SYSTEM –

1Butanol & Methacrylic Acid

Activity Coefficient Model –

NRTL

Type of Equation	Parameters	$\ln \gamma_1$ = $\ln \gamma_2$ =		Notation of Parameters in Data Sheet
NRTL [9] (continued)	$g_{12} - g_{22}$ [2] $g_{21} - g_{11}$ α_{12}	$x_2^2 \left[\tau_{21} \left(\frac{G_{21}}{x_1 + x_2 G_{21}} \right)^2 + \left(\frac{\tau_{12} G_{12}}{(x_2 + x_1 G_{12})^2} \right) \right]$ $x_1^2 \left[\tau_{12} \left(\frac{G_{12}}{x_2 + x_1 G_{12}} \right)^2 + \left(\frac{\tau_{21} G_{21}}{(x_1 + x_2 G_{21})^2} \right) \right]$	(31a) (31b)	A 12 A 21 ALPHA 12

2) $\tau_{12} = \frac{g_{12} - g_{22}}{RT}$ $\tau_{21} = \frac{g_{21} - g_{11}}{RT}$

$G_{12} = \exp(-\alpha_{12} \tau_{12})$ $G_{21} = \exp(-\alpha_{21} \tau_{21})$

g_{ij} parameter for interaction between components i and j; $g_{ij} = g_{ji}$

α_{ij} nonrandomness parameter; $\alpha_{ij} = \alpha_{ji}$

•) Wilson, NRTL, and UNIQUAC parameters are given in cal/mol with the gas constant R = 1.98721 cal/mol K and the temperature T in K.

Parameters are given in cal/mol with the gas.

2. Antoine Vapor Pressure Equation

The Antoine vapor pressure equation is used in the following form:

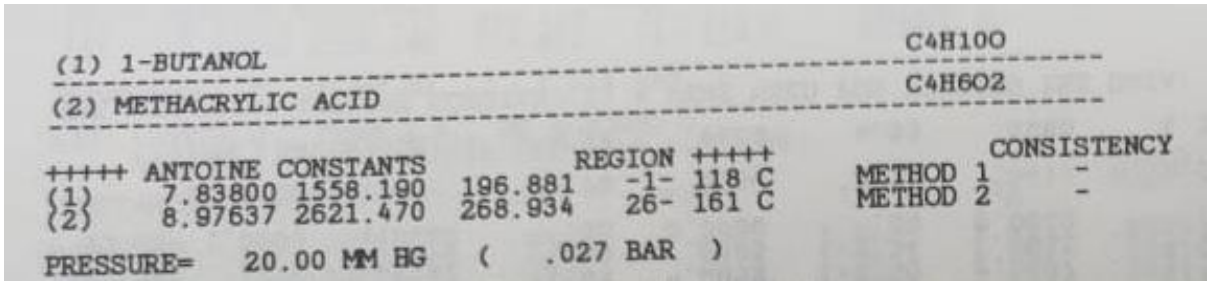
$$\log[p_i^0] = A - \frac{B}{t + C} \qquad (70)$$

with $[p_i^0]$ vapor pressure of pure component i in mm Hg
t temperature in degrees Celsius (° C)

The Antoine constants A, B, and C are given with respective temperature regions (in ° C).

Note- Here it is log (Base 10).

Value of Constants



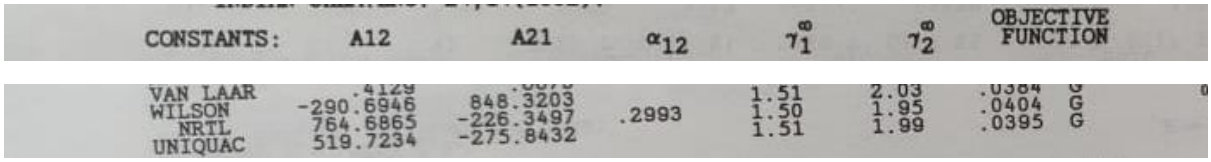
(1) 1-BUTANOL — C4H10O

(2) METHACRYLIC ACID — C4H6O2

+++++ ANTOINE CONSTANTS

				REGION +++++		CONSISTENCY
(1)	7.83800	1558.190	196.881	-1- 118 C	METHOD 1	-
(2)	8.97637	2621.470	268.934	26- 161 C	METHOD 2	-

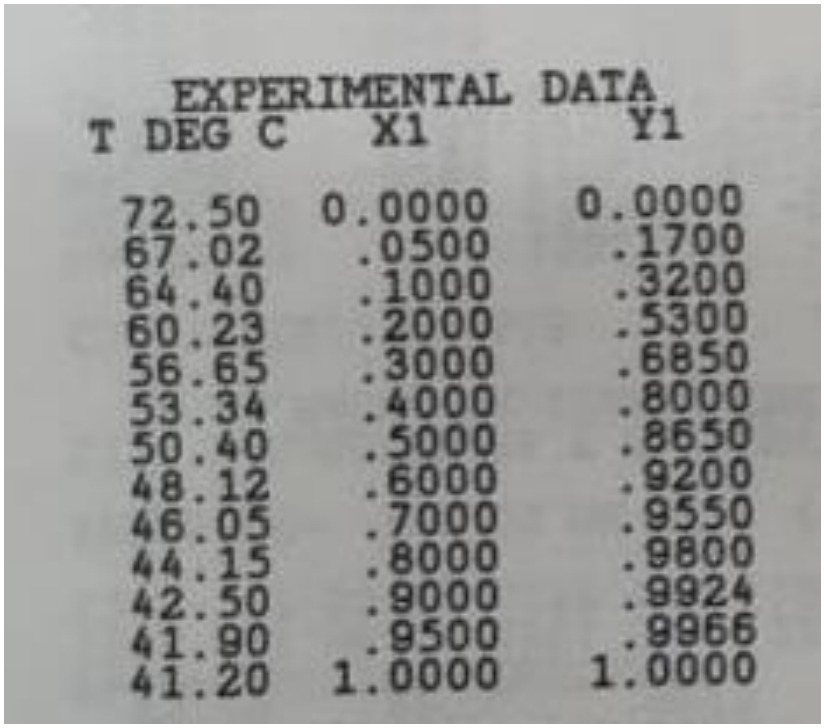
PRESSURE= 20.00 MM HG (.027 BAR)



CONSTANTS:	A12	A21	α_{12}	γ_1^∞	γ_2^∞	OBJECTIVE FUNCTION	
VAN LAAR	.4129	[illegible]		1.51	2.03	.0384	G
WILSON	-290.6946	848.3203	.2993	1.50	1.95	.0404	G
NRTL	764.6865	-226.3497		1.51	1.99	.0395	G
UNIQUAC	519.7234	-275.8432					

Please take data corresponding to NRTL

T-X-Y Data



EXPERIMENTAL DATA

T DEG C	X1	Y1
72.50	0.0000	0.0000
67.02	.0500	.1700
64.40	.1000	.3200
60.23	.2000	.5300
56.65	.3000	.6850
53.34	.4000	.8000
50.40	.5000	.8650
48.12	.6000	.9200
46.05	.7000	.9550
44.15	.8000	.9800
42.50	.9000	.9924
41.90	.9500	.9966
41.20	1.0000	1.0000

Take the molar volume from NIST Database. If not available there, please contact the TA's (Sandra and Krishna).

All data taken from Dechema Chemistry data series.