System:

1,4-Dioxane & Water

Type Of Equation:

UNIQUAC:

Type of Equation	Parameters	$\ln \gamma_1 =$ $\ln \gamma_2 =$	Notation of Parameters in Data Sheet
UNIQUAC [10]	$u_{12} - u_{22}$ [3]	$\ln \gamma_1^C + \ln \gamma_1^R$ [3] (32a)	A 12
	$u_{21} - u_{11}$	$\ln \gamma_2^C + \ln \gamma_2^R$ (32b)	A 21

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)

Table 4 UNIQUAC Activity Coefficient Equations [10] for Binary Systems

$$\ln \gamma_1 = \ln \gamma_1^C + \ln \gamma_1^R \tag{32a}$$

$$\ln \gamma_1^C = \ln \frac{\varphi_1}{x_1} + \frac{z}{2} q_1 \ln \frac{\vartheta_1}{\varphi_1} + \varphi_2 \left(l_1 - \frac{r_1}{r_2} l_2 \right) \tag{33a}$$

$$\ln \gamma_1^R = -q_1 \ln (\vartheta_1 + \vartheta_2 \tau_{21}) + \vartheta_2 q_1 \left(\frac{\tau_{21}}{\vartheta_1 + \vartheta_2 \tau_{21}} - \frac{\tau_{12}}{\vartheta_1 \tau_{12} + \vartheta_2} \right) \tag{34a}$$

$$\ln \gamma_2 = \ln \gamma_2^C + \ln \gamma_2^R \tag{32b}$$

$$\ln \gamma_2^C = \ln \frac{\varphi_2}{x_2} + \frac{z}{2} q_2 \ln \frac{\vartheta_2}{\varphi_2} + \varphi_1 \left(l_2 - \frac{r_2}{r_1} l_1 \right) \tag{33b}$$

$$\ln \gamma_2^R = -q_2 \ln (\vartheta_1 \tau_{12} + \vartheta_2) + \vartheta_1 q_2 \left(\frac{\tau_{12}}{\vartheta_1 \tau_{12} + \vartheta_2} - \frac{\tau_{21}}{\vartheta_1 + \vartheta_2 \tau_{21}} \right) \tag{34b}$$

$$l_i = \frac{z}{2}(r_i - q_i) - (r_i - 1) \qquad z = 10 \tag{35}$$

Symbols

l_i see equation (35)

q_i area parameter of component i *)

r_i volume parameter of component i *)

u_{ij} Parameter of interaction between components i and j; $u_{ij} = u_{ji}$

z coordination number

γ_i^C combinatorial part of activity coefficient of component i

γ_i^R residual part of activity coefficient of component i

$\vartheta_i = \dfrac{q_i x_i}{\sum_j q_j x_j}$ area fraction of component i

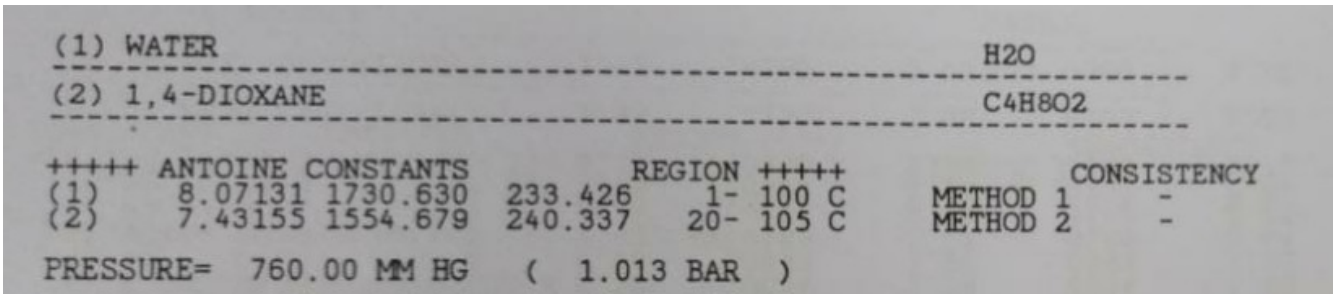
$\varphi_i = \dfrac{r_i x_i}{\sum_j r_j x_j}$ volume fraction of component i

τ_{ij} see Table 3

*) For values of r_i and q_i see Appendix A

*) 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.

Value of constants:



(1) WATER H2O

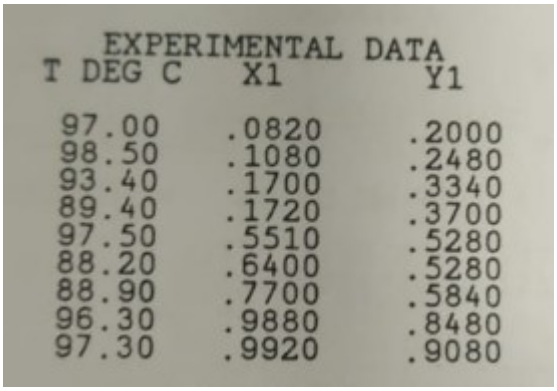
(2) 1,4-DIOXANE C4H8O2

+++++ ANTOINE CONSTANTS			REGION +++++		CONSISTENCY
(1)	8.07131 1730.630	233.426	1- 100 C	METHOD 1	-
(2)	7.43155 1554.679	240.337	20- 105 C	METHOD 2	-

PRESSURE= 760.00 MM HG (1.013 BAR)

CONSTANTS:	A12	A21	α_{12}	γ_1^∞	γ_2^∞	OBJECTIVE FUNCTION	
UNIQUAC	-19.1253	323.7097		3.03	14.31	.4613	G

T_{X-Y} Data:



EXPERIMENTAL DATA

T DEG C	X1	Y1
97.00	.0820	.2000
98.50	.1080	.2480
93.40	.1700	.3340
89.40	.1720	.3700
97.50	.5510	.5280
88.20	.6400	.5280
88.90	.7700	.5840
96.30	.9880	.8480
97.30	.9920	.9080

Take the molar volume from NIST Database. If not available, please contact the TA's (Krishna, Nikil & Adithya)

Note: All the data are taken from Dechema Chemistry Data Series