

**Table 1 Some Models for Excess Gibbs Energy and Activity Coefficients**

| Name                  | $G^E$                                                                                                      | Binary Parameters                              | $\ln \gamma_1$ and $\ln \gamma_2$                                                                                                                                                                                                                                                                                                                                                                                                  |
|-----------------------|------------------------------------------------------------------------------------------------------------|------------------------------------------------|------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Two-suffix Margules   | $\frac{G^E}{RTx_1x_2} = A$                                                                                 | $A$                                            | $\ln \gamma_1 = Ax_2^2$<br>$\ln \gamma_2 = Ax_1^2$                                                                                                                                                                                                                                                                                                                                                                                 |
| Three-suffix Margules | $\frac{G^E}{RTx_1x_2} = A_{21}x_1 + A_{12}x_2$                                                             | $A_{12}, A_{21}$<br>or<br>$A, B$               | $\ln \gamma_1 = x_2^2 [A_{12} + 2(A_{21} - A_{12})x_1]$<br>$\ln \gamma_2 = x_1^2 [A_{21} + 2(A_{12} - A_{21})x_2]$                                                                                                                                                                                                                                                                                                                 |
| Four-suffix Margules  | $\frac{G^E}{RTx_1x_2} = A_{21}x_1 + A_{12}x_2 - Cx_1x_2$                                                   | $A_{12}, A_{21}, C$                            | $\ln \gamma_1 = x_2^2 [A_{12} + 2(A_{21} - A_{12} - C)x_1 + 3Cx_1^2]$<br>$\ln \gamma_2 = x_1^2 [A_{21} + 2(A_{12} - A_{21} - C)x_2 + 3Cx_2^2]$                                                                                                                                                                                                                                                                                     |
| Van Laar              | $\frac{G^E}{RTx_1x_2} = \frac{A'_{12}A'_{21}}{A'_{12}x_1 + A'_{21}x_2}$                                    | $A'_{12}, A'_{21}$                             | $\ln \gamma_1 = A'_{12} \left( 1 + \frac{A'_{12}x_1}{A'_{21}x_2} \right)^{-2}$<br>$\ln \gamma_2 = A'_{21} \left( 1 + \frac{A'_{21}x_2}{A'_{12}x_1} \right)^{-2}$                                                                                                                                                                                                                                                                   |
| Wilson                | $\frac{G^E}{RT} = -x_1 \ln(x_1 + x_2\Lambda_{12}) - x_2 \ln(x_2 + x_1\Lambda_{21})$                        | $\Lambda_{12}, \Lambda_{21}$ ,<br>See Eq 13.53 | $\ln \gamma_1 = -\ln(x_1 + x_2\Lambda_{12}) + x_2 \left( \frac{\Lambda_{12}}{x_1 + x_2\Lambda_{12}} - \frac{\Lambda_{21}}{x_2 + x_1\Lambda_{21}} \right)$<br>$\ln \gamma_2 = -\ln(x_2 + x_1\Lambda_{21}) - x_1 \left( \frac{\Lambda_{12}}{x_1 + x_2\Lambda_{12}} - \frac{\Lambda_{21}}{x_2 + x_1\Lambda_{21}} \right)$                                                                                                             |
| NRTL                  | $\frac{G^E}{RTx_1x_2} = \frac{G_{21}\tau_{21}}{x_1 + x_2G_{21}} + \frac{G_{12}\tau_{12}}{x_2 + x_1G_{12}}$ | $\alpha, b_{12}, b_{21}$                       | $\ln \gamma_1 = x_2^2 \left[ \tau_{21} \left( \frac{G_{21}}{x_1 + x_2G_{21}} \right)^2 + \frac{G_{12}\tau_{12}}{(x_2 + x_1G_{12})^2} \right]$<br>$\ln \gamma_2 = x_1^2 \left[ \tau_{12} \left( \frac{G_{12}}{x_2 + x_1G_{12}} \right)^2 + \frac{G_{21}\tau_{21}}{(x_1 + x_2G_{21})^2} \right]$<br>$G_{12} = \exp(-\alpha\tau_{12}), G_{21} = \exp(-\alpha\tau_{21}), \tau_{12} = \frac{b_{12}}{RT}, \tau_{21} = \frac{b_{21}}{RT}$ |
| UNIQUAC               | See Appendix G                                                                                             | Appendix G                                     | See Appendix G                                                                                                                                                                                                                                                                                                                                                                                                                     |