CONCLUSION

Water activity prediction equations can be a very powerful tool for formulation development and humectant selection. This application note has introduced a method of using both the Ross equation and the Norrish equation to predict the water activity of a dried meat product.

Other equations can be used as well and additional information about prediction equations is available from Decagon Devices. Decagon is willing and able to assist you in predicting the water activity of your product.

Reference List

1. Norrish,R.S. 1966. An equation for the activity coefficients and equilibrium relative humidities of water in confectionary syrups. J Food Technol 1:25-39.
2. Ross,K.D. 1975. Estimation of water activity in intermediate moisture foods. Food Tech 29:26-34.

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Water Activity Prediction

The use of water activity lowering humectants is a powerful way to turn a perishable product into a shelf stable product. There are a wide variety of humectants available and the choice of humectant will depend on many factors including the impact of the added humectant on product quality. Another challenge is knowing how much humectant to add to lower the water activity to a desired level. The water activity of complex, multi-component foods can be difficult to determine without performing an actual water activity test. However, reformulating and testing the water activity of the new formula until the right combination is found can be time consuming and expensive. Thankfully, several good water activity prediction equations are available to provide a good estimate of the final water activity based on the ingredients of the product. These equations try to factor in the non-ideality of food systems and some give better estimations than others. Below is an introduction to the most common methods used to predict the water activity of product.

ROSS EQUATION

The best equation for predicting the water activity of a multi-component product is the Ross equation (Ross, 1975). This equation assumes that each solute (or ingredient) behaves independently and dissolves or interact with all of the water in the system. The relationship is based on the Gibbs-Duhem relationship and shows that:

$$a_w = a_{w\,initial} \times a_{w1} \times a_{w2} \times \ldots a_{wi}$$

Where a_w is the final water activity, $a_{w\,initial}$ is the initial a_w before adding solute *i*, and a_{wi} is the a_w the solute would have if it dissolved in all the water. This equation requires determination of the a_w of each component separately using another a_w prediction equation or using the component's sorption isotherm data if available.

NORRISH EQUATION

The Norrish equation (Norrish, 1966) is the most common prediction equation used to calculate the water activity of the individual ingredients for use in the Ross Equation. This equation uses the Hildebrand and Scott assumptions and shows that:

$$a_w = X_w [e^{(KX_s^2)}]$$

Where X_w = mole fraction of water, X_s= mole fraction of solute, and K is the empirical constant for the solute. The mole fraction of water and solute are determined based on the assumption that the solute is dissolved in all of the water in the product. The water activity as determined by the Norrish equation is then used in the Ross equation to determine the water activity of the product. The K values for the Norrish equation can be found in the original paper and some common K values are listed in Table 1.

Table 1: Norrish equation K values of common humectants

Compound	K	Compound	K
DE 43	-5.31	Mannose	-2.28 ± 0.22
Glactose	-2.24 ± 0.07	Xylose	-1.54 ± 0.04
Glucose	-2.25 ± 0.02	Sucrose	-6.47 ± 0.06
Glucose	-2.11 ± 0.11	PEG 400	-26.6 ± 0.8
Fructose	-2.15 ± 0.08	PEG 600	-56 ± 2
Glycerol	-1.16 ± 0.01	Citric Acid	-6.17 ± 0.49
Mannitol	-0.91 ± 0.27	Tartaric Acid	-4.68 ± 0.5
Propylene Glycol	-1	Malic Acid	-1.82 ± 0.13
Alanine	-2.52 ± 0.37	Glycine	+0.87 ± 0.11

SORPTION ISOTHERM

The K value for the Norrish equation is available for a limited number of potential ingredients. For ingredients that do not have a K value, it is necessary to use the sorption isotherm data for that ingredient. The sorption isotherm data can be obtained from the literature or can be generated using Decagon's AquaLab water activity meter (see isotherm application note). The grams of water per grams of solid for the ingredient can be determined from the product formula under the assumption that the new ingredient dissolves in all of the water in the product. This value and the sorption isotherm are used to determine the water activity of the ingredient, which is then used in the Ross equation.

EXAMPLE PROBLEM

Imagine that a company has a dried meat product that has a water activity of 0.92 and they want to know how much adding 20 grams of glycerol will lower the water activity. They also want to know how much glycerol needs to be added to make a product that has a water activity of 0.85. There is 50 total grams of water in the product and assume that the glycerol dissolves in all of the water.

Problem 1: What is the final a_W when the initial a_W is 0.92 and 20 grams of glycerol is added? First, the water activity of the 20 grams of glycerol dissolved in 50 gram of water must be determined using the Norrish equation. The mole fraction (X) of water and glycerol are needed to solve the Norrish equation and are calculated by:

$$N_{glycerol} = \frac{20 grams}{92.0944\ grams/mole} = 0.21717\ moles$$

$$N_{water} = \frac{50 grams}{18.02\ grams/mole} = 2.775\ moles$$

$$X_{water} = \frac{2.775\ moles}{2.775\ moles\ +\ 0.21717\ moles} = 0.92742$$

$$X_{glycerol} = 1 - 0.92742 = 0.07258$$

The mole fraction for water and glycerol can now by inserted into the Norrish equation along with the K value for glycerol to give:

$$a_w = 0.92742\left[e^{-1.16*0.07258^2}\right] = 0.922$$

Now the water activity of glycerol is inserted into the Ross equation along with the initial water activity to give:

$$a_w = 0.91x0.922 = 0.839$$

Adding 20 grams of glycerol to the dried meat product would lower the water activity from 0.91 to approximately 0.839.

Problem 2: How much glycerol needs to be added to make a product with a final water activity of 0.85 when the initial water activity is 0.92. The water activity of the added glycerol is determined by solving the Ross equation for the water activity of the glycerol as illustrated

$$a_{w\ glycerol} = \frac{a_{final}}{a_{w\ initial}} = \frac{0.85}{0.92} = 0.924$$

Next, the Norrish equation is used to solve for the mole fraction of glycerol:

$$\ln(0.924) = (\ln(X_{water}))(-1.16((X_{water})^2))$$

This equation cannot be easily solved directly, but by calculating the water activity of several different weights of glycerol, a plot can be constructed and the regression line can be used to determine the amount of glycerol that will produce a water activity of 0.924 (Table 2). This can easily be done using Microsoft Excel. When this plot is created, the equation of the line is:

$$\text{grams of glycerol} = -276a_{w\ glycerol} + 274.36$$

$$\text{grams of glycerol} = -276 * 0.924 + 274.36$$

$$\text{grams of glycerol} = 19.336$$

To reduce the water activity of a dried meat product from 0.92 to 0.85 requires the addition of 19.336 grams of glycerol

Table 2. Water activity calculated using the Norrish equation for various amounts of glycerol.

Grams of Glycerol Added	Norrish Calculated Water Activity
10	0.901
20	0.922
30	0.884
40	0.846
50	0.811
60	0.777
70	0.744