

# GMcal\_TieLinesLL: GUI for the Topological Analysis of Calculated $G^{M(L)}$ Surfaces and Curves, including Tie-Lines, Hessian Matrix, Spinodal Curve, Critical Point Location, etc. for Binary and Ternary LLE Data

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**TOPOLOGICAL ANALYSIS OF LIQUID-LIQUID EQUILIBRIUM DATA CORRELATIONS**  
 GUI v.2.2. Graphical User interface for the representation of  $G^M(L)$  surfaces for binary and ternary systems, including LL tie-lines, Tjessian matrix analysis, Spinodal curve, Flat Point Location, etc. (using NRTL, UNIQUAC or an alternative model)  
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**Institutional Repository RUA:** <http://hdl.handle.net/10045/51725>

Data source: Introduce Excel file name and press enter:

Remark: parameters: NRTL Tj=ajj/T and qj=aj, UNIQUAC Tj=exp(-ajj/T), ai, qj and Z

Calculated  $G^M(L)$  function and LL Tie-Lines:

Hessian Matrix Determinant & Flat point location:

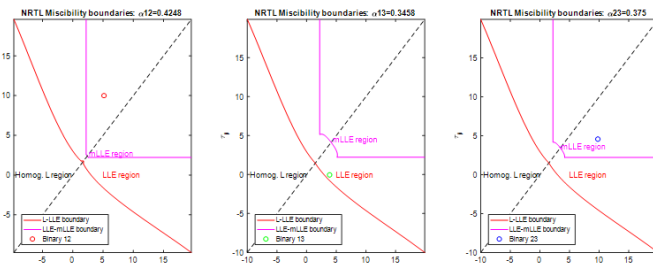
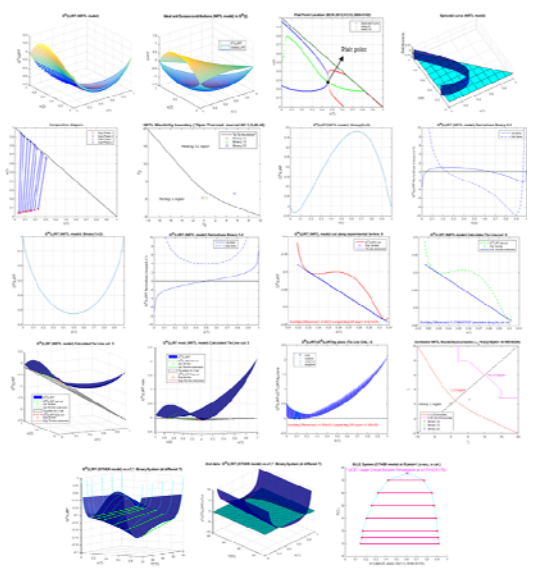
Ref. [12] I&ECCR 2012, 51(13), 5099-5102  
<http://dx.doi.org/10.1021/iecr2012793r>

NRTL Binary Parameter Boundaries (Tj vs Tj) for Total and Partial Miscibility:  Ref. [18] GUI/RUA, 2022 <http://hdl.handle.net/10045/121471>

GM(L) Surface cuts along the selected tie-lines: Number of the Tie-line to represent a GM/RT cut (if zero all the tie-line cuts will be represented)   Tie-Line GM(L) cuts

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Parameters		T12	-0.271955	Tj=ajj/T		NRTL		Fluid Phase Equilibria, 2017, 433, 243-252.	
1	Parameters	T12	-0.271955	Tj=ajj/T		NRTL		Fluid Phase Equilibria, 2017, 433, 243-252.	
2	F(alm)=	T21	0.2934596	Tj=ajj/T		NRTL		<a href="http://dx.doi.org/10.1016/j.fluid.2016.11.009">http://dx.doi.org/10.1016/j.fluid.2016.11.009</a>	
3	Tj [°C]	T13	0.4239739	Tj=ajj/T		NRTL		GMcal_TieLinesLL (v.2.2). Graphical User Interface (GUI) f	
4	N Tie-Lines=	T31	0.2818906	Tj=ajj/T		NRTL		<a href="http://hdl.handle.net/10045/51725">http://hdl.handle.net/10045/51725</a>	
5	Model used:	T23	5.4643647	Tj=ajj/T		NRTL		Test 5: LLE ternary system. NRTL model (with calculated)	
6	Experimental Data:	T32	1.6201092	Tj=ajj/T		NRTL		Consistent with the experimental data	
7	Experimental Data:			Tj=ajj/T		NRTL		Mean dev between cal and exp. conc. in mol fractions [ 0.025; 0.173]	
8	Experimental Data:			Tj=ajj/T		NRTL		0.002552986, 0.00252986, 0, 0.01983576, 0.01078454, 0.00232888	
9	Experimental Data:			Tj=ajj/T		NRTL		dev_xF1, dev_xF2, dev_xF3, dev_xF4, dev_xF5, dev_xF6, dev_xF7, dev_xF8, dev_xF9, dev_xF10	
10	Experimental Data:			Tj=ajj/T		NRTL		0.00466184, 0.00466184, 0, 0.000521499, 0.000009972, 0.000558494	
11	Experimental Data:			Tj=ajj/T		NRTL		0.00084482, 0.00084482, 0, 0.0199544, 0.01967028, 0.000495621	
12	Experimental Data:			Tj=ajj/T		NRTL		0.000422474, 0, 0.000351977, 0.000352932, 0.000694485	
13	Experimental Data:			Tj=ajj/T		NRTL		0.000433064, 0.000433064, 0, 0.000172568, 0.000507434, 0.000200001	
14	Experimental Data:			Tj=ajj/T		NRTL		0.000822347, 0.000822347, 0, 0.01747432, 0.0247487, 0.000491945	
15	Experimental Data:			Tj=ajj/T		NRTL		0.000427991, 0.000427991, 0, 0.009044075, 0.007952882, 0.000105184	
16	Experimental Data:			Tj=ajj/T		NRTL		0.000329705, 0.000329705, 0, 0.03707089, 0.034416227, 0.002780941	
17	Experimental Data:			Tj=ajj/T		NRTL		0.00256732, 0.00256732, 0, 0.00260702, 0.01041264, 0.000760562	
18	Experimental Data:			Tj=ajj/T		NRTL		0.000353632, 0.000353632, 0, 0.00959228, 0.01029595, 0.000526377	
19	Experimental Data:			Tj=ajj/T		NRTL			
20	Experimental Data:			Tj=ajj/T		NRTL			
21	Experimental Data:			Tj=ajj/T		NRTL			
22	Experimental Data:			Tj=ajj/T		NRTL			
23	Experimental Data:			Tj=ajj/T		NRTL			
24	Experimental Data:			Tj=ajj/T		NRTL			
25	Experimental Data:			Tj=ajj/T		NRTL			
26	Experimental Data:			Tj=ajj/T		NRTL			
27	Experimental Data:			Tj=ajj/T		NRTL			
28	Experimental Data:			Tj=ajj/T		NRTL			
29	Experimental Data:			Tj=ajj/T		NRTL			
30	Experimental Data:			Tj=ajj/T		NRTL			
31	Experimental Data:			Tj=ajj/T		NRTL			
32	Experimental Data:			Tj=ajj/T		NRTL			
33	Experimental Data:			Tj=ajj/T		NRTL			
34	Experimental Data:			Tj=ajj/T		NRTL			
35	Experimental Data:			Tj=ajj/T		NRTL			
36	Experimental Data:			Tj=ajj/T		NRTL			
37	Experimental Data:			Tj=ajj/T		NRTL			
38	Experimental Data:			Tj=ajj/T		NRTL			

Parameters		param.1 13.30		more parameters 7-9		more parameters 10-19		Fluid Phase Equilibria, 2017, 433, 243-252	
1	Parameters	param.1 13.30		more parameters 7-9		more parameters 10-19		Fluid Phase Equilibria, 2017, 433, 243-252	
2	F(alm)=	param.2 -172.62		more parameters 7-9		more parameters 10-19		<a href="http://dx.doi.org/10.1016/j.fluid.2016.11.009">http://dx.doi.org/10.1016/j.fluid.2016.11.009</a>	
3	Tj [°C]	param.3 -2423.78		more parameters 7-9		more parameters 10-19		GUI v.2.1 for the representation of GM surfaces	
4	N Tie-Lines=	param.4 8782.76		more parameters 7-9		more parameters 10-19		<a href="http://hdl.handle.net/10045/51725">http://hdl.handle.net/10045/51725</a>	
5	Model used:	param.5 0.20		more parameters 7-9		more parameters 10-19		Test 5: BINARY SYSTEM (UNIQUAC with T dependence)	
6	Experimental Data:	param.6 23.88		more parameters 7-9		more parameters 10-19		UCST: Upper Critical Solution Temperature	
7	Experimental Data:	param.6 23.88		more parameters 7-9		more parameters 10-19		Boundaries_LL_NRTL. Graphical User Interface (GUI) f	
8	Experimental Data:	param.6 23.88		more parameters 7-9		more parameters 10-19		<a href="http://hdl.handle.net/10045/121471">http://hdl.handle.net/10045/121471</a>	
9	Experimental Data:	param.6 23.88		more parameters 7-9		more parameters 10-19		Model 5	
10	Experimental Data:	param.6 23.88		more parameters 7-9		more parameters 10-19		UNIQUAC with T dependence	
11	Experimental Data:	param.6 23.88		more parameters 7-9		more parameters 10-19		for binary systems (15 parameters)	
12	Experimental Data:	param.6 23.88		more parameters 7-9		more parameters 10-19		Tj = exp (aij + bjj/T + cij ln T + dij T)	
13	Experimental Data:	param.6 23.88		more parameters 7-9		more parameters 10-19			
14	Experimental Data:	param.6 23.88		more parameters 7-9		more parameters 10-19			
15	Experimental Data:	param.6 23.88		more parameters 7-9		more parameters 10-19			
16	Experimental Data:	param.6 23.88		more parameters 7-9		more parameters 10-19		aij/R	
17	Experimental Data:	param.6 23.88		more parameters 7-9		more parameters 10-19		13.30	
18	Experimental Data:	param.6 23.88		more parameters 7-9		more parameters 10-19		-172.62	
19	Experimental Data:	param.6 23.88		more parameters 7-9		more parameters 10-19		-2423.78	
20	Experimental Data:	param.6 23.88		more parameters 7-9		more parameters 10-19		8782.76	
21	Experimental Data:	param.6 23.88		more parameters 7-9		more parameters 10-19		0.20	
22	Experimental Data:	param.6 23.88		more parameters 7-9		more parameters 10-19		23.88	
23	Experimental Data:	param.6 23.88		more parameters 7-9		more parameters 10-19		0.023	
24	Experimental Data:	param.6 23.88		more parameters 7-9		more parameters 10-19		0.0197	
25	Experimental Data:	param.6 23.88		more parameters 7-9		more parameters 10-19			
26	Experimental Data:	param.6 23.88		more parameters 7-9		more parameters 10-19			
27	Experimental Data:	param.6 23.88		more parameters 7-9		more parameters 10-19			
28	Experimental Data:	param.6 23.88		more parameters 7-9		more parameters 10-19			
29	Experimental Data:	param.6 23.88		more parameters 7-9		more parameters 10-19			
30	Experimental Data:	param.6 23.88		more parameters 7-9		more parameters 10-19			
31	Experimental Data:	param.6 23.88		more parameters 7-9		more parameters 10-19			
32	Experimental Data:	param.6 23.88		more parameters 7-9		more parameters 10-19			
33	Experimental Data:	param.6 23.88		more parameters 7-9		more parameters 10-19			
34	Experimental Data:	param.6 23.88		more parameters 7-9		more parameters 10-19			
35	Experimental Data:	param.6 23.88		more parameters 7-9		more parameters 10-19			
36	Experimental Data:	param.6 23.88		more parameters 7-9		more parameters 10-19			
37	Experimental Data:	param.6 23.88		more parameters 7-9		more parameters 10-19			
38	Experimental Data:	param.6 23.88		more parameters 7-9		more parameters 10-19			

UCST: Upper Critical Solution Temperature  
 Calculated (approx.)  
 Tj [°C]    x1    x2  
 103    0.697    0.303  
 I&ECCR, 2020, 59(17), 8463-8475.  
<https://doi.org/10.1021/acs.iecr.0c00141>