



Conventional empirical modelling of moisture sorption isotherms of 'Nutrimix' powder

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ABSTRACT : Conventional empirical models have been proposed to predict sorption (adsorption and desorption) isotherms of fortified weaning food 'Nutrimix' (an Indian dairy product), at four temperatures, *i.e.*, 15°, 25°, 35° and 45°C over a water activity range of 0.11–0.97. Five conventional empirical sorption models (Halsey, Caurie, BET, Oswin and GAB models) have been explored for fitting the sorption data. The dataset comprised 192 data points. Halsey model having accuracy as 93.37 per cent, Caurie model having accuracy as 91.45 per cent, BET model having accuracy as 81.21 per cent, Oswin model having accuracy as 94.42 per cent and GAB model having accuracy as 94.52 per cent. Comparing all five conventional empirical models, GAB was found the best conventional empirical sorption model having accuracy as 94.52 per cent.

KEY WORDS : Empirical sorption models, Milk, Moisture sorption isotherms, Nutrimix, Prediction, Weaning food

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INTRODUCTION

Iron and zinc fortified Nutrimix powder is a dairy product based on milk and pearl millet. It was developed by Sahare and Singh (2012) at Dairy Technology Division, National Dairy Research Institute, Karnal (India). This is used as a kind of weaning food that provides adequate amount of micronutrients good for human health.

All dehydrated products absorb moisture at moderate and high water activities that lead to protein insolubility and accelerated flavour deterioration. Equilibrium relationship between moisture content of food and the water activity at any temperature is quantified in the form of Moisture Sorption Isotherms (MSI). Knowledge of sorption isotherms of a food product is essential for product and process development,

besides food engineering applications (Delgado and Sun, 2002). The deteriorative mechanisms in food system are dependent on water activity and, therefore, water activity modifications are suggested for storage stability (Asbi and Bainu, 1986). Besides, the evaluation of thermodynamic functions of water sorbed provides valuable information to characterise storage and packaging problems and in appraising the shelf-life of food product under varying product, package and environment interactions (Roman *et al.*, 1979).

MSI of food products have been described mathematically with the help of several empirical, semi-empirical and theoretical models. Boquet *et al.* (1978) described the models proposed by Oswin (1946) and Halsey (1948) as the most versatile two-parameter equations for describing the sorption isotherms. Caurie (1981) developed a model, which could help in evaluating properties of sorbed water. In the COST 90 project on water activity, Bizot (1983) demonstrated that the 'Guggenheim-Anderson-de Boer' (GAB) equation was the three-parameter theoretical model giving best fit for most food isotherms over a wide water activity range.

Therefore, the objective of this paper is to analyse the experimental data on MSI of the fortified Nutrimix at different temperatures using conventional empirical models and generate information to quantify moisture sorption parameters, which

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could help in developing the fortified Nutrimix.

MATERIAL AND METHODS

Data :

The data on Equilibrium Moisture Content (EMC) of the fortified Nutrimix (called Nutrimix now onwards) at different temperatures and water activities for adsorption and desorption have been generated by the authors through an academic exercise. Adsorption and desorption isotherms of Nutrimix were determined at four temperatures, *i.e.*, 15°, 25°, 35° and 45°C over a water activity range of 0.11–0.97. Eight reagent grade salts (lithium chloride, magnesium chloride, potassium carbonate, magnesium nitrate, sodium chloride, potassium chloride, potassium nitrate and potassium sulphate) were chosen to cover the entire range of water activity. Three measurements for each experiment were taken. As a whole, there were 192 data points that have been utilised for developing the proposed conventional empirical models given in Table A.

Conventional empirical sorption models :

Five conventional empirical models have been explored to fit the experimental data on moisture sorption; and the relevant isotherm equations are presented in Table B. The notations: w , w_m and a_w in Table B denote equilibrium moisture content, monolayer moisture content and water activity, respectively. The other symbols are the model constants. The linearised forms of the two-parameter models, *viz.*, Oswin, BET,

Halsey and Caurie were used for evaluating the best fit values of constants using the linear regression technique. For three-parameter models, *viz.*, GAB, the regression coefficients/ constants: a , b and c significantly depend on the type of regression analysis. A nonlinear least squares procedure was chosen because it is widely considered as a reliable technique (Ramesh, 2003).

Table B : Conventional empirical moisture sorption models

Name of model	Equation	
Oswin (Oswin, 1946)	$W N a \frac{a_w^b}{1 > a_w}$(1)
BET (Brunauer <i>et al.</i> , 1938)	$W N \frac{C.W_m.a_w}{(1 - a_w).[1 < (C > 1)a_w]}$(2)
Halsey (Halsey, 1948)	$a_w N e^{-a/w^b}$(3)
Caurie (Caurie, 1970)	$a_w = e^{[a+ba_w]}$(4)
GAB (Van Den Berg and Bruin, 1981)	$w N w_m \frac{Cka_w}{1 > a_w [1 > a_w < Cka_w]}$(5)

Measure of prediction accuracy :

The accuracy of fit of different models was evaluated by calculating the Root Mean Square per cent error (RMS%) of moisture between the experimental and predicted EMC using the following formula :

Table A : Equilibrium moisture content (g water/100 g solids) of fortified nutrimix at different temperatures and water activities for adsorption and desorption

a_w	15°C			25°C			35°C			45°C		
	M*	s.d.**		a_w	M*	s.d.**	a_w	M*	s.d.**	a_w	M*	s.d.**
Adsorption												
0.113	5.92	0.06	0.113	5.79	0.10	0.112	5.32	0.09	0.111	5.01	0.31	
0.333	9.64	0.37	0.328	9.53	0.40	0.320	9.22	0.10	0.310	9.17	0.44	
0.431	11.05	0.42	0.432	10.98	0.14	0.432	10.80	0.15	0.433	10.79	0.29	
0.559	12.81	0.36	0.529	12.64	0.30	0.499	12.54	0.43	0.469	12.01	0.13	
0.756	17.66	0.14	0.759	17.28	0.25	0.749	16.81	0.29	0.745	16.43	0.25	
0.817	24.15	0.17	0.810	23.15	0.54	0.802	22.78	0.37	0.795	22.49	0.58	
0.953	42.92	0.38	0.936	41.63	0.46	0.907	40.98	0.41	0.869	39.38	0.28	
0.979	56.35	0.44	0.973	55.50	0.35	0.967	54.99	0.15	0.961	54.78	0.22	
Desorption												
0.113	7.03	0.09	0.113	6.91	0.27	0.112	6.55	0.39	0.111	6.13	0.24	
0.333	9.75	0.23	0.328	9.67	0.38	0.320	9.42	0.51	0.310	9.33	0.75	
0.431	11.25	0.07	0.432	11.08	0.44	0.432	10.93	0.15	0.433	10.84	0.06	
0.559	13.01	0.40	0.529	12.89	0.14	0.499	12.71	0.34	0.469	12.15	0.25	
0.756	17.87	0.54	0.759	17.55	0.01	0.749	17.13	0.13	0.745	16.87	0.10	
0.817	24.57	0.20	0.810	24.01	0.69	0.802	23.47	0.59	0.795	23.07	0.40	
0.953	44.32	0.29	0.936	43.98	0.50	0.907	42.27	0.54	0.869	40.37	0.17	
0.979	56.64	0.13	0.973	55.92	0.06	0.967	55.07	0.44	0.961	54.90	0.50	

M*=Mean, s.d.**=Standard deviation and Replicate=3

Table 1 : Root mean square percent error for the conventional empirical models of moisture sorption isotherms for fortified nutrimix at different temperatures

Temperature (°C)	RMS%				
	Halsey model	Caurie model	BET model	Oswin model	GAB model
Adsorption					
15	12.11	8.55	18.79	5.58	5.48
25	10.59	8.14	20.67	6.46	6.45
35	9.50	11.03	25.86	10.48	8.66
45	12.07	13.70	31.59	14.22	10.60
Desorption					
15	9.71	9.46	19.97	5.74	5.54
25	6.63	13.30	23.75	7.89	6.00
35	8.31	15.89	28.25	10.90	7.48
45	11.48	19.34	29.10	14.81	9.54

$$\text{RMS\%} = \sqrt{\frac{1}{n} \sum_{i=1}^n \frac{(W_{\text{EXP}} - W_{\text{PRE}})^2}{W_{\text{EXP}}} \times 100}$$

RESULTS AND DISCUSSION

The experimental data on moisture sorption was fitted to four different two-parameter and one three-parameter classical empirical models using Eq. 1 to 5. Root mean square per cent error (% RMS) for selected models of isotherm in the water activity and temperature ranges studied are presented in Table 1 for adsorption isotherm and desorption isotherm. The lower is the value of per cent RMS for predicted and experimental values; the better would be the goodness of fit. A good description of the isotherm is considered, on average, to be smaller than per cent RMS of 7.0 when a model is applied (Palou *et al.*, 1997).

Examination of the results in Table 1 indicated that the GAB models best described the experimental adsorption data for fortified Nutrimix throughout the entire range of water activity. In the present study, at 15, 25, 35 and 45°C the GAB model predicted the adsorption and desorption isotherm between 5.48 and 10.60 per cent RMS. This was followed by Oswin model with per cent RMS between 5.58 and 14.81 per cent. Since Oswin equation was not defined for the whole range of water activity (0.11-0.97), this study resulted in the GAB as best fitted equation for both adsorption and desorption isotherms. GAB equation was fitted precisely up to 0.90 a_w as well as it provided the better evaluation of amount of water tightly bound by primary adsorption sites.

Conclusion :

Conventional empirical sorption model (GAB, BET, Halsey, Caurie and Oswin) has been developed to EMC of fortified nutrimix powder (weaning food) at four different temperatures, *i.e.*, 15, 25, 35 and 45°C for adsorption and

desorption. Comparing all five conventional empirical models, GAB as the best conventional empirical sorption model appeared to be the best fitted one.

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