Boundaries_LL_NRTL

Graphical User Interface (GUI) for the Characterization of the NRTL Model: Binary Spinodal Surfaces (in the $\tau_{i,j}$-$\tau_{j,i}$-x_i space), LLE Maps, and Miscibility Boundaries

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1. INTRODUCTION

In a similar way to the previous MatLab Graphical User Interfaces (GUI's) developed to systematically check the consistency of LLE or VLE data correlation results, GMcal_TieLinesLL [1,2] GMcal_TieLinesVL [3] respectively, this Graphical User Interface (Boundaries_LL_NRTL) has been developed as a friendly tool for the analysis of the NRTL model, and it is directly related with the *AIChE Journal* research paper: ***"What does the NRTL model look like? Determination of boundaries for different fluid phase equilibrium regions"*** [4]. This GUI allows the direct visualization and calculation of 3D representations (in the $\tau_{i,j}$-$\tau_{j,i}$-x_i space) and 2D projections (in the $\tau_{i,j}$-$\tau_{j,i}$ plane) of binary spinodal surfaces, LLE maps, and miscibility boundaries of the NRTL model for different values of the non-randomness parameter ($\alpha_{i,j}$) between 0 and 0.95.

The analysis of all these figures allows researchers involved in the correlation of experimental liquid-liquid equilibrium data, to establish relations between the typology of the system under study (regarding the behavior of all the binary subsystems) and the values of the NRTL binary interaction parameters $\tau_{i,j}$-$\tau_{j,i}$ consistent with that typology.

NRTL model for non-ideal liquid mixtures

➢ ***Gibbs energy of mixing***

$$\mathbf{g^{M(L)} = G^{Mixture,L}/RT} = G^{Ideal}/RT + G^{Excess}/RT) = x_i \cdot ln\,(x_i) + G^E/RT$$

➢ ***Excess Gibbs energy:***

$$\frac{G^{E\,(NRTL)}}{RT} = \sum_{i=1}^{C} x_i \cdot \frac{\sum_{j=1}^{C} \tau_{j,i} \cdot G_{j,i} \cdot x_j}{\sum_{k=1}^{C} G_{k,i} \cdot x_k}$$

➢ ***Activity coefficient:***

$$ln\,\gamma_i \;\; = \frac{G^E}{RT} + \sum_{j=1}^{C} x_i \cdot \left(\frac{\partial (G^E/RT)}{\partial x_i} - \frac{\partial (G^E/RT)}{\partial x_j} \right)$$

$$ln\,\gamma_i^{NRTL} = \frac{\sum_{j=1}^{C} \tau_{j,i} \cdot G_{j,i} \cdot x_j}{\sum_{k=1}^{C} G_{k,i} \cdot x_k} + \sum_{j=1}^{C} \frac{G_{i,j} \cdot x_j}{\sum_{k=1}^{C} G_{k,j} \cdot x_k} \cdot \left(\tau_{i,j} - \frac{\sum_{m=1}^{C} \tau_{m,j} \cdot G_{m,j} \cdot x_m}{\sum_{k=1}^{C} G_{k,j} \cdot x_k} \right)$$

with $\tau_{j,i} = \frac{A_{j,i}}{RT}$; $G_{j,i} = exp(-\alpha_{j,i} \cdot \tau_{j,i})$; $A_{i,i}=0$ and $\alpha_{i,j} = \alpha_{j,i}$

For a binary system ($C=2$):

$$\frac{G^{E(NRTL)}}{RT} = x_1 \cdot \frac{\tau_{21} \cdot G_{21} \cdot x_2}{x_1 + G_{21} \cdot x_2} + x_2 \cdot \frac{\tau_{12} \cdot G_{12} \cdot x_1}{G_{12} \cdot x_1 + x_2}$$

$$\frac{\partial (G^{E(NRTL)}/RT)}{\partial x_1} = \frac{\tau_{21} \cdot (G_{21} \cdot x_2)^2}{(x_1 + G_{21} \cdot x_2)^2} + \frac{\tau_{12} \cdot G_{12} \cdot x_2^2}{(G_{12} \cdot x_1 + x_2)^2}$$

$$\frac{\partial (G^{E(NRTL)}/RT)}{\partial x_2} = \frac{\tau_{21} \cdot G_{21} \cdot x_1^2}{(x_1 + G_{21} \cdot x_2)^2} + \frac{\tau_{12} \cdot (G_{12} \cdot x_1)^2}{(G_{12} \cdot x_1 + x_2)^2}$$

$$ln\,\gamma_1^{NRTL} = x_2^2 \cdot \left[\frac{\tau_{21} \cdot G_{21}^2}{(x_1 + x_2 \cdot G_{21})^2} + \frac{\tau_{12} \cdot G_{12}}{(x_2 + x_1 \cdot G_{12})^2} \right]$$

$$ln\,\gamma_2^{NRTL} = x_1^2 \cdot \left[\frac{\tau_{12} \cdot G_{12}^2}{(x_2 + x_1 \cdot G_{12})^2} + \frac{\tau_{21}.G_{21}}{(x_1 + x_2 \cdot G_{21})^2} \right]$$

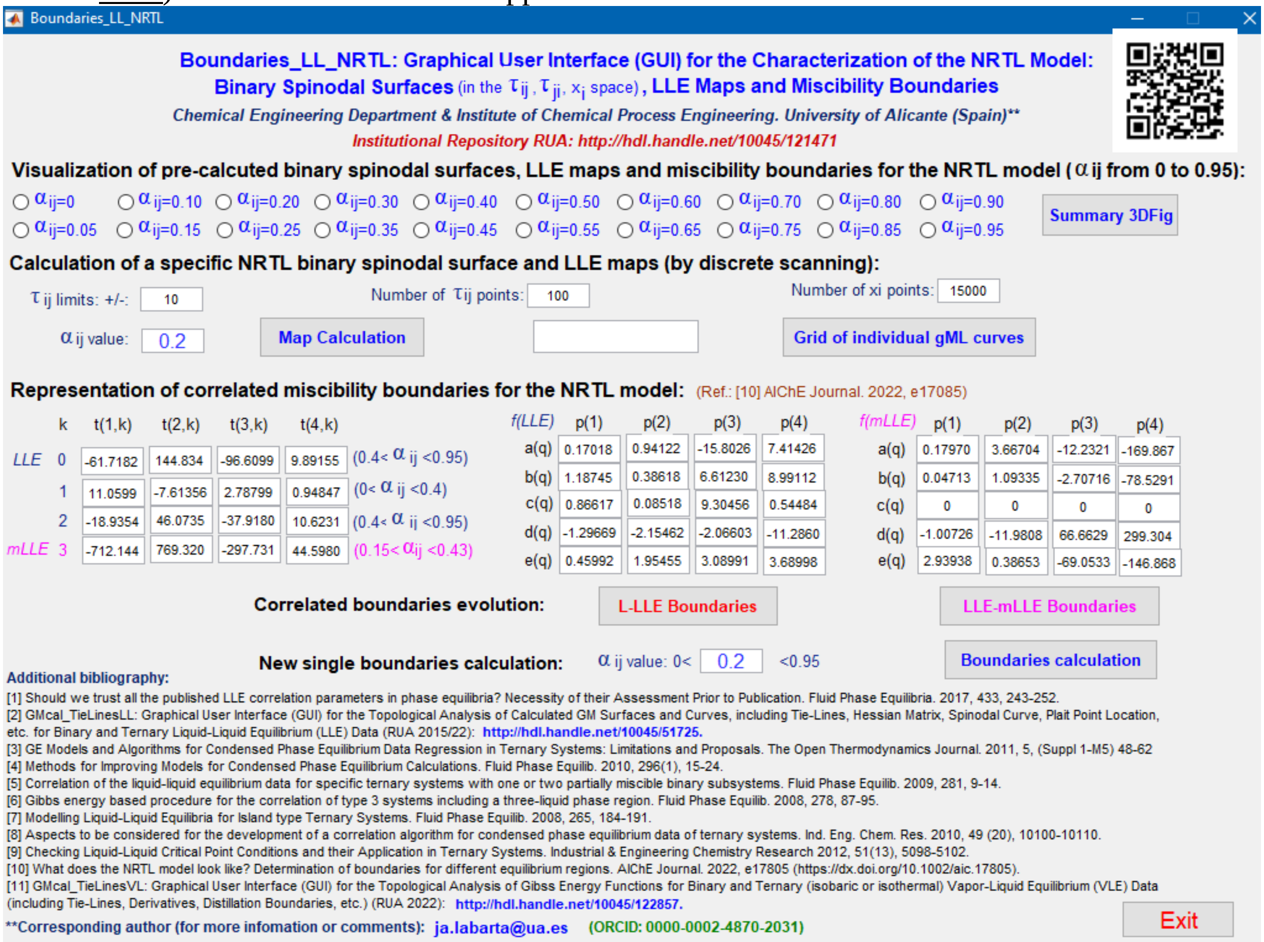
2. USER INSTRUCTIONS

1. *Download instructions*

1. Download the file to your computer in a known folder: **Boundaries_LL_NRTL.zip**
2. Unzip the file

2. *Using the GUI Boundaries_LL_NRTL*

1. Open Matlab software
2. Once in MatLab, select the folder where the file **Boundaries_LL_NRTL.zip** was unzipped as "current folder".
3. Localize and execute the file Boundaries_LL_NRTL.p from the MatLab Command Window (i.e.: writing Boundaries_LL_NRTL in the Command Window, and pressing enter). The next windows will appear.



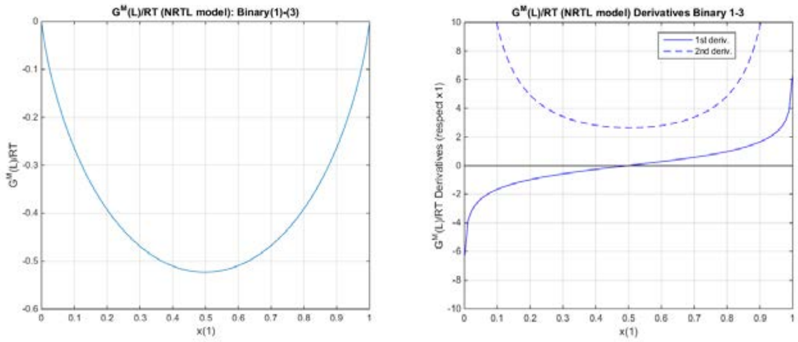
4. Once the main window of the GUI appears, it is possible to create different diagrams by using the corresponding push buttons:

   - Pre-calculated 3D binary spinodal surfaces (in the $\tau_{i,j}$-$\tau_{j,i}$-x_i space) and miscibility boundaries (2D projections in the $\tau_{i,j}$-$\tau_{j,i}$ plane) for the NRTL model for different $\alpha_{i,j}$ values (from 0 to 0.95). (e.g. Figures 1a).

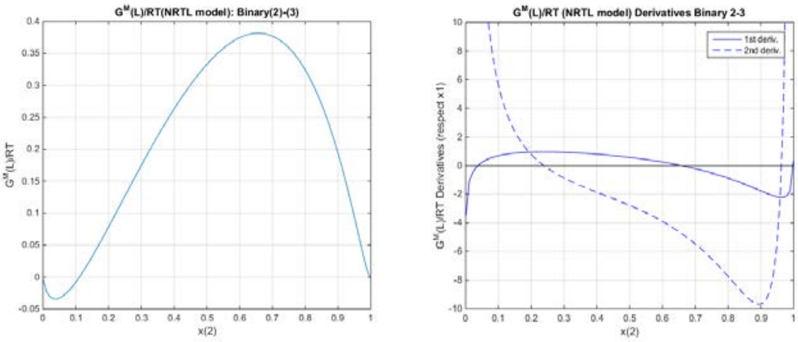
   - Figure 3D resume with all the 2D projections for different $\alpha_{i,j}$ values, from 0 to 0.95 (Figure 1b).

   - Calculation and representation of a specific NRTL binary spinodal surface and its 2D projection for a concrete value of $\alpha_{i,j}$ (by discrete scanning of the binary parameters $\tau_{i,j}$ and $\tau_{j,i}$). It is possible to choose the $\alpha_{i,j}$ value, the upper/lower limits of the tau parameters, and the number of tau and x points used in the corresponding scanning. The default values are respectively: 0.2; +/- 10; 100 and 15000. (e.g. Figures 1c)

     Remark: The possibility of the existence of LL phase splitting has been analyzed through zeros of the second derivative of the Gibbs energy of mixing (with respect to the molar fraction), for each set of $\tau_{i,j}$-$\tau_{j,i}$ values, in the whole composition range ($x_i \in [0,1]$). That is due because the presence of a LL splitting requires the existence of two zeros in the second derivative of the Gibbs energy of mixing, as can be observed in the following figures: Case a represents a totally homogeneous binary mixture in the whole range of compositions, while cases b-e correspond to binary systems with two partially miscible components just one LLE. When there are more than two compositions with a value of zeros in the second derivative of the Gibbs energy of mixing, more than one LL spliting exists (case f or g):



a)



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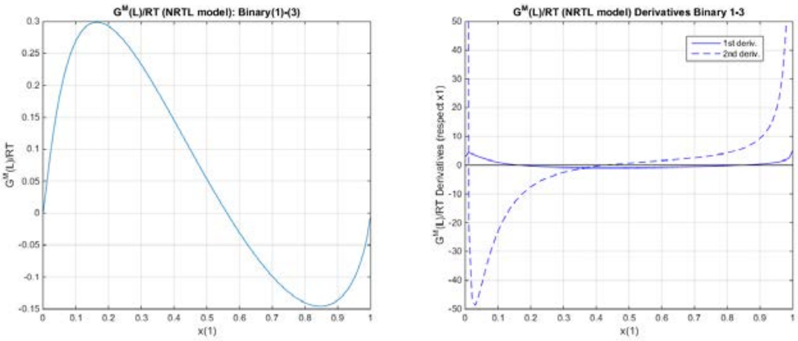
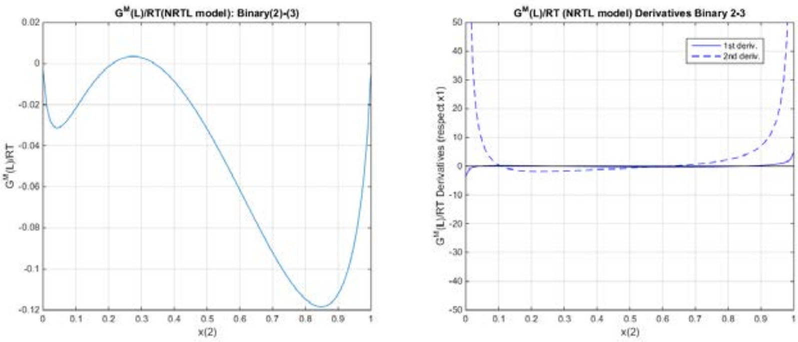
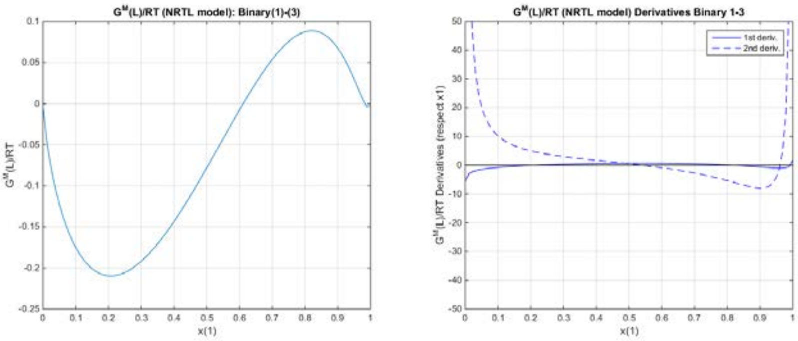


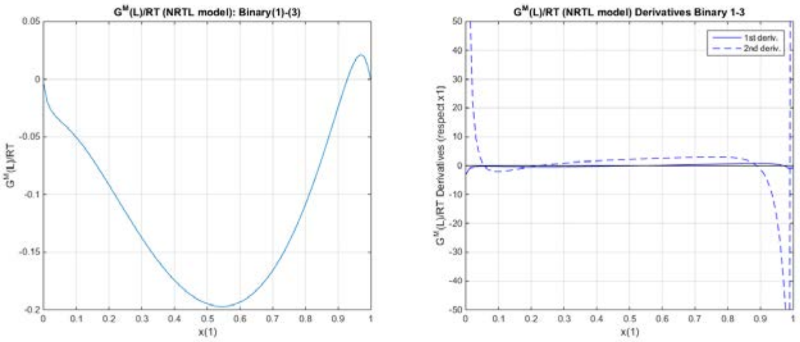
c)



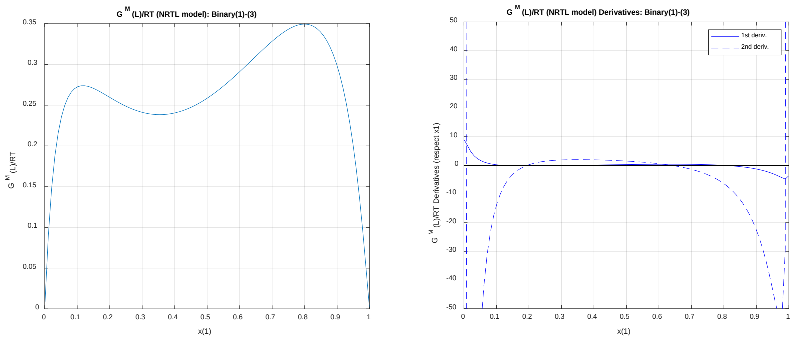
d)



e)



f)



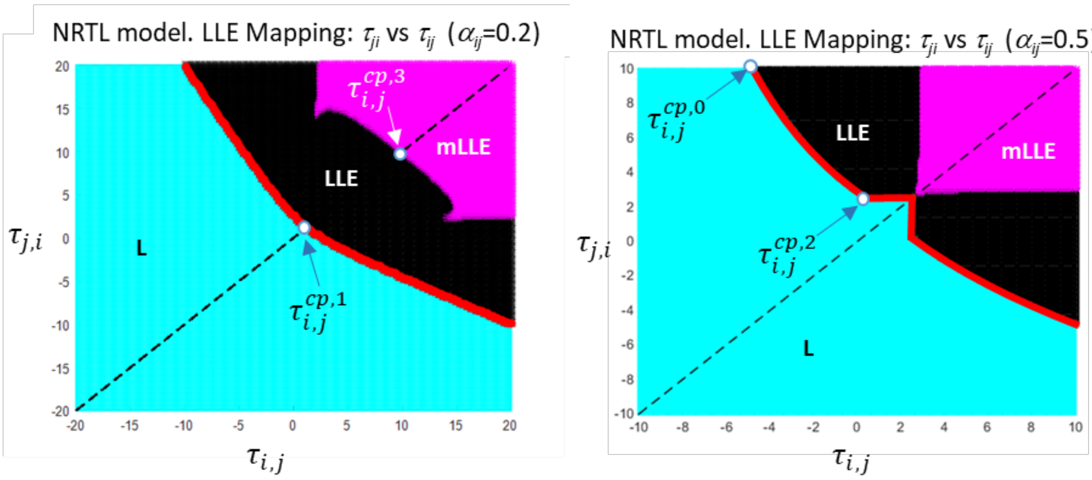
g)

- Calculation and representation of a grid of individual Gibbs energy of mixing curves specific NRTL binary spinodal surface for a concrete value of $\alpha_{i,j}$ and different pairs of the binary parameters $\tau_{i,j}$ and $\tau_{j,i}$. (e.g. Figure 1d).
- Representation of the evolution of the correlated L-LLE and LLE-mLLE boundaries observed for the NRTL by using the set of parameters included as default corresponding with the following equations and definitions [3]) (Figures 1e).

$$f(\tau_{i,j},\alpha_{i,j}) \equiv \tau_{j,i}^{cal} = p_1 \cdot \tau_{i,j}^3 + p_2 \cdot \tau_{i,j}^2 + p_3 \cdot \tau_{i,j} + p_4$$

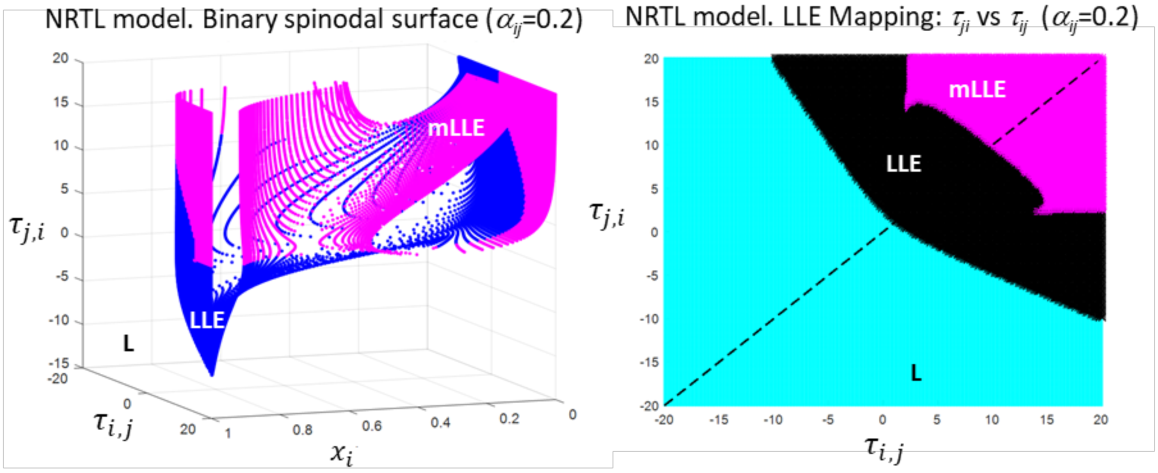
$$p_q = a_q + b_q \cdot ln\left(\alpha_{i,j} + c_q\right) + d_q \cdot \alpha_{i,j} + e_q \cdot \alpha_{i,j}^2 \qquad q = \{1,2,3,4\}$$

$$g_k\left(\alpha_{i,j}\right) \equiv \tau_{i,j}^{cp,k} = t_{1,k} \cdot \alpha_{i,j}^3 + t_{2,k} \cdot \alpha_{i,j}^2 + t_{3,k} \cdot \alpha_{i,j} + t_{4,k}$$

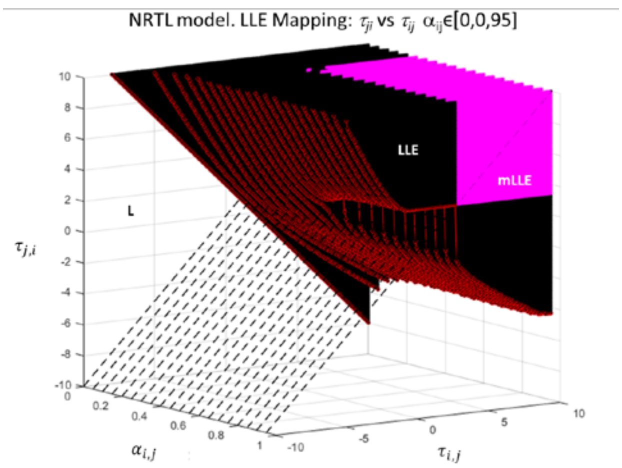


If we use the value of 10 as the upper bound for $\tau_{j,i}$, in both cases, the miscibility boundary (red line) exists in the range of values of $\tau_{i,j}$ from -5 to 10, i.e. $\tau_{i,j}{}^{cp,0}=-5$.

- Calculation and representation of the correlated NRTL miscibility boundaries for a specific value of $\alpha_{i,j}$ and different pairs of the binary parameters $\tau_{i,j}$ and $\tau_{j,i}$. (e.g. Figure 1f).



a)



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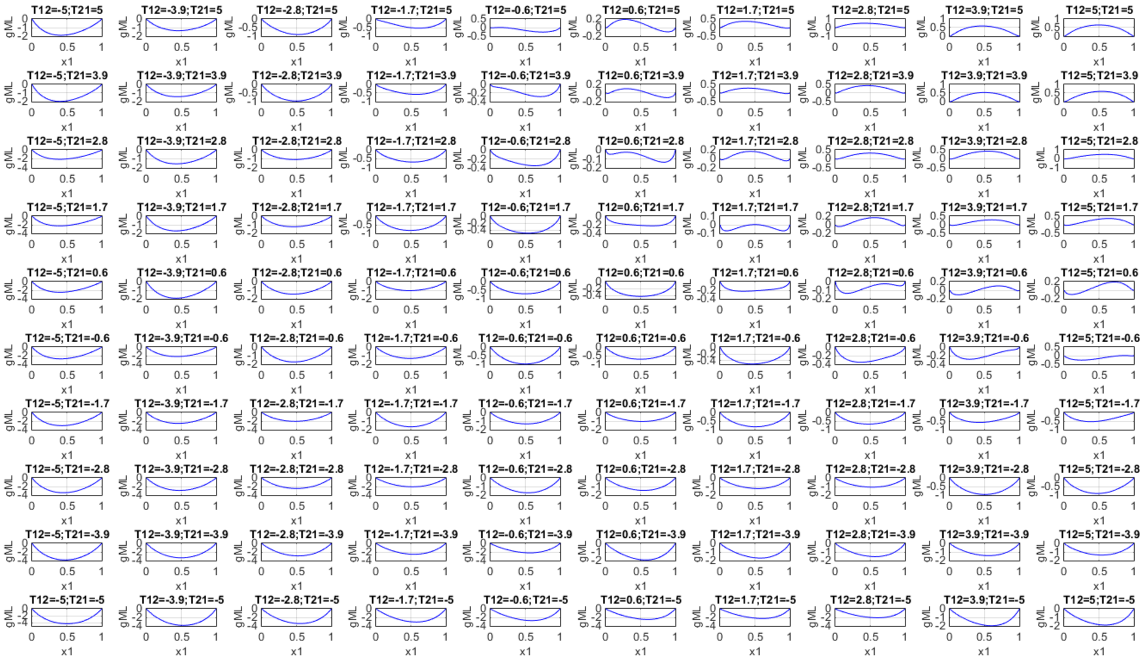

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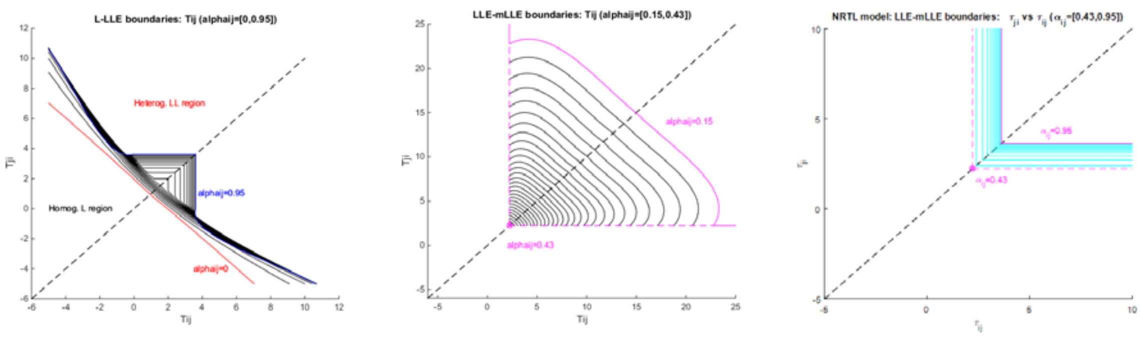

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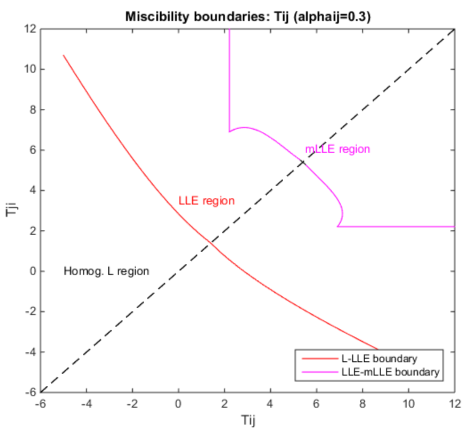
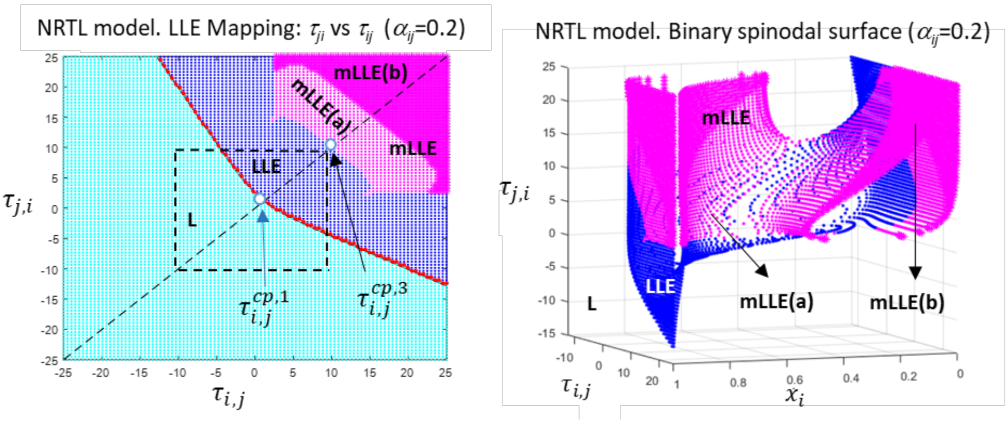


f)

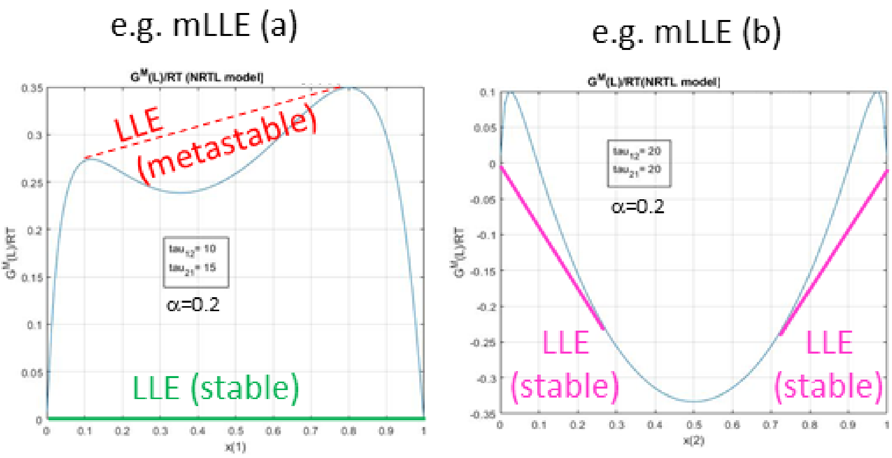
Figure 1. Examples of different individual graphs that can be generated with the GUI developed: Boundaries_LL_NRTL (RUA).

A deeper analysis of the mLLE region for $\alpha_{i,j}$=0.2, indicates that this region presents two different behaviors (see Figure 2a,b): mLLE(a) where one of the LL splittings is metastable and mLLE(b) where both LL splittings are stable (Sapkowski & Hofman, Fluid Phase Equilibria, 2023). In any case, both regions mLLE(a) and (b) present values of the $\tau_{i,j}$ too large (larger than 10) in order to correlate correctly LLE data, especially in multicomponent systems, because e.g. in ternary systems they produce Gibbs energy of mixing functions so flattened that produce too much uncertainty in the solutions obtained.

On the other hand, the region mLLE(a) decreases when the $\alpha_{i,j}$ value increases, and it disappears at an α_{ij} value around 0.45 (Figure 2c).



a)



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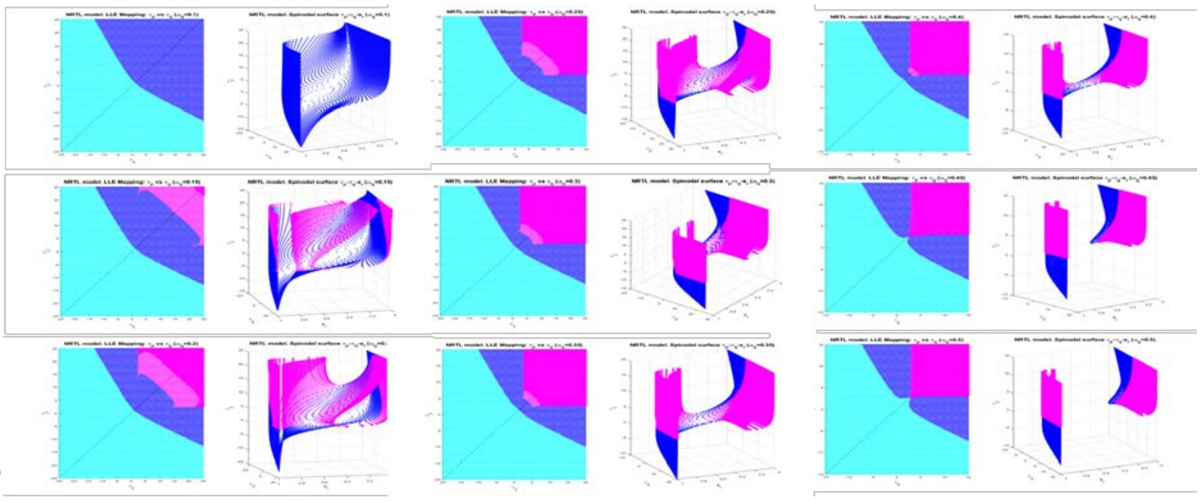

c)

Figure 2. Evolucion of the mLLE region with the $\alpha_{i,j}$ value.

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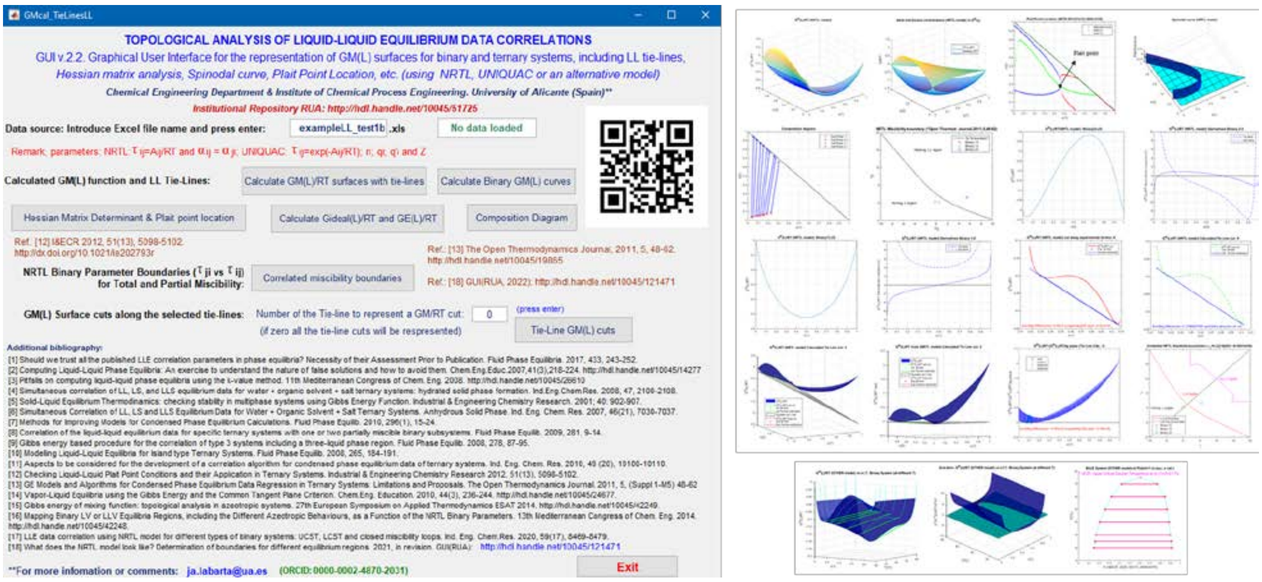

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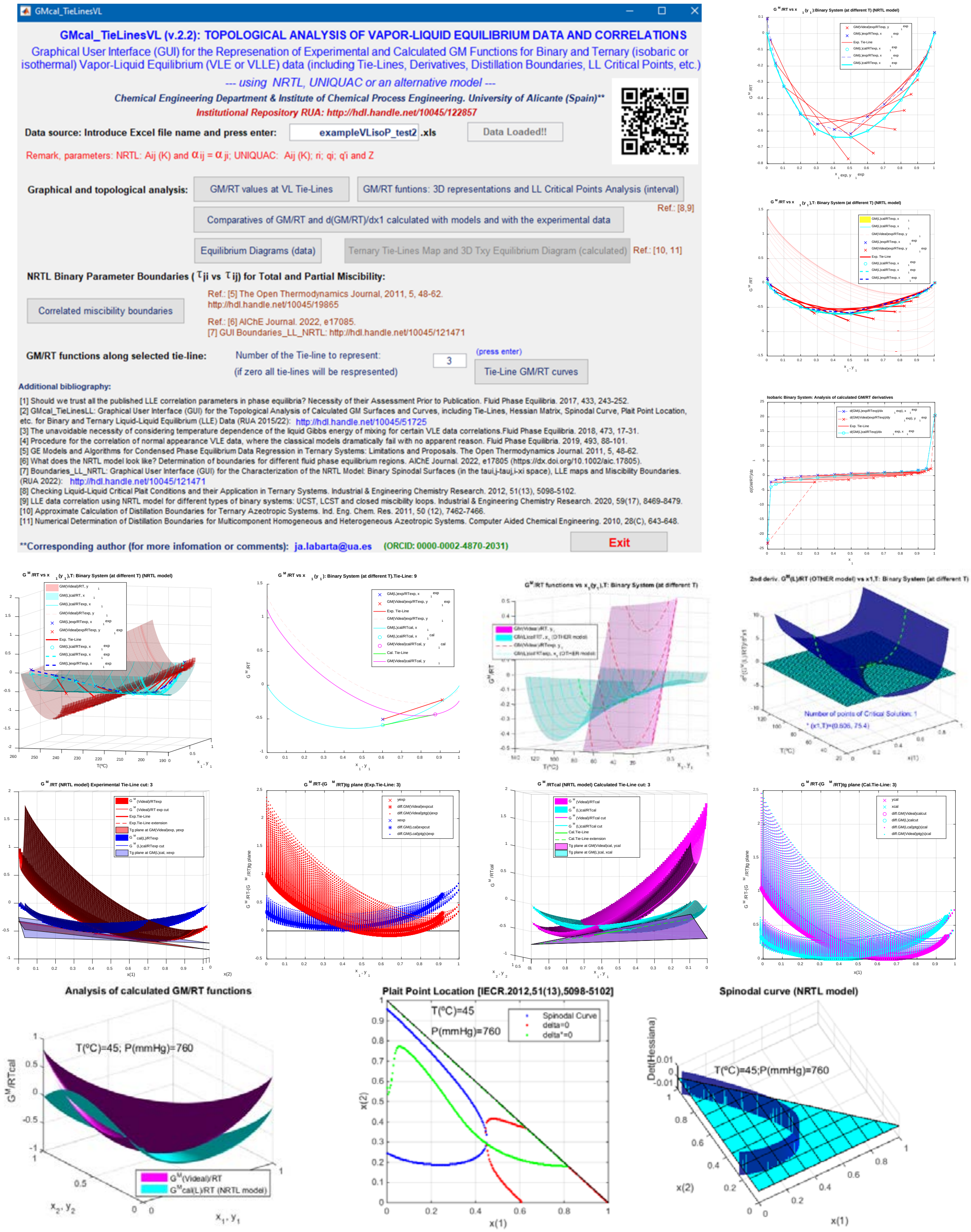

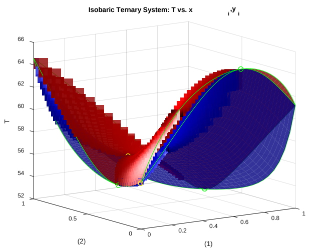

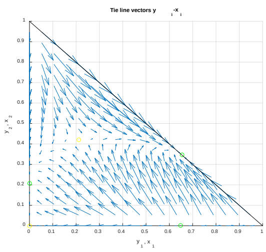

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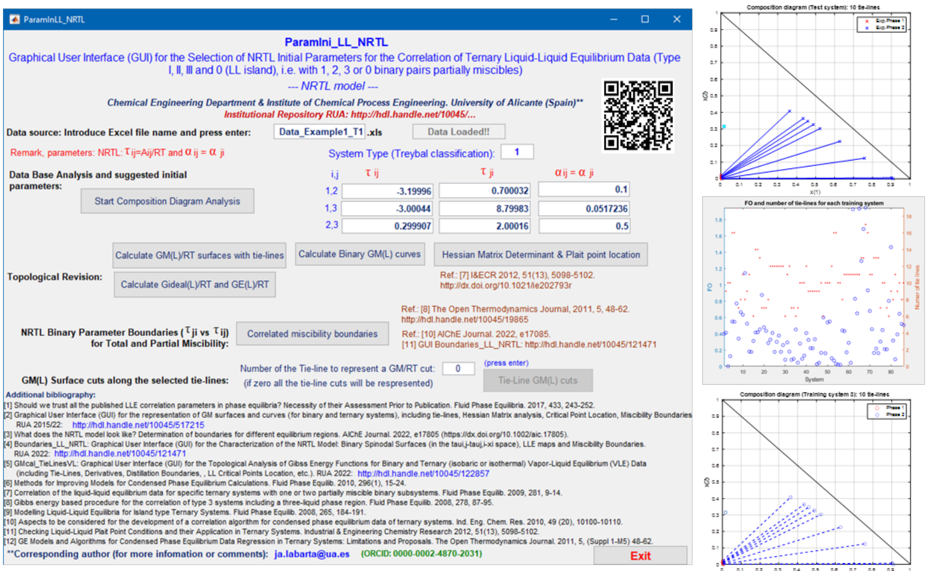

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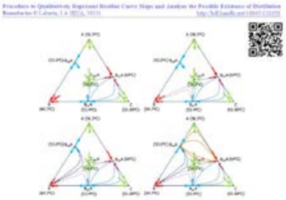

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REMARK: IF YOU WANT TO RECEIVE A NOTIFICATION WITH POSSIBLE UPDATES OF THIS GUI. PLEASE SENT AN E-MAIL TO: ja.labarta@ua.es (ORCID: http://orcid.org/0000-0002-4870-2031)