Simulator Data

For the system methanol / diethylketone, the default binary parameters for the NRTL equation are given in the database of a particualr process simulator as follows:

23.1766 (A12)
25.0239 (A21)
-6644.97 (B12)
-9051.47 (B21)
0.3 (alpha)

The intial analysis indicates that the parameters are okay. One would expect slightly positive deviations from Raoult's law ($\gamma \sim 2$ as guess), as the OH-group in methanol cannot be well combined with the hydrocarbon tails of the ketone.

However, when plotting the Px diagrams for t = 30°C, t = 65°C and t = 100°C one observes strongly negative deviations from Raoult's law at low temperatures, with azeotrope and strongly positive deviations from Raoult's law at high temperatures, which is very unusual.

Further analysis indicates that the data base contains only one isobaric data set. It is generally not a good idea to model one isobaric data set with so many adjustable parameters, and any results should be treated with caution. The binary parameters have most likely been calcualted by a generic fitting program with no critical review of the experimental data.

Conclusion: It is dangerous to trust simulator default parameters without check.