Chemical Instrument

ERH to EMC Conversion

Ref:ERHtoEMC_Model_DS_E

Evaluation of isotherm's Model

Bradley's equation has been reported to fit the experimental data for proteins such as myosin, ovalbumin etc. (Palnitkar and Heldman, 1971)
The BET equation is used most frequently to characterize the monolayer water.
GAB(Guggenheim,Anderson and Brunauer) equation is considered one of the best equations for fitting siotherms of many food materials. It does require five experimental data points, but is good up to aw 0.94.
Oswin's equation is a series expansion for S-shaped curves.
Henderson's equation is good for describing globular proteins(Okos et al., 1992).
Ferro Fontan et al., (1982) investigated the Hailwood and Horrobin isotherm equation, which was applied to collagen and fish protein concentrates.

Equation used in MS2100 Instrument's Software

1. Chen-Clayton Equation (CHCE):

$$r.h. = \exp\left[-\frac{C_1}{T_K{}^{C_2}}\exp\left(-C_3 T_K{}^{C_4} M\right)\right]$$

EMC=-log(-pow(Tk,C2)* log(WaterActivity)/C1)/(C3*pow(Tk,C4))

2. Modified-Chung-Pfost Equation (MCPE):

$$r.h. = \exp\left[-\frac{C_1}{T + C_2}\exp\left(-C_3 M\right)\right]$$

EMC=-log(-log(WaterActivity)* (Temperature+C2)/C1)/C3

3. Modified-Halsey Equation (MHAE):

$$r.h. = \exp\left(-\exp\left(C_1 + C_2 T\right) M^{-C_3}\right)$$

EMC=exp(- log(-log(WaterActivity)/ exp(C1+C2*Temperature))/ C3)

4. Modified-Henderson Equation (MHEE):

$$r.h. = 1 - \exp\left[-C_1\left(T + C_2\right) M^{C_3}\right]$$

EMC=exp(log(-log(1-WaterActivity)/(C1*(Temperature+C2)))/C3)

5. Modified-Oswin Equation (MOSE):

$$r.h. = \frac{1}{1+\left(\frac{C_1 + C_2 T}{M}\right)^{C_3}}$$

EMC=(C1+C2*Temperature)/ exp((1- WaterActivity)/ (WaterActivity*C3))

6. Strohman-Yoerger Equation (STYE):

$$r.h. = \exp\left[C_1 \exp(-C_2 M) \ln P_s - C_3 \exp(-C_4 M)\right]$$

*Not available

7. Brunauer-Emmett-Teller (BET)

$$X_{eq} = \frac{(XM \cdot C \cdot a_w)\left[1-(n+1)\cdot a_w{}^{n} + n \cdot a_w^{n+1}\right]}{(1-a_w)\left[1+(C-1)\, a_w - C \cdot a_w{}^{n+1}\right]} \qquad Xe = \frac{(X_m a_w C)(1-(n+1)a_w{}^{n} + na_w{}^{n+1})}{(1-a_w)[1+(C-1)a_w - Ca_w{}^{n+1})]}$$

EMC=(C1*C2* WaterActivity)*(1-(C3+1)*pow(WaterActivity,C3)+C3*pow(WaterActivity,C3+1))/((1-WaterActivity)*(1+(C2-1)* WaterActivity-C2*pow(WaterActivity,C3+1)))
Note: C1=Xm; C2=C;C3=n;
Initial Data: C1= 0.104; C2= 0.876;C3=107.07;(30C°)
C1=3.9478; C2=0.1058;C3=43.76; (40C°)

8.BET Linear

$$X_{eq} = \frac{a_w \cdot XM \cdot C}{(1-a_w)\cdot(1+(C-1)\cdot a_w)}$$

EMC= WaterActivity*C1*C2/((1- WaterActivity)*(1+(C2-1)* WaterActivity))
Note: C1=Xm; C2=C;
Initial Data: C1= 0.104; C2= 0.876; (30C°)

9. Guggenheim-Anderson-deBoer (GAB)

$$X_{eq} = \frac{XM \cdot C \cdot K \cdot a_w}{(1-K\cdot a_w)\cdot(1-K\cdot a_w + C\cdot K\cdot a_w)} \qquad Xe = \frac{(C-1).X_m.K.a_w}{1+(C-1).K.a_w} + \frac{X_m.K.a_w}{1-a_w K}$$

$$c = 0.00218 e^{\left(\frac{2520.3}{T}\right)}$$

c=0.00218*exp(2520.3/Tk)= C2*exp(2520.3/Tk)

$$k = 0.19423 e^{\left(\frac{435.7}{T}\right)}$$

k=0.19423*exp(435.7/Tk)= C3*exp(435.7/Tk)

EMC=C1*C2*exp(2520.3/Tk)*C3*exp(435.7/Tk)* WaterActivity /((1- WaterActivity)*(1-C3*exp(435.7/Tk)* WaterActivity +C2*exp(2520.3/Tk)* C3*exp(435.7/Tk)* WaterActivity));
Note: C1=Xm=0.0598; C2=0.00218;C3= 0.19423;

Table 1. Estimated Values and Regression Coefficients for G.A.B. Model

T /°C	X_m/mc·(d.b.)	c/-	k/-	r^2
25	0.0598	11.85	0.82	0.998
40		5.67	0.80	0.995
55		4.27	0.75	0.996
70		3.87	0.68	0.991

10. LANGMUIR

$$X_{eq} = \frac{XM \cdot C \cdot a_w}{1 + C \cdot a_w} \qquad Xe = \frac{A.B.a_W}{1 + a_W.B}$$

Xe=C1* C2*WaterActivity/(1+C2* WaterActivity)
Note: C1=Xm; C2=C;
Initial Data: C1=1011.181; C2= 0.00059;

Useful data colected for reference

Data from literature: “DESORPTION ISOTHERMS OF CALENDULA OFFICINALIS L”
Franceli da Silva1 , Kil Jin Park 1, Pedro Melillo Magalhães 2 and Marina Pozitano 1.

Table 2: The sorption isotherm model

NAME OF THE MODEL	MODEL	
BET	$X_{eq} = \frac{(XM \cdot C \cdot a_w)\left[1-(n+1)\cdot a_w{}^n + n \cdot a_w^{n+1}\right]}{(1-a_w)\left[1+(C-1)\, a_w - C \cdot a_w{}^{n+1}\right]}$	(1)
BET LINEAR	$X_{eq} = \frac{a_w \cdot XM \cdot C}{(1-a_w)\cdot(1+(C-1)\cdot a_w)}$	(2)
GAB	$X_{eq} = \frac{XM \cdot C \cdot K \cdot a_w}{(1-K \cdot a_w)\cdot(1-K \cdot a_w + C \cdot K \cdot a_w)}$	(3)
HALSEY	$X_{eq} = XM\left(\frac{-A}{\log(a_w)}\right)^{1/n}$	(4)
HENDERSON	$X_{eq} = \left(-\frac{\log(1-a_w)}{K}\right)^{1/n}$	(5)
LANGMUIR	$X_{eq} = \frac{XM \cdot C \cdot a_w}{1+C \cdot a_w}$	(6)
OSWIN	$X_{eq} = A\left(\frac{a_w}{1-a_w}\right)^B$	(7)
PELEG	$X_{eq} = K_1 . a_w{}^{n_1} + K_2 . a_w{}^{n_1}$, $n_1 < 1$ e $n_2 > 1$	(8)
CHUNG & PFOST	$X_{eq} = \left(\frac{-1}{B}\right)\cdot \log\left(\frac{\log(a_w)\cdot(R \cdot T)}{-A}\right)$	(9)
HENDERSON	$X_{eq} = \left(-\frac{\log(1-a_w)}{K \cdot (T+C)}\right)^{1/n}$	(10)

Table 4: Estimates of parameters of empirical models.

Model	Constants, R2 and error	TEMPERATURE		
		30 °C	45 °C	60 °C
BET	XM	0.104	70.324	285.428
	C	0.876	0.001	0.001
	N	107.070	2.016	0.875
	R2	0.955	0.979	0.944
	E (%)	34.99	23.28	28.37
BET LINEAR	XM	0.104	0.042	0.039
	C	0.876	30.833	22.77
	R2	0.955	0.971	0.990
	E (%)	34.99	11.95	9.23
GAB	XM	0.038	0.062	0.033
	C	7.11×10^5	6.914	41.062
	K	1.175	0.889	1.072
	R2	0.993	0.986	0.993
	E (%)	7.95	16.18	6.76
HALSEY	A	0.050	0.044	0.028
	B	1.172	1.127	1.236
	R2	0.972	0.988	0.988
	E (%)	280.68	359.50	419.44
LAGMUIR	XM	1096.117	734.300	146.517
	C	0.000	0.000	0.001
	R2	0.831	0.950	0.943
	E (%)	38.53	26.78	28.77
OSWIN	A	0.098	0.094	0.079
	B	1.021	0.551	0.518
	R2	0.955	0.988	0.981
	E (%)	34.85	14.50	15.82
PELEG	K1	0.135	0.013	0.025
	N1	0.492	-0.285	-0.034
	K2	5.592	0.293	0.216
	N2	11.490	1.946	2.129
	R2	0.993	0.997	0.999
	E (%)	9.40	5.71	3.36

R^2 – determination coefficient.

Data from literature: "APPLICATION OF MATHEMATICAL MODELS OF TWO AND THREE PARAMETERS IN THE PREDICTION OF SORPTION ISOTHERMS FOR INGÁ (Ingáedulis) PULP" Franceli da Silva1 , Kil Jin Park, Pedro Melillo Magalhães and Marina Pozitano.

Model	Equation	
Anderson	$Xe = \frac{A.B.C.a_w}{1+(B-2).C.a_w.+(1-B).C^2.a_w}$	(1)
BET modified	$Xe = \frac{(X_m a_w C)(1-(n+1)a_w{}^n + na_w{}^{n+1})}{(1-a_w)[1+(C-1)a_w - Ca_w{}^{n+1})]}$	(2)
GAB	$Xe = \frac{(C-1).X_m.K.a_w}{1+(C-1).K.a_w} + \frac{X_m.K.a_w}{1-a_w K}$	(3)
Langmuir	$Xe = \frac{A.B.a_w}{1+a_w.B}$	(4)
Oswin	$Xe = A.[a_w/(1-a_w)]^B$	(5)
Smith	$Xe = A - B.\ln(1-a_w)$	(6)

Table 2. Estimated values of several models parameters, regression coefficients (R^2) and E (%).

Models	Parameters	ingá pulp	
		40 °C	60 °C
Anderson	A	0.2432	4.3718
	B	2.063	0.2762
	C	1.196	0.3658
	R^2, (E%)	0.993 , (1.78)	0.975 , (1.96)
BET modified	*Xm*	3.9478	7.8908
	N	43.76	51.947
	C	0.1058	0.0537
	R^2 , (E%)	0.993 , (1.68)	0.988 , (1.79)
GAB	*Xm*	0.2163	0.1951
	C	3.6914	5.3119
	K	0.7516	0.7139
	R^2 , (E%)	0.993 , (1.22)	0.990 , (1,45)
Langmuir	A	1011.181	225.051
	B	0.00059	0.0229
	R^2 , (E%)	0.950 , (2.33)	0.968 , (2.01)
Oswin	A	0.249	0.228
	B	0.3451	0.3084
	R^2 , (E%)	0.970 , (2.56)	0.965 , (2.67)
Smith	A	0.0899	0.0971
	B	0.2077	0.1622
	R^2 , (E%)	0.982 , (2.10)	0.971 , (2.79)

Data from literature:" Comparison and Selection of EMC/ERH Isotherm Equations for Drying and Storage of Grain and Oilseed"
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1. Chen-Clayton Equation (CHCE):

$$r.h. = \exp\left[-\frac{C_1}{T_K{}^{C_2}}\exp\left(-C_3 T_K{}^{C_4} M\right)\right] \tag{1}$$

2. Modified-Chung-Pfost Equation (MCPE):

$$r.h. = \exp\left[-\frac{C_1}{T + C_2}\exp(-C_3 M)\right] \tag{2}$$

3. Modified-Halsey Equation (MHAE):

$$r.h. = \exp\left(-\exp(C_1 + C_2 T) M^{-C_3}\right) \tag{3}$$

4. Modified-Henderson Equation (MHEE):

$$r.h. = 1 - \exp\left[-C_1 (T + C_2) M^{C_3}\right] \tag{4}$$

5. Modified-Oswin Equation (MOSE):

$$r.h. = \frac{1}{1 + \left(\frac{C_1 + C_2 T}{M}\right)^{C_3}} \tag{5}$$

6. Strohman-Yoerger Equation (STYE):

$$r.h. = \exp\left[C_1 \exp(-C_2 M) \ln P_s - C_3 \exp(-C_4 M)\right] \tag{6}$$

Table 5. The best fitted coefficients for adsorptive, desorptive and average isotherm equations.

Data Sets	Best Fitted Equation Coefficients				RSS	SEE	MRD
	C_1	C_2	C_3	C_4			
Wheat: Modified-Chung-Pfost Equation							
Adsorption	401.52	73.607	0.14974		1.1950	0.0558	0.16423
Desorption	545.25	64.047	0.17316		2.7264	0.0669	0.59591
Total	478.87	64.933	0.16558		4.8434	0.0662	0.55857
Shelled Corn: Modified-Oswin Equation							
Adsorption	13.1882	-0.058628	2.98726		0.19965	0.04013	0.06152
Desorption	13.9005	-0.076819	2.96243		1.71130	0.06093	0.10346
Total	13.7738	-0.074127	2.96856		1.93735	0.05740	0.09660
Rice: Strohman-Yoerger Equation							
Adsorption	2.60693	0.22350	8.48875	0.19608	0.83505	0.06527	0.10577
Desorption	1.03151	0.13755	7.73688	0.17268	2.77199	0.07042	0.12657
Total	1.15668	0.15345	7.78269	0.17828	4.17767	0.07419	0.13202
Rapeseed: Modified-Halsey Equation							
Adsorption	2.7812	-8.9162×10^{-4}	1.6685		0.86939	0.05477	0.09866
Desorption	2.8989	-1.4596×10^{-2}	1.5454		3.10511	0.09112	0.17269
Total	2.8380	-9.6915×10^{-3}	1.5845		4.38937	0.08124	0.14770