APPENDIX B

NRTL PARAMETERS AND ANTOINE COEFFICIENTS

Tables B.1, B.2, and B.3 give binary interaction parameters (a, b, and c, respectively) for the NRTL equation (Equations B.1 and B.2) for systems that have been used and discussed extensively throughout the book. All parameters are regressed values from the Dortmund databank, obtained from Aspen Plus®.

$$\gamma_i = \exp\left[\frac{\sum_j x_j \tau_{ji} G_{ji}}{\sum_k x_k G_{ki}} + \sum_j \frac{x_j G_{ij}}{\sum_k x_k G_{kj}}\left(\tau_{ij} - \frac{\sum_m x_m \tau_{mj} G_{mj}}{\sum_k x_k G_{kj}}\right)\right] \tag{B.1}$$

$$\text{where } \tau_{ij} = a_{ij} + b_{ij}/T(K) \quad \text{and} \quad G_{ij} = \exp(-c_{ij}\tau_{ij}) \tag{B.2}$$

Example of Using Tables B.1–B.3

Suppose the binary interaction coefficients are being sought for the benzene–water system. We shall designate benzene as component i and water as component j. Then, in Table B.1, progress down the first column until component i is found (benzene). Then, progress down the row where component i has been found and search for the cell intersection with component j in the first row. It can be seen that $a_{ij} = 45.191$. To find a_{ji}, repeat the procedure, but search for component j in the first column, and then for the cell intersection with component i in the first row. In this

Understanding Distillation Using Column Profile Maps, First Edition. Daniel Beneke, Mark Peters, David Glasser, and Diane Hildebrandt.

TABLE B.1 Binary Interaction Parameter a_{ij} for the NRTL Model for Selected Components

	Methanol	Ethanol	Benzene	*p*-Xylene	Toluene	Chloroform	Water	Acetone
Methanol	0.000	4.712	−1.709	0.678	0.000	0.000	−0.693	0.000
Ethanol	−2.313	0.000	0.569	4.075	1.146	0.000	−0.801	−1.079
Benzene	11.580	−0.916	0.000	0.000	−2.885	0.000	45.191	0.422
p-Xylene	−3.259	−5.639	0.000	0.000	0.000	0	2.773	0.000
Toluene	0.000	−1.722	2.191	0.000	0.000	0.000	−247.879	−1.285
Chloroform	0.000	0.000	0.000	0	0.000	0.000	−7.352	0.538
Water	2.732	3.458	140.087	162.477	627.053	8.844	0.000	0.054
Acetone	0.000	−0.347	−0.102	0.000	1.203	0.965	6.398	0.000

TABLE B.2 Binary Interaction Parameter b_{ij} for the NRTL Model for Selected Components

	Methanol	Ethanol	Benzene	*p*-Xylene	Toluene	Chloroform	Water	Acetone
Methanol	0.0	−1162.3	892.2	295.5	371.1	−71.9	173.0	114.1
Ethanol	483.8	0.0	−54.8	−1202.4	−113.5	−148.9	246.2	479.1
Benzene	−3282.6	882.0	0.0	122.7	1124.0	−375.4	591.4	−239.9
p-Xylene	1677.6	2504.2	−136.5	0.0	75.9	−17.7	296.7	173.6
Toluene	446.9	992.7	−863.7	−91.1	0.0	−57.0	14759.8	630.1
Chloroform	690.1	690.3	313.0	−120.2	−25.2	0.0	3240.7	−106.4
Water	−617.3	−586.1	−5954.3	−6046.0	−27269.4	−1140.1	0.0	420.0
Acetone	101.9	206.6	306.1	83.2	−400.5	−590.0	−1809.0	0.0

TABLE B.3 Binary Interaction Parameter c_{ij} for the NRTL Model for Selected Components

	Methanol	Ethanol	Benzene	*p*-Xylene	Toluene	Chloroform	Water	Acetone
Methanol	0.0	0.3	0.4	0.5	0.3	0.3	0.3	0.3
Ethanol	0.0	0.0	0.3	0.3	0.3	0.3	0.3	0.3
Benzene	0.0	0.0	0.0	0.3	0.3	0.5	0.2	0.3
p-Xylene	0.0	0.0	0.0	0.0	0.3	0.3	0.2	0.3
Toluene	0.0	0.0	0.0	0.0	0.0	0.3	0.2	0.3
Chloroform	0.0	0.0	0.0	0.0	0.0	0.0	0.2	0.3
Water	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.3
Acetone	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0

TABLE B.4 Antoine Equation Coefficients for Selected Components

	Methanol	Ethanol	Benzene	*p*-Xylene	Toluene	Chloroform	Water	Acetone
A	8.07240	8.1122	6.90565	6.99052	6.95464	6.93710	8.01767	7.23160
B	1574.990	1592.864	1211.033	1453.430	1344.800	1171.200	1715.7	1277.030
C	238.870	226.184	220.790	215.307	219.482	227.000	234.268	237.230

example, $a_{ji} = 140.087$. Using a similar procedure, values for parameters b and c can also be found.

The Antoine equation for calculating vapor pressure is given in Equation B.3, with the relevant constants in Table B.4.

$$\ln\left(P_i^{\mathrm{VAP}}\right) = A_i - \frac{B_i}{T + C_i} \tag{B.3}$$