

Boundaries_LL_NRTL: GUI for the Characterization of the NRTL Model: Binary Spinodal Surfaces (in the τ_{ij} - τ_{ji} - x_i space), LLE Maps, and Miscibility Boundaries

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**Boundaries_LL_NRTL: Graphical User Interface (GUI) for the Characterization of the NRTL Model:
Binary Spinodal Surfaces (in the τ_{ij} - τ_{ji} - x_i space), LLE Maps and Miscibility Boundaries**

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Visualization of pre-calculated binary spinodal surfaces, LLE maps and miscibility boundaries for the NRTL model (α_{ij} from 0 to 0.95):

$\alpha_{ij}=0$ $\alpha_{ij}=0.10$ $\alpha_{ij}=0.20$ $\alpha_{ij}=0.30$ $\alpha_{ij}=0.40$ $\alpha_{ij}=0.50$ $\alpha_{ij}=0.60$ $\alpha_{ij}=0.70$ $\alpha_{ij}=0.80$ $\alpha_{ij}=0.90$
 $\alpha_{ij}=0.05$ $\alpha_{ij}=0.15$ $\alpha_{ij}=0.25$ $\alpha_{ij}=0.35$ $\alpha_{ij}=0.45$ $\alpha_{ij}=0.55$ $\alpha_{ij}=0.65$ $\alpha_{ij}=0.75$ $\alpha_{ij}=0.85$ $\alpha_{ij}=0.95$ Summary 3Dfig

Calculation of a specific NRTL binary spinodal surface and LLE maps (by discrete scanning):

τ_{ij} limits: +/-: Number of τ_{ij} points: Number of x_i points:

α_{ij} value: Map Calculation Grid of individual gM.L curves

Representation of correlated miscibility boundaries for the NRTL model: (Ref: [10] AIChE Journal, 2022, e17085)

k	t(1,k)	t(2,k)	t(3,k)	t(4,k)	f(LLE)	p(1)	p(2)	p(3)	p(4)	f(mLLE)	p(1)	p(2)	p(3)	p(4)	
LLE 0	-61.7182	144.834	-96.6099	9.89155	(0.4 < α_{ij} < 0.95)	a(q)	0.17018	0.94122	-15.8926	7.41426	a(q)	0.17970	3.66704	-12.2321	-169.867
1	11.0599	-7.61356	2.78799	0.94847	(0 < α_{ij} < 0.4)	b(q)	1.18745	0.39818	6.61230	8.99112	b(q)	0.04713	1.09335	-2.70716	-70.5291
2	-18.9354	46.9735	-37.9100	10.6231	(0.4 < α_{ij} < 0.95)	c(q)	0.96617	0.85518	9.30456	9.54404	c(q)	0	0	0	0
mLLE 3	-712.144	789.320	-297.731	44.5960	(0.15 < α_{ij} < 0.43)	d(q)	-1.29669	-2.15482	-2.96603	-11.2090	d(q)	-1.00726	-11.9808	66.6629	299.304
						e(q)	0.45992	1.95455	3.08991	3.68998	e(q)	2.93930	0.38653	49.0533	-146.868

Correlated boundaries evolution: LLE Boundaries LLE mLLE Boundaries

New single boundaries calculation: α_{ij} value: 0 < < 0.95 Boundaries calculation

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