

Table 12.5: Parameter Values for the Wilson and NRTL Equations.

Parameters a_{12} , a_{21} , b_{12} , and b_{21} have units of cal mol^{-1} , and V_1 and V_2 have units of $\text{cm}^3 \text{mol}^{-1}$. Values are those recommended by Gmehling et al. *Vapor-Liquid Equilibrium Data Collection*, Chemistry Data Series, vol. I, parts 1a, 1b, 2c and 2e, DECHEMA, Frankfurt/Main, 1981–1988.

System	V_1 V_2	Wilson equation		NRTL equation		
		a_{12}	a_{21}	b_{12}	b_{21}	α
Acetone(1) Water(2)	74.05 18.07	291.27	1,448.01	631.05	1,197.41	0.5343
Methanol(1) Water(2)	40.73 18.07	107.38	469.55	-253.88	845.21	0.2994
1-Propanol(1) Water(2)	75.14 18.07	775.48	1,351.90	500.40	1,636.57	0.5081
Water(1) 1,4-Dioxane(2)	18.07 85.71	1,696.98	-219.39	715.96	548.90	0.2920
Methanol(1) Acetonitrile(2)	40.73 66.30	504.31	196.75	343.70	314.59	0.2981
Acetone(1) Methanol(2)	74.05 40.73	-161.88	583.11	184.70	222.64	0.3084
Methyl acetate(1) Methanol(2)	79.84 40.73	-31.19	813.18	381.46	346.54	0.2965
Methanol(1) Benzene(2)	40.73 89.41	1,734.42	183.04	730.09	1,175.41	0.4743
Ethanol(1) Toluene(2)	58.68 106.85	1,556.45	210.52	713.57	1,147.86	0.5292

12.18. For one of the binary systems listed in the preceding table, based on Eq. (10.5) and the Wilson equation make the following calculations:

(a) *BUBL T*: $P = 101.33 \text{ kPa}$, $x_1 = 0.3$.

(b) *DEW T*: $P = 101.33 \text{ kPa}$, $y_1 = 0.3$.

(c) *P, T-flash*: $P = 101.33 \text{ kPa}$, $T = \frac{1}{2}(T_{\text{bubble}} + T_{\text{dew}})$, $z_1 = 0.3$.

(d) If an azeotrope exists at $P = 101.33 \text{ kPa}$, find T^{az} and $x_1^{\text{az}} = y_1^{\text{az}}$.

12.19. Work the preceding problem for the NRTL equation: