8	1.12
23	2.13
32	2.88
42	3.9
59	6.29
74	7.99
80	10.09

Linear isotherm: slope = 0.117, intercept = -0.37

2. Package
   - Permeability coefficient (P) = 4.49 x 10^{-16} (kg.m)/(m^2.s.Pa)
   - Surface area of package (A) = 0.02 m^2
   - Thickness (ℓ) = 1.25 mil = 0.000032 m
3. Distribution environment
   - Temperature (T) = 23°C
   - Relative humidity (RH) = 50%