

ParamIni_LL_NRTL: GUI for the Selection of NRTL Initial Parameters for the Correlation of Ternary Liquid-Liquid Equilibrium Data (Type I, II, III and 0 (LL island), i.e. with 1, 2, 3 or 0 binary pairs partially miscible)
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ParamIni_LL_NRTL

Graphical User Interface (GUI) for the Selection of NRTL Initial Parameters for the Correlation of Ternary Liquid-Liquid Equilibrium Data (Type I, II, III and 0 (LL island), i.e. with 1, 2, 3 or 0 binary pairs partially miscible)

--- NRTL model ---

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 Institutional Repository RUA: <http://hdl.handle.net/10045/130017>

Data source: Introduce Excel file name and press enter: Data Loaded!!

Remark, parameters: NRTL: $\tau_{ij} = A_{ij}/RT$ and $\alpha_{ij} = \alpha_{ji}$

System Type (Treybal classification):

i,j	τ_{ij}	τ_{ji}	$\alpha_{ij} = \alpha_{ji}$
1,2	-3.19996	0.700032	0.1
1,3	-3.00044	8.79983	0.0517236
2,3	0.299907	2.00016	0.5

Data Base Analysis and suggested initial parameters:

Buttons: Calculate GM(L)/RT surfaces with tie-lines, Calculate Binary GM(L) curves, Hessian Matrix Determinant & Plait point location

Topological Revision:

Ref: [7] I&ECR 2012, 51(13), 5098-5102. <http://dx.doi.org/10.1021/ie202793r>
 Ref: [8] The Open Thermodynamics Journal, 2011, 5, 48-62. <http://hdl.handle.net/10045/19865>
 Ref: [10] AIChE Journal, 2022, e17085.
 [11] GUI Boundaries_LL_NRTL: <http://hdl.handle.net/10045/121471>

NRTL Binary Parameter Boundaries (τ_{ij} vs τ_{ji}) for Total and Partial Miscibility:

Number of the Tie-line to represent a GM/RT cut: (press enter)

GM(L) Surface cuts along the selected tie-lines: (if zero all the tie-line cuts will be respresented)

Additional bibliography:

- Should we trust all the published LLE correlation parameters in phase equilibria? Necessity of their Assessment Prior to Publication. Fluid Phase Equilibria, 2017, 433, 243-252.
- Graphical User Interface (GUI) for the representation of GI surfaces and curves (for binary and ternary systems), including tie-lines, Hessian Matrix analysis, Critical Point Location, Miscibility Boundaries RUA 2015/22: <http://hdl.handle.net/10045/517215>
- What does the NRTL model look like? Determination of boundaries for different equilibrium regions. AIChE Journal, 2022, e17805 (<https://dx.doi.org/10.1002/aic.17805>).
- Boundaries_LL_NRTL: Graphical User Interface (GUI) for the Characterization of the NRTL Model: Binary Spinodal Surfaces (in the tau-ij-tau-ji-xi space), LLE maps and Miscibility Boundaries. RUA 2022: <http://hdl.handle.net/10045/121471>
- GMcal_TieLinesVL: Graphical User Interface (GUI) for the Topological Analysis of Gibbs Energy Functions for Binary and Ternary (isobaric or isothermal) Vapor-Liquid Equilibrium (VLE) Data (Including Tie-Lines, Derivatives, Distillation Boundaries, LL Critical Points Location, etc.). RUA 2022: <http://hdl.handle.net/10045/122857>
- Methods for Improving Models for Condensed Phase Equilibrium Calculations. Fluid Phase Equilib. 2010, 296(1), 15-24.
- Correlation of the liquid-liquid equilibrium data for specific ternary systems with one or two partially miscible binary subsystems. Fluid Phase Equilib. 2009, 281, 9-14.
- Gibbs energy based procedure for the correlation of type 3 systems including a three-liquid phase region. Fluid Phase Equilib. 2008, 278, 87-95.
- Modeling Liquid-Liquid Equilibria for Island type Ternary Systems. Fluid Phase Equilib. 2008, 285, 184-191.
- Aspects to be considered for the development of a correlation algorithm for condensed phase equilibrium data of ternary systems. Ind. Eng. Chem. Res. 2010, 49 (20), 10100-10110.
- Checking Liquid-Liquid Plait Point Conditions and their Application in Ternary Systems. Industrial & Engineering Chemistry Research 2012, 51(13), 5098-5102.
- GE Models and Algorithms for Condensed Phase Equilibrium Data Regression in Ternary Systems: Limitations and Proposals. The Open Thermodynamics Journal, 2011, 5, (Suppl 1-M5) 48-62.

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