

GMcal_TieLinesVL: GUI for the Topological Analysis of Experimental and Calculated G^M Functions for Binary and Ternary (isobaric or isothermal) VLE Data (including Tie-Lines, Derivatives, Distillation Boundaries, LL Critical Points Location etc.)

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GMcal_TieLinesVL (v.2.2): TOPOLOGICAL ANALYSIS OF VAPOR-LIQUID EQUILIBRIUM DATA AND CORRELATIONS
 Graphical User Interface (GUI) for the Representation of Experimental and Calculated G^M Functions for Binary and Ternary (isobaric or isothermal) Vapor-Liquid Equilibrium (VLE or VLLE) data (including Tie-Lines, Derivatives, Distillation Boundaries, LL Critical Points, etc.)
 -- using NRTL, UNIQUAC or an alternative model --
 Chemical Engineering Department & Institute of Chemical Process Engineering, University of Alicante (Spain)**
 Institutional Repository RUA: <http://hdl.handle.net/10045/122857>

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

Remark, parameters: NRTL: Aij (K) and $\alpha_{ij} = \alpha_j$; UNIQUAC: Aij (K); n; q; q1 and Z

Graphical and topological analysis: Ref: [8,9]

Comparatives of GM/RT and $d(GM/RT)/dx_1$ calculated with models and with the experimental data

Equilibrium Diagrams (data) Ref: [10, 11]

NRTL Binary Parameter Boundaries (τ_{ij} vs τ_{ji}) for Total and Partial Miscibility:
 Ref: [5] The Open Thermodynamics Journal, 2011, 5, 48-62. <http://hdl.handle.net/10045/19865>
Ref: [6] AIChE Journal, 2022, e17085. <https://doi.org/10.1002/aic.17805>
[7] GUI Boundaries_LL_NRTL: <http://hdl.handle.net/10045/121471>

GM/RT functions along selected tie-line: Number of the Tie-line to represent: (press enter)

Additional bibliography:
 [1] 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.
 [2] GMcal_TieLinesVL: Graphical User Interface (GUI) for the Topological Analysis of Calculated G^M Surfaces and Curves, including Tie-Lines, Hessian Matrix, Spinodal Curve, Plait Point Location, etc. for Binary and Ternary Liquid-Liquid Equilibrium (LLE) Data (RUA 2015/22): <http://hdl.handle.net/10045/1725>
 [3] The unavoidable necessity of considering temperature dependence of the liquid Gibbs energy of mixing for certain VLE data correlations Fluid Phase Equilibria 2016, 473, 17-31.
 [4] Procedure for the correlation of normal appearance VLE data, where the classical models dramatically fail with no apparent reason. Fluid Phase Equilibria. 2019, 423, 88-101.
 [5] GE Models and Algorithms for Condensed Phase Equilibrium Data Regression in Ternary Systems: Limitations and Proposals. The Open Thermodynamics Journal. 2011, 5, 48-62.
 [6] What does the NRTL model look like? Determination of boundaries for different fluid phase equilibrium regions. AIChE Journal, 2022, e17805 (<https://doi.org/10.1002/aic.17805>).
 [7] Boundaries_LL_NRTL: Graphical User Interface (GUI) for the Characterization of the NRTL Model Binary Spinodal Surfaces (in the tau_{ij}-tau_{ji}-x₁ space), LLE maps and Miscibility Boundaries. (RUA 2022): <http://hdl.handle.net/10045/121471>
 [8] Checking Liquid-Liquid Critical Point Conditions and their Application in Ternary Systems. Industrial & Engineering Chemistry Research. 2012, 51(13), 5098-5102.
 [9] LLE data correlation using NRTL model for different types of binary systems: UCST, LCST and closed miscibility loops. Industrial & Engineering Chemistry Research. 2020, 59(17), 8469-8479.
 [10] Approximate Calculation of Distillation Boundaries for Ternary Azeotropic Systems. Ind. Eng. Chem. Res. 2011, 50 (12), 7462-7466.
 [11] Numerical Determination of Distillation Boundaries for Multicomponent Homogeneous and Heterogeneous Azeotropic Systems. Computer Aided Chemical Engineering. 2010, 28(C), 643-648.

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