

# SORPTION ISOTHERMS FOR FOOD PRODUCTS: STUDY OF MODELS AGREEMENT

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The knowledge of sorption isotherms is important for establishing conditions of storage and of processes like drying. There are several models for fitting sorption isotherms. This work presents a study about the agreement of 40 mathematical models of sorption isotherms to experimental data of 53 food products. The quadratic residual sum and the standard error were the criteria of evaluation. For the major part of the products, the best agreement was obtained with equation of Jaafar and Michalowski, if temperature or saturation pressure were not considered as a variable. For cases where temperature or saturation pressure were considered, the equation of Strohman and Yoerger was the one with the best agreement for most of the products. Ross equation, based on thermodynamics aspects, was also tested for some products, but the agreement was just satisfactory.

*KEY-WORDS: FOOD –STORAGE, DRYING; THERMODYNAMICS; SORPTION ISOTHERMS.*

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## 1 INTRODUCTION

Water represents the compound of biological materials of higher percentage in most of food products. It is a vehicle to biological, chemical and enzymatic reactions. It also influences sensorial properties. Moisture content of a product in equilibrium with the boundary atmosphere is called equilibrium moisture content. It is function of relative humidity, air temperature and interactions between water and solid material. The relationship between moisture content and its water activity (or relative humidity) in a certain temperature is called sorption isotherm.

Sorption isotherms are important, among other factors, to establish storage conditions of certain food and to report adsorptions properties of food products (DU, ZHOU and YANG, 2007; ASSUNÇÃO and PENA, 2007; YANG *et al.*, 2009). Iglesias and Chirife (1982) published a study of agreement of equations of sorption isotherms of several food products. Those authors worked only with models of two parameters and noted that there is not an universal equation that fits all the tested food experimental isotherm data. The differences among the isotherm behavior for different products result, among other factors, from the relationship between moisture content and the structure of the food. Basu, Shivhare & Mujumdar (2006) in a review of sorption isotherms presented a great discussion about thermodynamic aspect, determination methods, with 19 mathematical models and 12 products. Those authors verified that GAB model (VAN DEN BERG, 1983) was the one with best agreement for most of the food products. The GAB (VAN DEN BERG, 1983) and BET (BRUNAUER, EMMETT & TELLER., 1938) equations are commonly used for food products (GOULA *et al.*, 2008; VEGA-GALVÉZ *et al.*, 2009; FARAHNAKY, ANSARI & MAJZOBI, 2009; FABRA *et al.*, 2009; THYS *et al.*, 2010; SYAMALADEVI *et al.*, 2010; KOC *et al.*, 2010). Limousin *et al.* (2007) observed that the choice for a model should be based on the simplest model, with physical argument. Roman *et al.* (2004) recommended the use of an equation based on the components of the food, the Ross one.

The goal of this work was the obtainment of agreement of mathematical models for food products experimental data of isotherms. Experimental data were obtained in the literature. Such data were extracted only from tables. Data from graphics were not used here, for a greater reliance. Until the present moment, there is not a work with the great number of equations and products reported in this study.

## 2 MATERIAL AND METHODS

### 2.1 MATERIALS

The food products tested in the present work were the following ones: acacia, açai, alginic acid, amaranth seeds, apple, apricot, banana, barley, black bean seed, buckwheat, coffee cherry, benefited coffee, coffee products, colza, corn, cotton seed, cowpea, cupuaçu, dry beans, soy bran, flaxseed, flour, gluten, grape, kiwi, lean beef, maize starch, mushroom, oats, peanuts, pear, pork muscle, potato, potato starch, pulp of West Indian cherry, quinoa grains, rice (milled, rough and whole grain), rye, shelled corn, shelled popcorn, sorghum, soybeans, pink shrimp, starch, sugar beet seeds, tragacanth and wheat.

### 2.2 MATHEMATICAL MODELS

The mathematical models used are presented in Table 1.

### 2.3 METHODOLOGY

The equations used and its references are presented in Table 1. These equations were adjusted with a non-linear estimation method and quasi-Newton approach with convergence criterion of  $1.00 \times 10^{-4}$ . Initial value of 0.10 and initial estimative of 0.50 were used for all the estimated parameters. The agreements were selected based on determination coefficient ( $r^2$ ) and estimative standard error (SE) given by equations 41 and 42, respectively, as recommended and used by Basu, Shivhare &

Mujumdar (2006). Only values of  $r^2$  higher than 0.99 were considered for equations that do not take temperature and/or vapor pressure of saturation into account. The best agreement was the criterion for equations that consider at least one of these variables (temperature or vapor pressure):

$$r^2 = \frac{\sum_1^n (PRED - OBS)^2}{\sum_1^n (OBS - \overline{OBS})^2} \quad (41)$$

$$SE = \sqrt{\frac{\sum_1^n (OBS - PRED)^2}{n}} \quad (42)$$

Where: OBS = observed value;  $\overline{OBS}$  = the average value of observed values; PRED = the predict value; and n = the number of observations.

**TABLE 1 - MATHEMATICAL MODELS OF SORPTION ISOTHERMS**

Equation	Ref	N°	Equation	Ref°	N°
$\varphi = \frac{X/s_1}{s_2(1-X/s_1)}$	38	1	$\varphi = \frac{s_1}{\exp(s_2 X^{-s_3})}$	59	21
$X = \frac{s_1 s_2}{(1-\varphi)[1+(s_2-1)\varphi]}$	9	2	$h(1-\varphi) = -s_1 T + s_2 X^{s_3}$	45	22
$\log(\log(100\varphi)) = s_2 \log\left(\frac{X}{s_1}\right)$	24	3	$\varphi = s_3 \left( -\exp\left(-s_1 X^{-s_2}\right) \right)$	45	23
$X = \frac{s_1}{\ln(\varphi)} + s_2$	37	4	$\varphi = 1 - \exp\left[-s_1(s_2 + T)X^{s_3}\right]$	41	24
$h(\varphi) = s_1 - \frac{s_2}{X^2}$	25,26	5	$\varphi = \exp\left[-X^{s_3} \exp(s_1 - s_2 T)\right]$	41	25
$X = \frac{s_1 s_2 \varphi}{1 + \varphi s_2} (1 + \varphi)$	30	6	$\varphi = \exp\left[-\frac{s_1}{s_3 + T} \exp(-s_2 X)\right]$	41	26
$h(h(1/\varphi)) = h s_1 + X h s_2$	7	7	$h(1-\varphi) = -s_1 X^{s_2} T^{s_3}$	41	27
$h(1-\varphi) = -s_1 X^{-s_2}$	29	8	$X = (-s_2 T + s_3) \frac{s_1 \varphi}{(1-\varphi)[1+(s_1-1)\varphi]}$	43	28
$h(X) = \ln(s_1) - s_2 \varphi$	12	9	$\varphi = \exp\left[-s_1 T^{s_2} \exp(-s_3 T^{s_4} X)\right]$	14	29

Equation	Ref	N°	Equation	Ref°	N°
$h(\varphi) = -\frac{s_1}{R} \exp(-s_2 X)$	15	10	$1 - \varphi = \exp\left[-s_1 T^{s_2} X^{s_3} T^{s_4}\right]$	17	30
$\varphi = \frac{s_1 + X}{s_2 + X}$	42	11	$h \varphi = s_1 h P_s(T) \exp(s_2 X) + s_3 \exp(s_4 X)$	54	31
$X = s_1 \left(\frac{\varphi}{1-\varphi}\right)^{s_2}$	44	12	$X = \frac{s_1 s_2 s_3 \varphi}{(1-s_3 s_4 \varphi)[1+(s_2-s_4)s_3 \varphi]}$	4	32
$X = \frac{s_1 s_2 \varphi}{(1-\varphi)[1+(s_2-1)\varphi]}$	33	13	$X = s_1 \exp(s_2 h \varphi) + s_3 \varphi^{s_4}$	46	33
$\ln(\varphi) = \frac{-s_1 s_2 X}{(1/S_3) - (1/T) - 1}$	2	14	$\varphi = \exp\left[s_1 \exp(s_2 - s_3 T) X^{s_4}\right]$	16	34
$X = \frac{s_1 s_2 \varphi (-\varphi^{s_3})}{(1-\varphi)[1+(s_2-1)\varphi]}$	49	15	$\varphi = s_1 + s_2 X + s_3 X^2 + s_4 X^3 + s_5 X^4$	45	35
$X = \frac{1}{s_2} h \left[ \frac{1}{s_1} (h \varphi - s_3) \right]$	13	16	$h[\varphi P_s(T)] = (s_1 + s_2 X) \ln(P_s(T)) + (s_3 + s_4 X + s_5 X^2)$	28	36
$\frac{\varphi}{X} = s_1 + s_2 \varphi + s_3 \varphi^2$	23	17	$h(\varphi) = -\frac{s_1}{R} \exp(-s_2 X)$	54	37
$h \left[ X + (X^2 + s_1)^{s_2} \right] = s_2 \varphi + s_3$	31	18	$h[\varphi P_s(T)] = s_1 + s_2 X - \frac{\left(s_3 + s_4 X + \frac{s_5}{X} + \frac{s_6}{X^2}\right)}{T}$	62	38
$X = s_1 \left(\frac{\varphi}{s_3 - \varphi}\right)^{s_2}$	21	19	$1 - \varphi = \exp\left[-s_1 (s_5 T + s_6)^{s_2} (100X)^{s_3} (s_5 T + s_6)^{s_4}\right]$	17	39
$X = \frac{s_1 s_2 s_3 \varphi}{(1-s_3 \varphi)[1+(s_2-1)s_3 \varphi]}$	59	20	$X = (-s_4 T + s_5) \frac{\left[\exp\left(\frac{s_1}{T} + s_2\right)\right] (s_5 T + s_6)}{(1-K\varphi)[1+(C-1)K\varphi]}$	43	40
			$K = S_5 + S_6 \quad C = \exp\left(\frac{s_1}{T} + s_2\right)$		

Ref corresponds to: 2 - AGUERRE, SUAREZ & VIOLLAZ (1983); 4 - ANDERSON & HALL (1948); 7 - BRADLEY (1936); 9 - BRUNAUER, EMMETT & TELLER (1938); 12 - CAURIE (1970); 13 - CHEN (1971); 14 - CHEN & CLAYTON (1971); 15 - CHUNG & PFOST (1967); 16 - COSTA, MURATA & BARROZO (1997); 17 - DAY & NELSON (1965); 21 - GINZBURG & SAVINA (1982); 23 - HAILWOOD & HORROBIN (1946); 24 - HALSEN (1948); 25 - HARKINS & JURA (1944a); 26 - HARKINS & JURA (1944b); 28 - HAYNES (1978); 29 - HENDERSON (1952); 30 - HUTTIG (1948); 31 - IGLESIAS & CHERIFE (1976b); 33 - JAAFAR & MICHALOWSKI (1990); 37 - KUHN (1964); 38 - LANGMUIR (1916); 41 - MADAMBA, DRISCOLL & BUCKLE (1995); 42 - MIZRAHI, LABUZA & KAREL (1970); 43 - MOTARJEMI (1988); 44 - OSWIN (1946); 45 - PAKOWSKI (1995); 46 - PELEG (1992); 49 - ROUNSLEY (1961); 54 - STROHMAN & YOERGER (1967); 59 - VAN DEN BERG (1983); 62 - WERLING (1978).

### 3 RESULTS AND DISCUSSION

Table 2 and 3 present the agreements obtained for several products. The references of the experimental data, the number of experimental points, temperature and range of relative humidity are also presented in such tables. Besides the products in Table 2, it was tried to adjust data from isotherms of fat cattle (TRUJILLO, YEOW & PHAM 2003) but, no model presented  $r^2 \geq 0.99$  for this product. Trujillo, Yeow & Pham (2003) presented adjust for fat cattle with GAB (VAN DEN BERG, 1983) equation, but did not present  $r^2$  values.

**TABLE 2 - AGREEMENT PARAMETERS OF MATHEMATICAL MODELS TO EXPERIMENTAL DATA OF SORPTION ISOTHERMS OF SEVERAL FOOD PRODUCTS**

Product (Ref., NP)	T [K]	$\phi$	Eq.	$S_1$	$S_2$	$S_3$	$S_4$	$S_5$	$r^2$ $\times 10^4$	S E $\times 10^2$
Açaí <sup>a(52)</sup> , 12 for each temperature	288	0.13-0.96	17	0.331345	-1.63259	5.323191	-	-	9558	5.56
	298	0.11-0.93	17	0.259707	-1.05888	4.403736	-	-	9365	6.45
	308	0.10-0.93	17	0.280826	-1.53972	6.031590	-	-	9761	4.58
Açaí <sup>d(52)</sup> , 12 for each temperature	288	0.14-0.96	17	0.645017	-4.40031	10.97147	-	-	9887	2.53
	298	0.12-0.93	17	0.542244	-3.41149	9.210610	-	-	9735	4.60
	308	0.14-0.93	17	0.438836	-2.86611	8.810009	-	-	9772	4.04
Alginate acid <sup>(51),5</sup>	298	0.34-1.00	13	0.0587	1.9265x10 <sup>-6</sup>	0.8048	-	-	9965	0.46
Amaranth seeds <sup>(47),7</sup>	308	0.03-0.98	15	0.3974	1.3899	0.3421	-	-	9963	0
Apple <sup>a(34)</sup> , 10	303	0.11-0.90	13	0.1736	8.645	0.9083	-	-	9947	1.81
Apple <sup>d(34)</sup> , 10	303	0.11-0.90	35	0.6469	-6.7077	26.8163	-33.8385	13.9568	9924	2.19
Apricot <sup>(34)</sup> , 10 for each temperature	303	0.11-0.90	13	0.0920	6.2722	0.9907	-	-	9989	0.76
	318	0.11-0.88	4	-0.096	-0.0155	-	-	-	9964	1.29
Apricot <sup>(34)</sup> , 30	303	0.11-0.90	4	-0.1026	0.0896	-	-	-	9957	1.81
	318	0.11-0.88	13	0.0778	10.7716	1.0314	-	-	9979	1.07
Banana <sup>(35),29</sup>	318	0.03-0.39	35	0.4044	-2.069	36.5398	-130.933	147.3786	9664	2.25
Barley <sup>(8),10</sup>	298	0.10-1.00	33	0.1827	0.5758	0.183	8.9122	-	9996	0.17
Black bean seed, CAMILO <sup>(11),5</sup>	298	0.58-0.93	12	0.0896	0.5981	-	-	-	9995	0.18
Black bean seed, JEO1 <sup>(11),5</sup>	298	0.58-0.93	12	0.0860	0.626	-	-	-	9980	0.36
Black bean seed, JEO2 <sup>(11),5</sup>	298	0.58-0.93	12	0.0870	0.6149	-	-	-	9995	0.18
Black bean seed, NAG12 <sup>(39),5</sup>	298	0.58-0.93	12	0.0887	0.6119	-	-	-	9963	0.68
Black bean seed, TUC500 <sup>(11),5</sup>	298	0.58-0.93	12	0.0897	0.5997	-	-	-	9988	0.37
Buckwheat <sup>(8),10</sup>	298	0.10-1.00	13	0.0829	19.2425	0.7431	-	-	9940	0.59
Coffee cherry <sup>d(1),4</sup>	298	0.20-0.75	17	-5.391	45.7164	-49.4577	-	-	9931	2.10
Colza <sup>(60)</sup>	298	0.10-0.90	17	198.74	18.8988	-079	-	-	9951	0.19
Coffee products FDDC <sup>(27),8</sup>	293	0.00-0.60	35	-0.015	1.3095	66.4305	-323.701	30.4328	9770	3.11
Coffee products FDDC <sup>(27),8</sup>	293	0.00-0.61	13	0.0396	22.8429	1.2584	-	-	9976	0.23
Coffee products RGDC <sup>(27),8</sup>	293	0.00-0.61	35	0.0740	-13.801	939.2347	-10572.7	2.20x10 <sup>4</sup>	9638	12.31
Coffee products RGUC <sup>(27),8</sup>	293	0.00-0.61	35	-041	24.8236	-1.3x10 <sup>3</sup>	2.94x10 <sup>4</sup>	-1.9x10 <sup>5</sup>	9666	3.74

Product (Ref.), NP	T [K]	$\varphi$	Eq.	$S_1$	$S_2$	$S_3$	$S_4$	$S_5$	$r^2$ $\times 10^4$	S E $\times 10^2$
Coffee products SDDC <sup>(27),8</sup>	293	0.00-0.61	13	0.0332	23.6737	1.3089	-	-	9933	0.37
Coffee products SDUC <sup>(27),8</sup>	293	0.00-0.61	13	0.0341	25.5487	1.3159	-	-	9903	0.46
Cotton seed <sup>(8),6</sup>	298	0.10-1.00	4	-0.020	0.0568	-	-	-	9977	0.28
Cowpea <sup>(3), 8</sup> for each temperature	313	0.43-0.98	35	0.6089	-6.8852	65.1851	12.5994	-599.481	9984	0.77
	333	0.43-0.95	35	1.0707	-24.8579	303.7234	-1237.9	1629.44	9987	0.69
	353	0.37-0.99	35	1.0707	-24.8579	303.7234	-1237.9	1629.44	9987	0.69
Cupuaçu <sup>a(52),12</sup> for each temperature	288	0.18-0.94	17	0.121477	0.584706	0.465717	-	-	9323	5.50
	398	0.13-0.94	17	0.178998	0.071454	1.405506	-	-	9533	6.03
	308	0.10-0.95	17	0.199202	-0.028952	1.460395	-	-	9562	5.86
Cupuaçu <sup>d(52),12</sup> for each temperature	288	0.27-0.94	17	0.188790	0.267102	0.809608	-	-	9834	3.06
	398	0.08-0.94	17	0.253008	-0.391976	2.026859	-	-	9462	5.78
	308	0.11-0.95	17	0.246861	-0.218345	1.625365	-	-	9511	6.50
Dry beans, dark red kidney <sup>(8),8</sup>	298	0.10-1.00	13	0.0735	25.8184	0.8516	-	-	9972	0.28
Dry beans, flat, small white <sup>(8),8</sup>	298	0.10-1.00	32	0.0737	5.7404	5.6272	0.1491	-	9994	0.12
Dry beans, great Northern <sup>(8),8</sup>	298	0.10-1.00	32	0.0741	5.9422	5.6744	0.147	-	9998	0.07
Dry beans, light red kidney <sup>(8),8</sup>	298	0.10-1.00	13	0.0755	35.4002	0.8377	-	-	9997	0.09
Dry beans, pinto <sup>(8),8</sup>	298	0.10-1.00	13	0.0748	35.5077	0.8343	-	-	9993	0.13
Dry beans, red Mexican <sup>(8),8</sup>	298	0.10-1.00	13	0.0743	36.3581	0.8479	-	-	9997	0.09
Soy bran <sup>(40), 6</sup>	323	0.11-0.80	13	0.042	20.8406	1.0362	-	-	9988	0.26
Flaxseed <sup>(8),10</sup>	298	0.10-1.00	13	0.0439	37.1743	0.8392	-	-	9984	0.27
Flour <sup>(10),6</sup>	293	0.12-0.89	13	0.0681	117.2592	0.8163	-	-	9978	0.29
Gluten <sup>(10),6</sup>	293	0.07-0.92	35	-0.277	9.839	-24.6865	18.6295	-2.5862	9924	2.72
Tragacanth <sup>(10),4</sup>	298	0.34-1.00	9	0.035	-2.5624	-	-	-	9979	0.41
Grape <sup>a(34), 10</sup>	303	0.11-0.90	21	1.0036	0.1049	1.3012	-	-	9975	1.25
Grape <sup>d(34), 10</sup>	303	0.11-0.90	21	1.0064	0.1282	1.3505	-	-	9985	0.99
Kiwi <sup>(35),28</sup>	298	0.27-0.88	35	0.3662	-2.6812	17.237	-28.044	14.1876	9673	3.68
Lean beef <sup>(58), 10</sup>	278	0.34-0.98	12	0.1069	0.6025	-	-	-	9995	0.85
Mushroom, Agaricus <sup>(50),5</sup>	303	0.22-0.40	13	0.083	3.9918	0.7453	-	-	9992	0.26
Mushroom, Pleurotus <sup>(50),5</sup>	303	0.22-0.40	13	0.1074	3.3038	0.776	-	-	9942	0.52
Oats <sup>(8),10</sup>	298	0.10-1.00	13	0.0724	17.1016	0.7719	-	-	9944	0.58
Peanuts, kernels <sup>(8),6</sup>	283	0.10-1.00	5	0.1484	0.0034	-	-	-	9900	1.70
Peanuts, pod <sup>(8),6</sup>	283	0.10-1.00	13	0.0502	15.6282	0.7986	-	-	9968	0
Pear <sup>(35),30</sup>	298	0.21-0.91	35	0.1976	0.5592	7.8229	-19.886	12.8643	9608	4.43
Pink Shrimp <sup>a(5),24</sup>	283	0.07-0.92	17	0.332459	-1.32220	4.247144	-	-	9495	5.28
	298	0.24-0.94	17	0.244509	-0.383894	2.091547	-	-	9760	3.07
	313	0.13-0.91	17	0.299176	-1.02548	3.786085	-	-	9590	4.29
Pink Shrimp <sup>d(5),24</sup>	283	0.06-0.92	17	0.484350	-2.23579	5.696980	-	-	9788	3.79
	298	0.09-0.94	17	0.380162	-1.18178	3.348690	-	-	9721	4.33
	313	0.15-0.91	17	0.439139	-1.97821	5.465058	-	-	9856	3.12

Product (Ref.), NP	T [K]	$\phi$	Eq.	$S_1$	$S_2$	$S_3$	$S_4$	$S_5$	$r^2$ x10 <sup>4</sup>	S E x10 <sup>2</sup>
Potato <sup>a(34)</sup> , 10 for each temperature	303	0.11-0.90	21	1.0771	0.0573	1.165	-	-	9977	1.22
	318	0.11-0.88	35	-0.303	13.038	-58.0187	117.795	-80.5684	9977	1.18
	333	0.11-0.84	15	278.48	0.3217	0.0009	-	-	9907	0.49
	303	0.11-0.90	21	0.9919	0.0309	1.5213	-	-	9964	1.51
	318	0.11-0.88	13	0.0604	21.4821	0.9305	-	-	9950	0.61
Potato starch <sup>(51),5</sup>	298	0.34-1.00	13	0.1003	1811190.1	0.7174	-	-	9994	0.20
Quinoa grains <sup>(57), 10</sup>	293	0.09-0.85	35	1.2616	-54.2659	806.5031	-4368	8207.42	9981	1.08
Rice, milled <sup>(6),10</sup>	298	0.10-1.00	35	0.6081	-22.1115	298.4938	-1248.2	1705.60	9937	2.28
Rice, rough <sup>(6),8</sup>	273	0.10-1.00	13	0.0979	19.7848	0.6592			9953	0.31
Rice, whole grain <sup>(6),10</sup>	298	0.10-1.00	35	-0.516	18.8067	-220.677	1410.02	-2986.71	9995	0.60
Rye <sup>(6),9</sup>	298	0.10-1.00	12	0.1218	0.3331	-	-	-	9940	0.45
Shelled corn WD <sup>(6),10</sup>	298	0.10-1.00	21	1.2817	0.0431	1.472	-	-	9924	2.50
Shelled corn YD <sup>(6),5</sup>	266	0.10-1.00	13	0.1211	5.3526	0.5758	-	-	9996	0.06
Shelled popcorn <sup>(6),10</sup>	298	0.10-1.00	35	0.5162	-20.1887	293.0418	-1274.7	1800.92	9981	1.24
Sorghum <sup>(6),7</sup>	272	0.10-1.00	21	8.5874	0.8074	0.6427	-	-	9976	0.83
Sorghum, kafir <sup>(6),8</sup>	277	0.10-1.00	21	1.4962	0.0668	1.4249	-	-	9996	0.47
Soybeans <sup>(6),8</sup>	298	0.10-1.00	13	0.052	50.5255	0.8654	-	-	9971	0.30
Starch <sup>(10),6</sup>	293	0.10-0.92	21	1.4754	0.1099	1.1014	-	-	9972	1.46
Sugar beet seeds <sup>(6),8</sup>	277	0.30-1.00	12	0.1425	0.3174	-	-	-	9933	0.46
	288	0.30-1.00	12	0.1273	0.3027	-	-	-	9993	0.13
West Indian cherry, Pulp <sup>(53),7</sup>	303	0.19-0.95	13	0.1494	92.0271	1.0682	-	-	9954	1.83
Wheat <sup>(6),7</sup>	272	0.10-1.00	13	0.1238	5.4292	0.5437	-	-	9980	0.17
Wheat, durum <sup>(6),10</sup>	298	0.10-1.00	13	0.0665	60.6882	0.8151	-	-	9936	0.69
Wheat, hard red spring <sup>(6),10</sup>	298	0.10-1.00	13	0.0802	15.4221	0.7601	-	-	9955	0.54
Wheat, hard red winter <sup>(6),10</sup>	298	0.10-1.00	13	0.0793	15.7338	0.763	-	-	9960	0.52
Wheat, soft red winter <sup>(6),5</sup>	266	0.10-1.00	13	0.1324	6.3960	0.5226	-	-	9981	0.12
Wheat, white <sup>(6),10</sup>	298	0.10-1.00	13	0.0710	37.2703	0.8000	-	-	997	0.47

Ref corresponds to 1 - AFONSO Jr (2001), 3 - AJIBOLA, AVIARA & AJETUMOBI (2003), 5 - ASSUNÇÃO & PENA (2007), 8 - BROOKER *et al.* (1974), 10 - BUSHUK & WINKLER (1957), 11 - CASTILLO *et al.* (2003), 27 - HAYAKAWA, MATAS & HWANG (1978), 34 - KAYMAK-ERTEKIN & GEDIK (2004), 35 - KIRANAUDIS *et al.* (1997), 40 - LUZ *et al.* (2006), 47 - POLLIO, TOLABA & SUAREZ (1988), 50 - SHIVHAREA *et al.* (2004), 51 - SHOTTON & HARB (1965), 52 - SILVA, SILVA & PENA (2008), 53 - SILVA *et al.* (2005), 57 - TOLABA *et al.* (2004), 58 - TRUJILLO, YEOW & PHAM (2003), 60 - VASCONCELOS (1998), NP: number of experimental points; <sup>a</sup>: Adsorption; <sup>d</sup>: Desorption; FDUC: freeze dried undecaffeinated; FDDC: freeze dried decaffeinated; SDUC: spray dried undecaffeinated; SDDC: spray dried decaffeinated; RGUC: roast & ground undecaffeinated; RGDC: roast & ground decaffeinated.

Table 2 shows that, among the models that do not consider temperature or vapor pressure as variables, the one that presented the higher number of agreement was Jaafar & Michalowski (1990) model, equation 13, followed by equations 35, 12, 32, 17, 4, 15, 33, 9 and 5, in this order. The great fitness of Jaafar and Michalowski (1990) model should be because it is a phenomenological modification of BET model (BRUNAUER, EMMETT & TELLER, 1938). That model was also among the best ones in a study with dry residue of pink shrimp, developed by Assunção and Pena (2007). Even though equation 35 presented very good agreements; it is a polynomial equation without phenomenological basis. Due to this fact, it was only presented in Table 2 for cases where no other model carried out to  $r^2 \geq 0.99$ .

**TABLE 3 - AGREEMENT PARAMETERS OF MATHEMATICAL MODELS OF ISOTHERMS WITH TEMPERATURE AND/OR VAPOR PRESSURE CONSIDERED AS VARIABLES**

Product <sup>(Ref)</sup> , NP, RT	Eq.	S <sub>1</sub>	S <sub>2</sub>	S <sub>3</sub>	S <sub>4</sub>	S <sub>5</sub>	S <sub>6</sub>	r <sup>2</sup> x10 <sup>4</sup>	SE x10 <sup>2</sup>
Acacia <sup>(51)</sup> , 16, 298-323	31	-0.0171	6.0912	-4.4444	-16.0803	-	-	9728	2.94
Açai <sup>(52)</sup> , 36, 288-308	36	0.284867	0.70117	-3.27602	0.02190	2.2033	-	9820	0.96
Pulp of West Indian cherry <sup>(53)</sup> , 21, 303-323	37	0.9824	-3.9542	-0.0339	1.6612	0.0249	-	9249	5.24
Alginate <sup>(41)</sup> , 24, 298-323	31		24.2137	-5.7191	-19.147	-	-	9772	3.51
Amaranth seeds <sup>(47)</sup> , 21, 308-338	31	0.9489	-17.6845	-6.6602	-19.855	-	-	9890	2.43
Apple <sup>a(34)</sup> , 30, 303-333	37	7.9293	-22.4151	-1.2748	-2.8965	0.0255	-	9844	0.98
Apple <sup>d(34)</sup> , 30, 303-333	26	154.5864	4.6377	-271.3408	-	-	-	9617	1.53
Apricot <sup>a(34)</sup> , 30, 303-333	28	2.0398	-0.0002	0.0202	-	-	-	9803	0.97
Apricot <sup>d(34)</sup> , 30, 303-333	28	8.3626	0.0005	0.2542	-	-	-	9655	1.47
Banana <sup>(55)</sup> , 56, 303-333	28	5.3350	0.0037	1.2456	-	-	-	9662	3.05
Beneficed coffee <sup>(1)</sup> , 16, 298-328	28	1.316x10 <sup>6</sup>	0.0007	0.2801	-	-	-	9715	0.86
Coffee cherry <sup>a(1)</sup> , 16, 298-328	40	30.1010	-1.989	-	0.0005	0.0205	-14.634	9752	2.28
Coffee cherry <sup>d(1)</sup> , 16, 298-328	24	0.0014	0.937	317.6441	-	-	-	8838	5.84
Cupuaçu <sup>a(52)</sup> , 36, 288-308	36	2.141804	-1.80427	-1.92489	-3.5011	4.7188	-	9694	2.52
Pelled Coffee <sup>a(1)</sup> , 16, 298-328	37	7.2823	-36.2975	-0.2594	0.1976	0.0302	-	9426	4.97
Pelled Coffee <sup>d(1)</sup> , 16, 298-328	28	0.0016	0.8589	288.6395	-	-	-	8913	5.31
Pulped Coffee <sup>a(1)</sup> , 16, 298-328	40	15.4335	-1.2370	-	0.0003	0.0143	-8.4196	9648	1.85
Colza <sup>(60)</sup> , 15, 298-308	37	-0.9789	-9.1054	19.0038	-5.0495	2.5147x10 <sup>7</sup>	-	9789	3.16
Coffee products FDCC <sup>(27)</sup> , 16, 293-303	36	2.0103	-7.1813	-4.6032	53.6349	-174.8835	-	9667	3.73
Coffee products FDUC <sup>(27)</sup> , 16, 293-303	37	2.417	-33.1918	-0.3692	1.8171	0.0394	-	9793	2.95
Coffee products SDUC <sup>(27)</sup> , 16, 293-303	37	4.0303	-47.3896	-0.7541	-2.5856	0.0863	-	9822	2.73
Cowpea <sup>(3)</sup> , 40, 313-353	36	1.1034	-0.3719	-1.9959	15.4359	-29.8465	-	9732	3.32
Dry beans Michelite <sup>(8)</sup> , 20, 277-327	23	0.4725	2.4337	0.8250	-	-	-	9908	1.92
Soy bran <sup>(40)</sup> , 18, 323-343	31	-0.2697	-4.9928	-4.0915	-34.6631	-	-	9530	5.58
Flour <sup>(10)</sup> , 24, 293-323	26	515.7182	18.7084	-2.18x10 <sup>2</sup>	-	-	-	9897	2.75
Gluten <sup>(10)</sup> , 24, 293-323	37	0.6921	-22.0328	-0.0475	3.7792	0.0001	-	9564	6.37
Tragacanth <sup>(10)</sup> , 20, 298-323	39	3.7426	-10.2467	0.3976	2.3615	0.0084	-0.903	9857	2.45
Grape <sup>a(34)</sup> , 30, 303-333	37	2.9192	-16.6127	-0.7433	-1.9644	0.0188	-	9858	0.93
Grape <sup>d(34)</sup> , 30, 303-333	28	6.6902	-0.0019	-0.4392	-	-	-	9808	1.52
Kiwi <sup>(35)</sup> , 57, 303-333	24	0.0998	-277.275	0.9813	-	-	-	9254	5.19
Lean beef <sup>(58)</sup> , 40, 278-313	37	0.9612	-22.99	-0.5431	-3.8554	0.0249	-	9771	3.08
Maize starch <sup>(51)</sup> , 24, 298-323	23	0.2064	2.1971	1.0149	-	-	-	9779	3.45
Mushroom, agaricus <sup>(50)</sup> , 25, 303-343	31	0.5170	-4.927	-4.1926	-7.3901	-	-	9942	1.65
Mushroom, pleurotus <sup>(50)</sup> , 25, 303-343	39	0.0045	0.5509	0.0031	1.6132	0.1575	-8.3019	9800	3.07
Pear <sup>(35)</sup> , 56, 303-333	37	0.2460	-8.1071	-0.3757	-1.0104	0.0002	-	9229	6.47
Pork muscle, <sup>(58)</sup> , 40, 298-303	36	0.9631	-0.0360	-2.1099	-3.345	5.4891	-	9545	6.12
Pink shrimp <sup>(5)</sup> , 80, 283-313	36	1.085395	-0.09714	-2.424	-1.20040	2.9577	-	9741	1.07
Pink shrimp <sup>(5)</sup> , 80, 283-313	36	0.875676	0.13382	-2.6494	0.21656	1.6116	-	9722	1.48
Potato <sup>a(34)</sup> , 30, 303-333	39	0.0406	-0.1439	0.0057	1.4222	0.1749	-8.2301	9670	1.42
Potato starch <sup>(51)</sup> , 24, 298-323	29	7.615x10 <sup>6</sup>	-2.3783	482.5275	-0.5949	-	-	9900	2.32
Quinoa grains <sup>(57)</sup> , 27, 293-313	37	0.6834	-16.0253	-0.0002	8.8652	0.0009	-	9488	5.83
Rice rough <sup>(8)</sup> , 34, 273-317	31	1.2719	-16.9299	-8.4443	-18.7186	-	-	9913	2.23



Product <sup>(Ref.)</sup> , NP, RT	Eq.	S <sub>1</sub>	S <sub>2</sub>	S <sub>3</sub>	S <sub>4</sub>	S <sub>5</sub>	S <sub>6</sub>	r <sup>2</sup> x10 <sup>4</sup>	SE x10 <sup>2</sup>
Rice whole grain <sup>(8)</sup> , 19, 298-311	36	1.5354	-2.3821	-4.7359	38.7978	-80.5366	-	998	1.14
Shelled corn YD <sup>(6)</sup> , 156, 273-317	29	35.1057	-0.3365	0.0046	1.4388	-	-	9545	5.18
Sorghum <sup>(8)</sup> , 48, 272-322	24	0.8339	-173.105	2.4289	-	-	-	9886	2.43
Sorghum, kafir <sup>(38)</sup> , 26, 277-305	37	0.6258	-10.7376	-8.2614	-15.4848	5.8267	-	9942	1.90
Starch <sup>(10)</sup> , 24, 293-323	29	14.8592	-0.1934	0.0058	1.3874	-	-	9906	2.66
Sugar beet seeds <sup>(8)</sup> , 28, 277-310	31	1.1242	-12.0045	-7.1809	-16.6978	-	-	9953	1.38
Wheat <sup>(6)</sup> , 110, 272-356	31	0.7917	-13.7295	-6.1830	-16.265	-	-	9704	3.88
Wheat (soft red winter) <sup>(8)</sup> , 29, 266-298	26	594.0084	18.0655	-203.2337	-	-	-	9948	1.47
Wheat starch <sup>(47)</sup> , 24, 298-323	30	2.3692x10 <sup>7</sup>	-2.1971	253.8559	-0.8206	-	-	9891	2.42

Ref corresponds to 1 - AFONSO Jr (2001), 3 - AJIBOLA, AVIARA & AJETUMOBI (2003), 5 - ASSUNÇÃO & PENA (2007), 8 - BROOKER *et al.* (1974), 10 - BUSHUK & WINKLER (1957), 11 - CASTILLO *et al.* (2003), 27 - HAYAKAWA, MATAS & HWANG (1978), 34 - KAYMAK-ERTEKIN and GEDIK (2004), 35 - KIRANAUDIS *et al.* (1997), 40 - LUZ *et al.* (2006), 47 - POLLIO, TOLABA & SUAREZ (1988), 50 - SHIVHAREA *et al.* (2004), 51 - SHOTTON & HARB (1965), 52 - SILVA, SILVA & PENA (2008), 53 - SILVA *et al.* (2005), 57 - TOLABA *et al.* (2004), 58 - TRUJILLO, YEOW & PHAM (2003), 60 - VASCONCELOS (1998), NP: number of experimental points; <sup>TR</sup>: Temperature range; <sup>a</sup>: Adsorption; <sup>d</sup>: Desorption; FDUC: freeze dried undecaffeinated; FDDC: freeze dried decaffeinated; SDUC: spray dried undecaffeinated; SDDC: spray dried decaffeinated; RGUC: roast & ground undecaffeinated; RGDC: roast & ground decaffeinated.

Table 3 shows the best agreements obtained with the equations that consider T and/or Ps as variables. According to Table 3, among the models that take in account temperature or vapor pressure as a variable, the one with the best agreements for a product majority was the Strohman and Yoerger (1967) model, equation 31. This model was the best one of rice, as reported by SUN (1999) and one of the best models (SUN and WOODS, 1993) in studies of isotherms of wheat.

The agreement of ROSS equation, as proposed by Roman *et al.* (2004) was tested here for some food sorption isotherms (Table 4). Even though this equation was based on thermodynamics aspects, considering the components of food products, the agreement was not so good.

Figure 1 shows adjustments of isotherms of corn grains (yd) with Jaafar & Michalowski (1990) equation and Figure 2 with Chen and Clayton (1971) equation (equations 13 and 29, Table 1, respectively) in several temperatures. These equations were the best for this product. It is possible to see in these Figures and in Tables 2 and 3, a very good agreement.

**TABLE 4 - AGREEMENT PARAMETERS OF ROSS EQUATION**

Product <sup>(Ref.)</sup>	T [K]	R <sup>2</sup> x10 <sup>4</sup>	SE x10 <sup>2</sup>
Apricot <sup>(34)</sup>	303.15	3117	60.76
Cowpea <sup>(3)</sup>	313.15	4006	86.75
	323.15	4171	90.34
	333.15	5669	93.65
	343.15	4370	96.05
	353.15	4674	97.75
Potato <sup>(34)</sup>	333.15	5627	72.47
	318.15	5938	74.00
	303.15	6342	83.97
Rice, milled <sup>(8)</sup>	298.15	9999	73.53

Ref. corresponds to 3 - AJIBOLA, AVIARA & AJETUMOBI (2003), 8 - BROOKER *et al.* (1974), 34 - KAYMAK-ERTEKIN and GEDIK (2004).

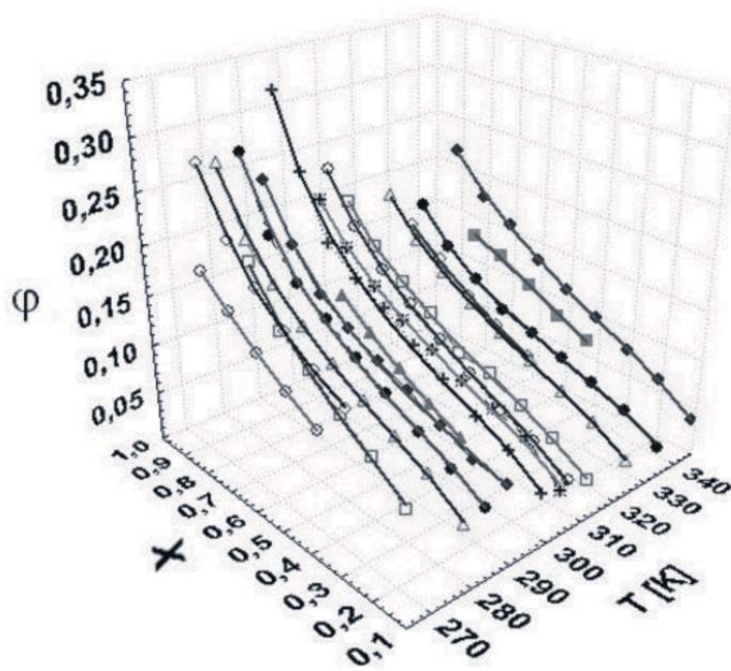


FIGURE 1 - ADJUSTMENTS OF SORPTION ISOTHERMS OF CORN GRAIN YD AT SEVERAL TEMPERATURES WITH JAAFAR & MICHALOWSKI (1990) EQUATION

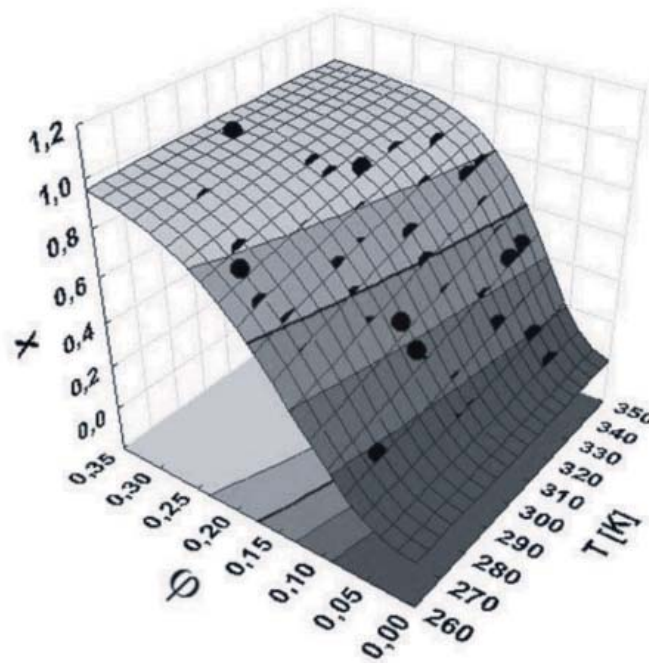


FIGURE 2 - ADJUSTMENTS OF SORPTION ISOTHERMS OF CORN GRAIN YD AT SEVERAL TEMPERATURES WITH CHEN & CLAYTON (1971) EQUATION

## 4 CONCLUSION

Among the mathematical models tested for food products, the one of Jaafar and Michalowski was the one with the greater number of best agreements, with respect to models that do not consider temperature or saturation pressure as a variable. It is interesting to note that this model is a phenomenological modification of BET model. Among the models that consider temperature or saturation pressure as a variable, the one of Strohman and Yoerger gave the best agreements. The agreement of Ross equation, based on thermodynamics aspects, was tested here for some food sorption isotherms and the agreement was satisfactory.

## NOMENCLATURE

$\varphi$	relative humidity	%
X	moisture content (d.b.)	kg kg <sup>-1</sup>
Ps	Saturation pressure	kPa
s <sub>1</sub> to s <sub>6</sub>	Equations parameters	-

## RESUMO

### ISOTERMAS DE SORÇÃO DE ALIMENTOS: ESTUDO DO AJUSTE DE MODELOS MATEMÁTICOS

O conhecimento das isotermas de sorção é importante para estabelecer as condições de armazenamento de alimentos e de processos como a secagem. Existem diversos modelos de ajuste de isotermas de sorção. Este trabalho apresenta estudo sobre o ajuste de 40 modelos matemáticos de isotermas de sorção para dados experimentais de 53 produtos alimentícios. A soma de resíduo quadrático e o erro padrão foram os critérios de avaliação. Para a maior parte dos produtos, o melhor ajuste foi obtido com a equação de Jaafar e Michalowski, quando a temperatura e a pressão de saturação não foram consideradas como variáveis. Para os casos em que a temperatura ou a pressão de saturação foram consideradas como variáveis, a equação de Strohman e Yoerger apresentou o melhor ajuste para a maioria dos produtos. A equação de Ross, baseada em aspectos termodinâmicos, também foi testada para alguns produtos, mas o ajuste mostrou-se somente satisfatório.

**PALAVRAS-CHAVE:** ALIMENTO - ARMAZENAMENTO; SECAGEM; TERMODINÂMICA; ISOTERMAS DE SORÇÃO.

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#### ACKNOWLEDGEMENTS

The authors thank Profa. Dra. Maria Aparecida Silva for the suggestion of the theme of this work.