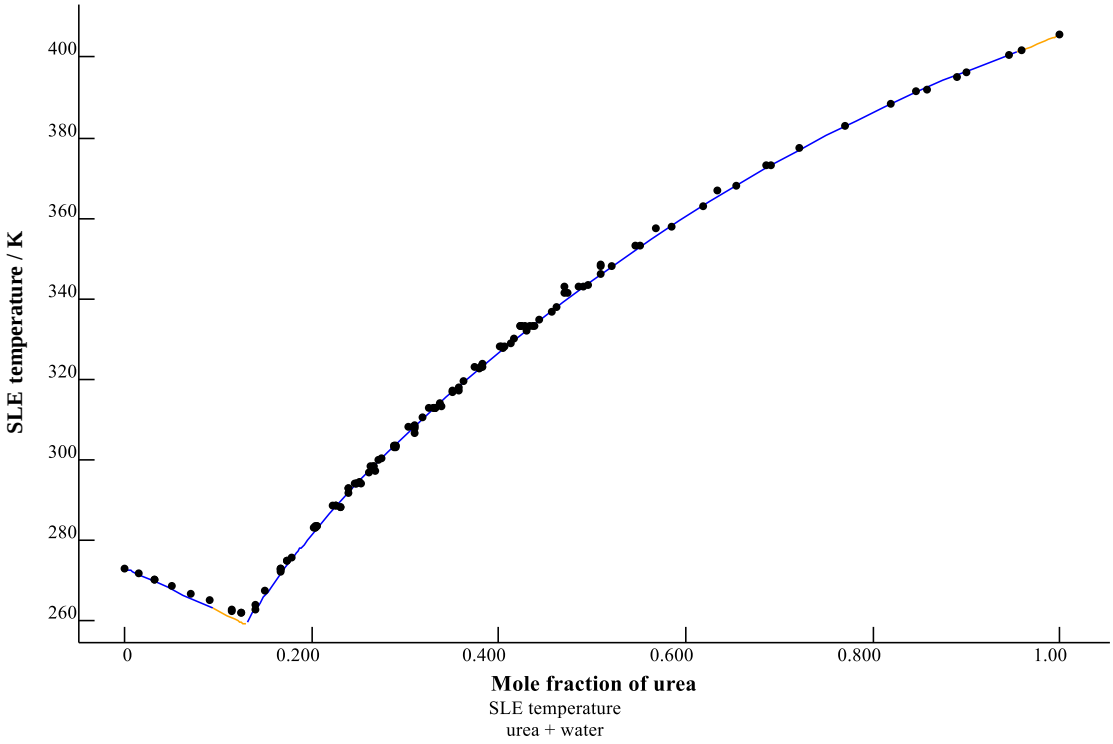
Preliminary selection for SLE (simple eutectics)

urea + water

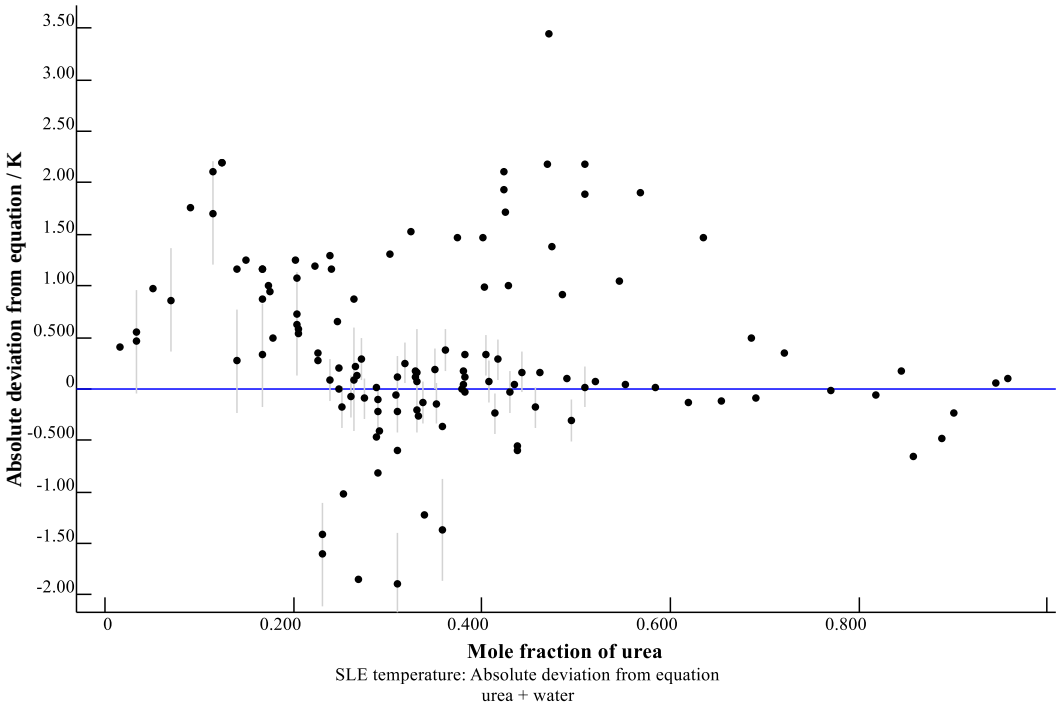
Model:

Wilson model with the following parameters (form: A + B/T)

	A	B
1	-2.00666	42.6832
2	0.592323	147.6



SLE temperature
urea + water



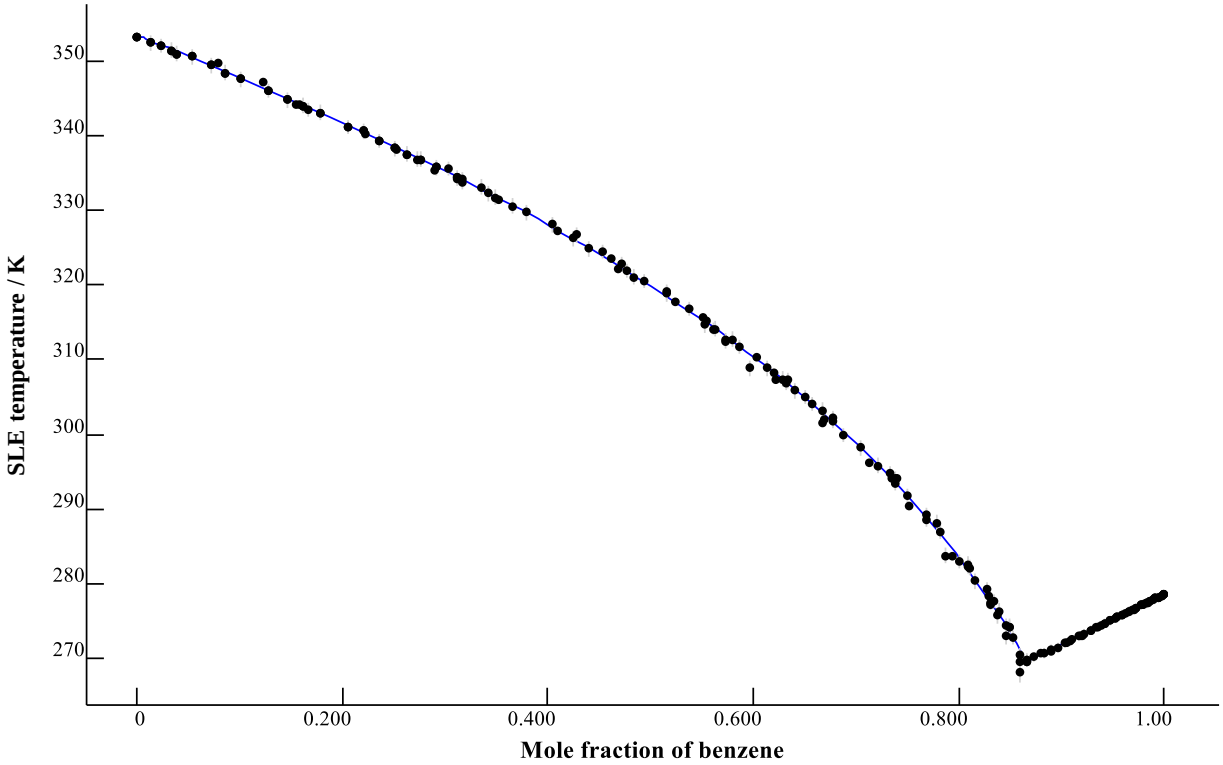
SLE temperature: Absolute deviation from equation
urea + water

Cryoscopic behavior of water is not adequately represented by the model and will not be part of recommendation. Some researchers claim 3 different states of solid urea that is not obviously true. Additional literature will be collected and reviewed. Consistency with other properties is reasonable.

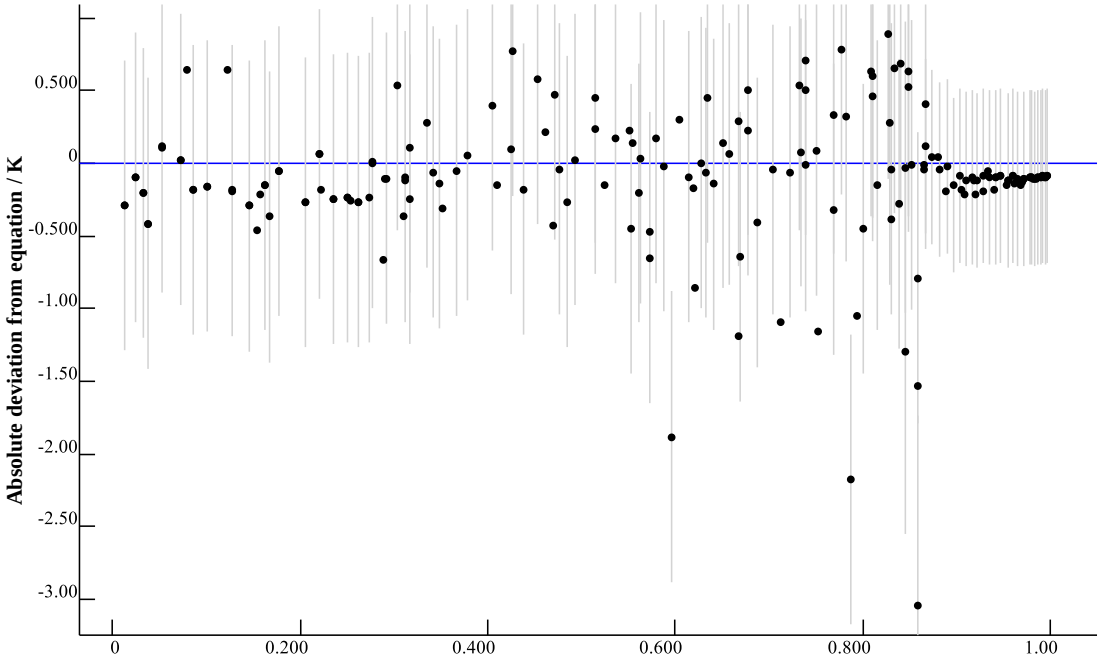
benzene + naphthalene

Model: NRTL with the following parameters:
Non-randomness parameter: 0.145198
Dimensionless interaction parameters (form: A + B/T):

	A	B
1	-1.41121	658.489
2	1.20467	-550.81



SLE temperature
benzene + naphthalene



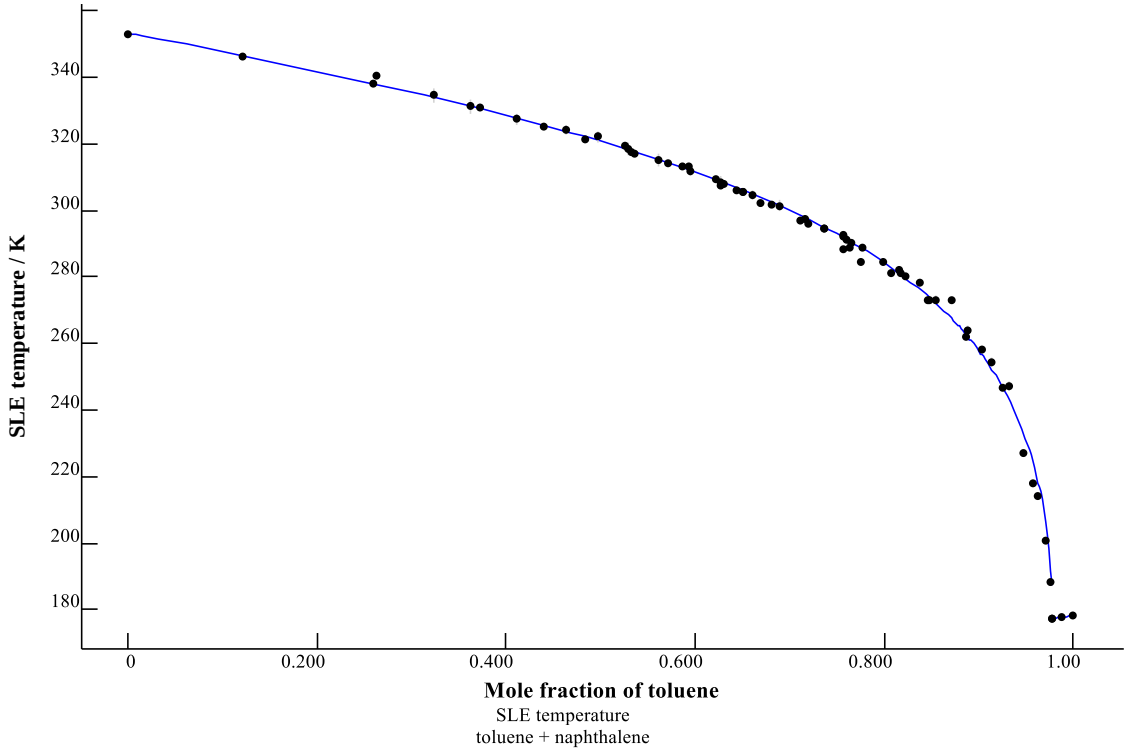
SLE temperature: Absolute deviation from equation
benzene + naphthalene

Nearly ideal. Consistent with other available property data. Consistency with Solubility Data Series is reasonable.

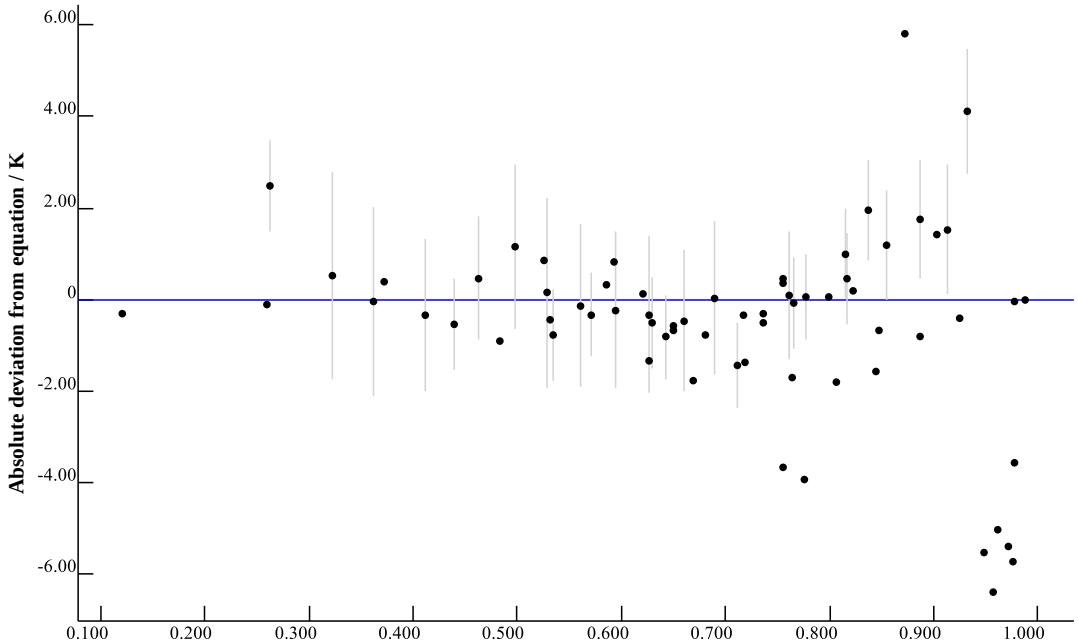
toluene + naphthalene

Model:
NRTL with the following parameters:
Non-randomness parameter: 0.442973
Dimensionless interaction parameters (form: A + B/T):

	A	B
1	1.86522	-688.106
2	-1.68996	733.55



SLE temperature
toluene + naphthalene



SLE temperature: Absolute deviation from equation
toluene + naphthalene

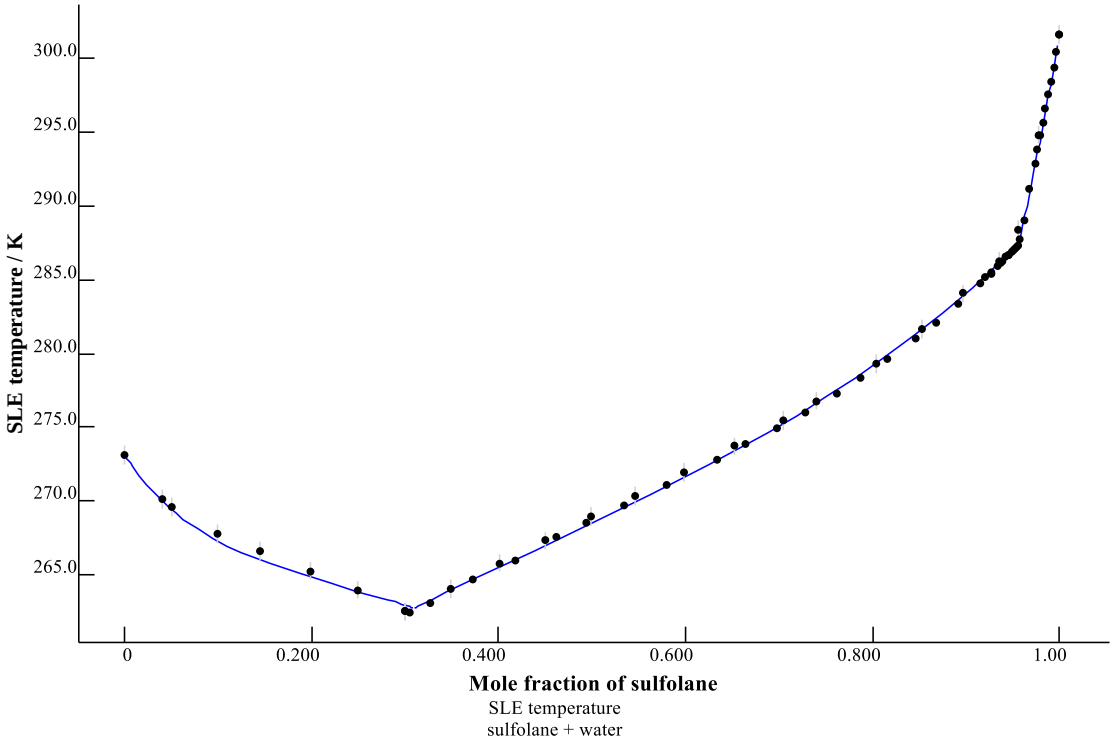
Close to ideal; reasonably agrees with the available VLE data. Has a region the solubility is nearly independent on T and non-isothermal methods (variation of T with constant composition) should not be adequate. Consistency with Solubility Data Series is reasonable.

sulfolane + water

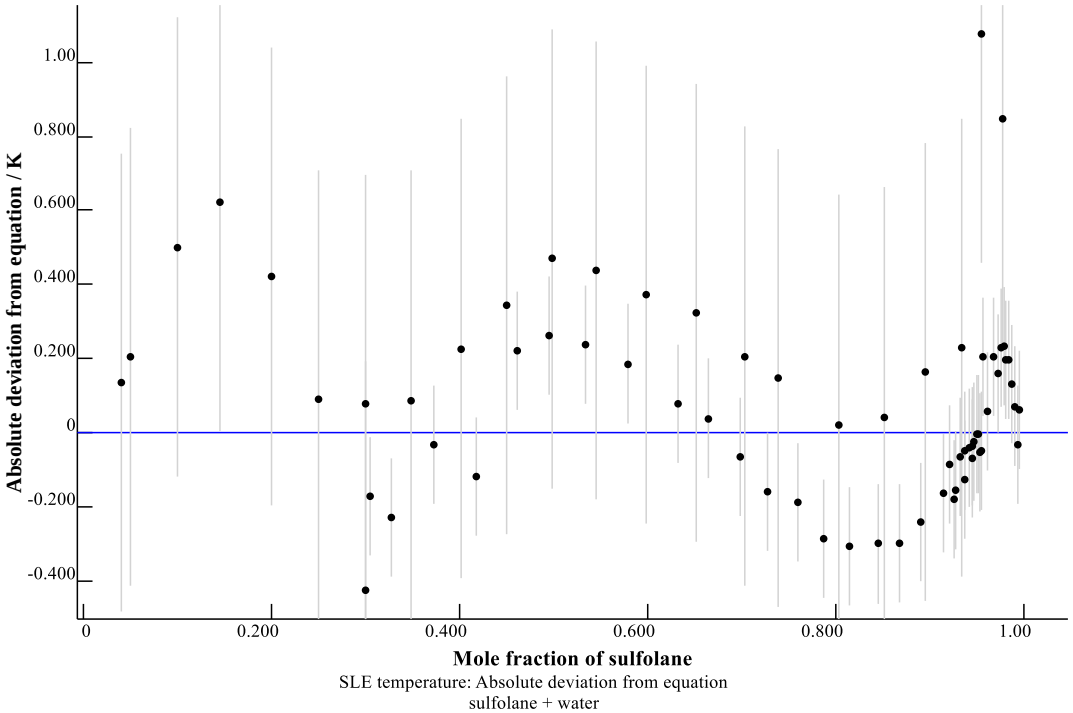
Model:

Wilson model with the following parameters (form: A + B/T):

	A	B
1	-2.22209	395.589
2	2.84798	-1336.3



SLE temperature
sulfolane + water



SLE temperature: Absolute deviation from equation
sulfolane + water

Models fit SLE data if melting enthalpy for sulfolane is modified from 1.4 kJ/mol to 2.1 kJ/mol (fusion). That is consistently observed for other mixtures with sulfolane. The water side of the SLE diagram is represented by models worse and will not be part of recommendation.

The high-temperature crystal of sulfolane can be easily supercooled, so a metastable SLE can be obtained. On the one hand, it creates difficulties for the researchers. On the other hand, it can be used to test the authors' methodology to get stable SLE (rather than metastable).

benzoic acid + water

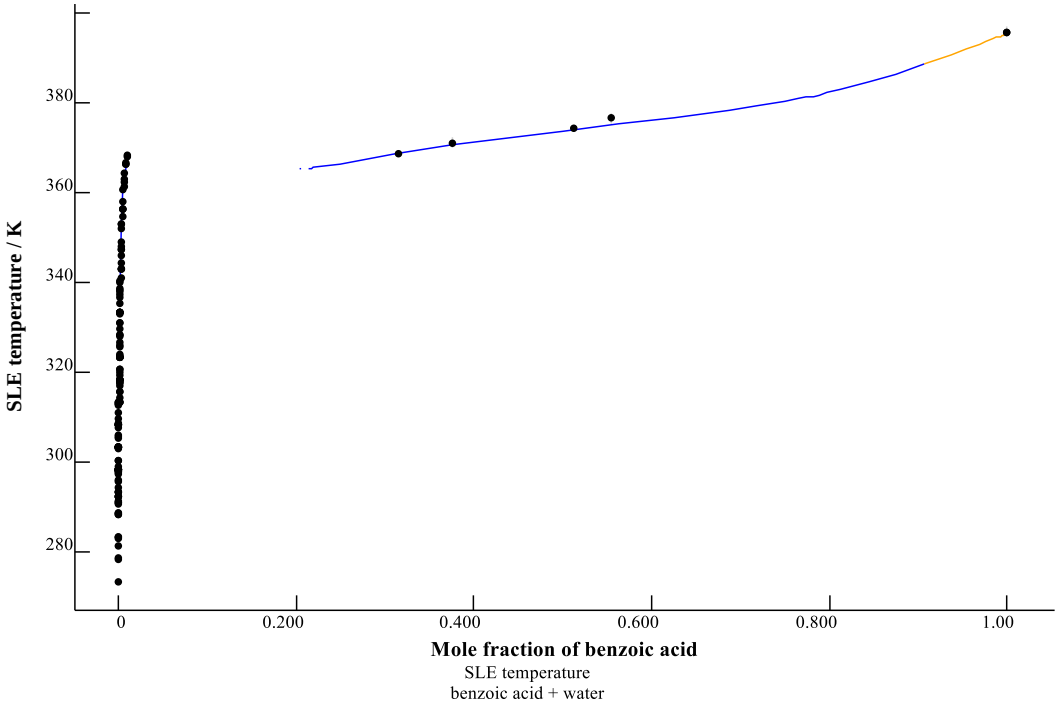
Model:

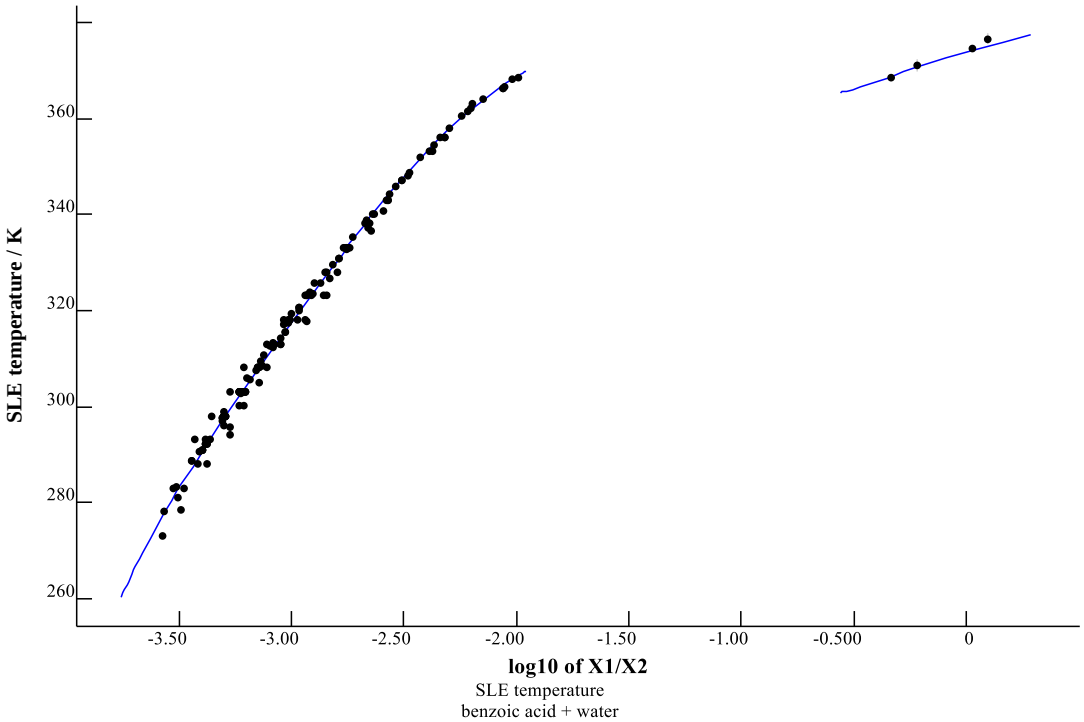
NRTL with the following parameters:

Non-randomness parameter: 0.477258

Dimensionless interaction parameters (form: A + B/T + DT):

	A	B	D
1	44.3515	-4795.43	-0.0742835
2	-22.3148	10216	-0.0096489





Probably, it is the best studied SLE with low solubility. The model is reasonably consistent with other properties. Temperature deviations on the steep part does not make sense; composition deviations (most within 10%) will be shown later.