Procedure to Qualitatively Represent Residue Curve Maps and Analyze the Possible Existence of Distillation Boundaries

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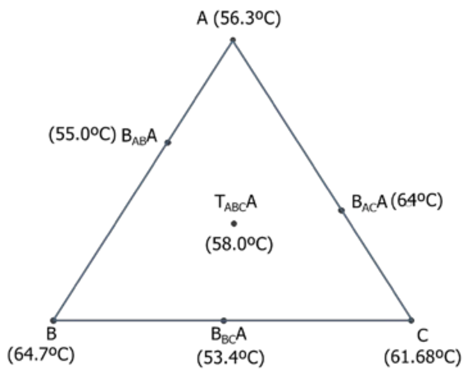
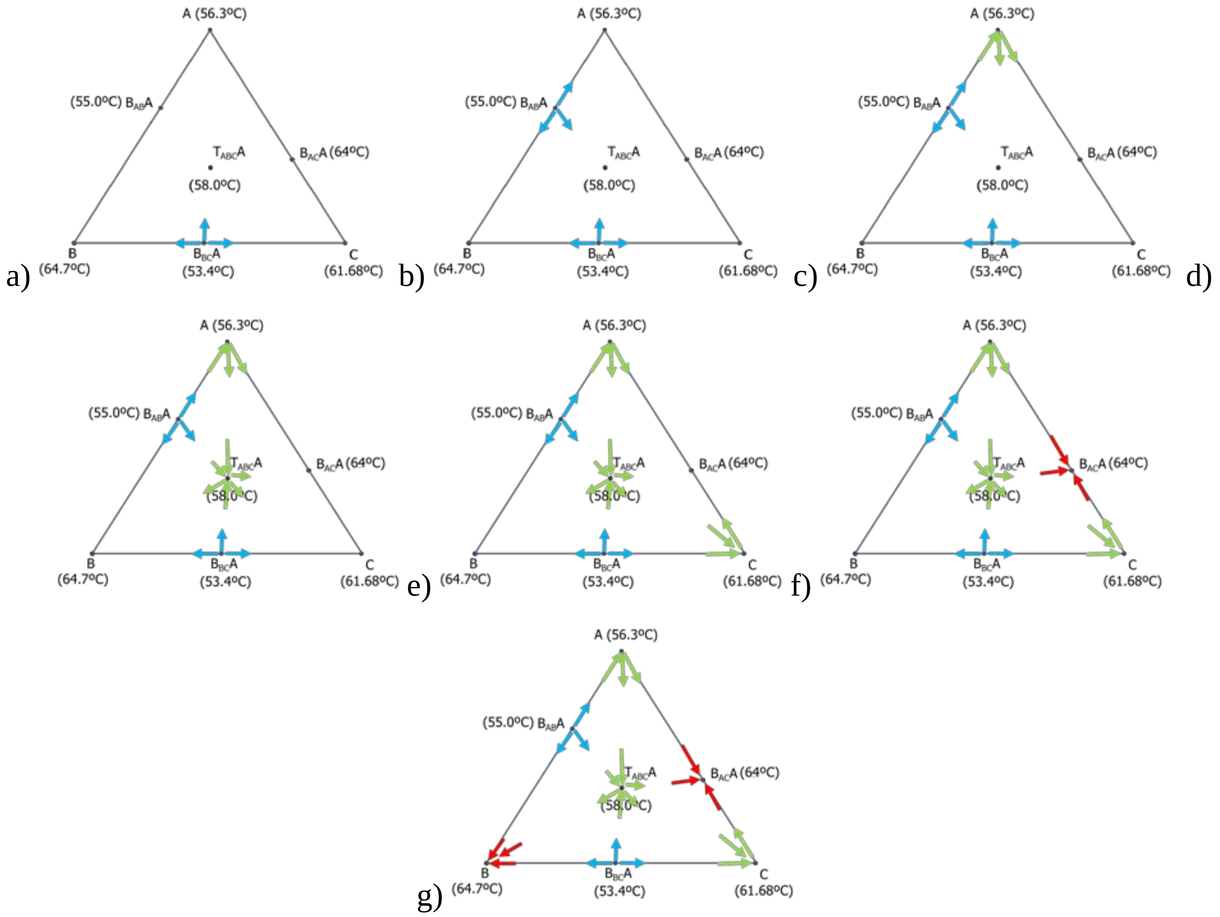
The analysis of residue curve maps is essential to know the VLE behavior of a ternary mixture, the possible existence of distillation boundaries and therefore different distillation regions in the ternary composition diagram, and the corresponding areas where the different distillation products are located. All this knowledge is necessary for the correct design of distillation column sequences especially when azeotropic distillation columns are included [1-4].

As a first step, it is possible to represent qualitative residue curve maps just by knowing the equilibrium temperature of all the characteristic points (nodes) of the ternary system, i.e. pure components, and binary and ternary azeotropes (if they exist). The procedure is the following:

1.- To draw the ternary composition diagram (equilateral or rectangular) including all the characteristic points (nodes) and their equilibrium temperatures:

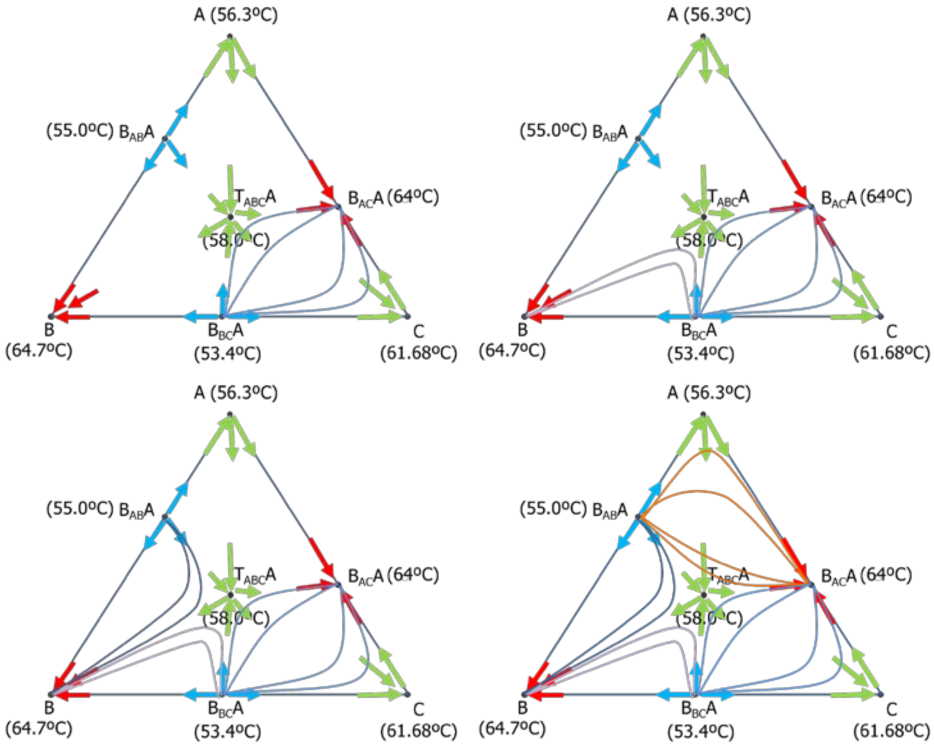


2.- To analyze the behavior of the residual curves (leave or enter) in the vicinity of each node starting for instance with the node with lower boiling (VLE) temperature. The residue curves represent the evolution of the liquid composition in a differential (simple open) distillation, and therefore the temperature increases along the residue curves.

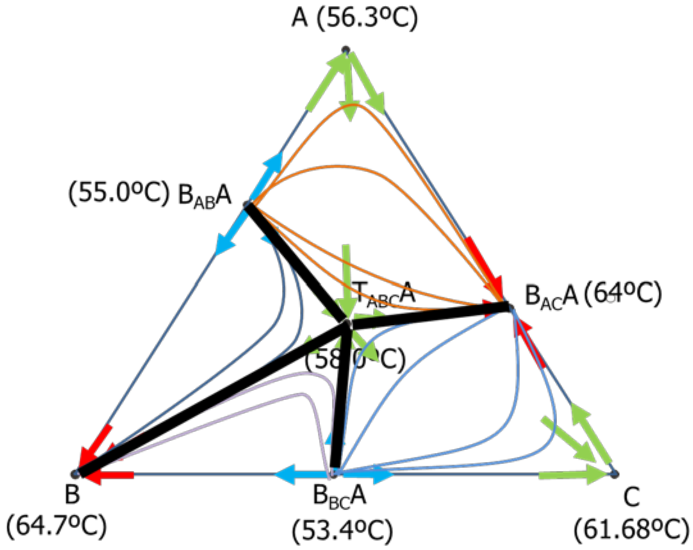


3.- To define the different nodes as stable (only residual curves enter, red arrows in the previous figure), unstable (only residual curves leave, blue arrows in the previous figure), and saddle (there are residual curves going in and going out, green arrows in the previous figure).

4.- To draw the corresponding qualitative residue curves connecting the corresponding unstable, saddle, and stable nodes. For instance, starting with the lowest temperature node and following in the first step the arrows of the edges of the triangle.



5.- Analyzing the existence of different distillation regions (regions in the composition diagram with residue curves with different topology, i.e. residue curves that start and/or end at different nodes), the corresponding distillation boundaries can be drawn. In our case study, there are 4 different distillation regions and four distillation boundaries.



Remark that the number of distillation regions and boundaries depends on the equilibrium temperatures of the different nodes and not are directly related to the number of azeotropes (binary and or ternary) that are present in the ternary system.

- **More information about distillat**
- **ion boundaries and residue curves maps definition and calculation [1-4]:**

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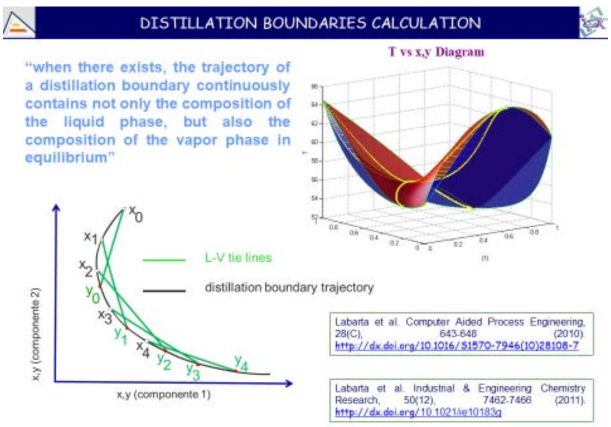

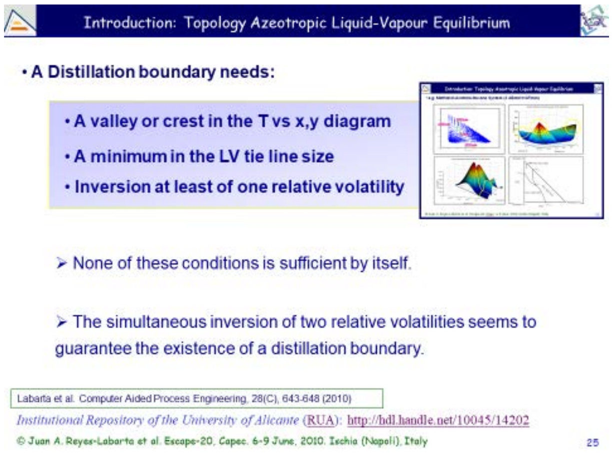

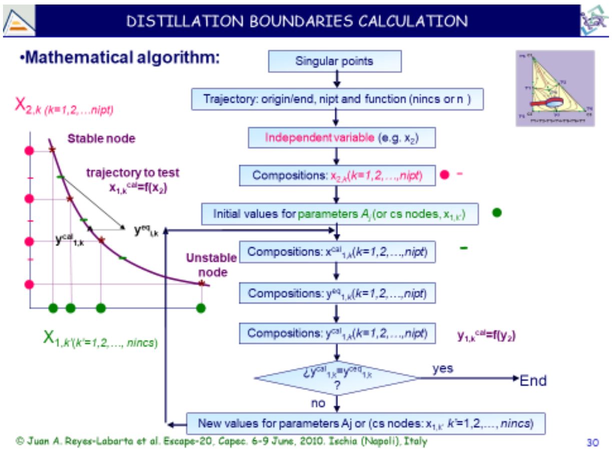

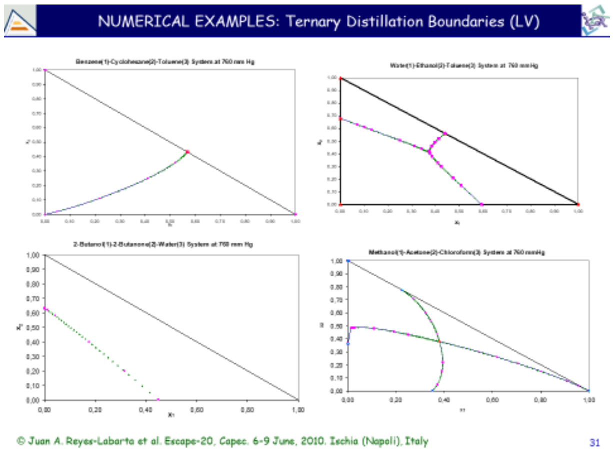

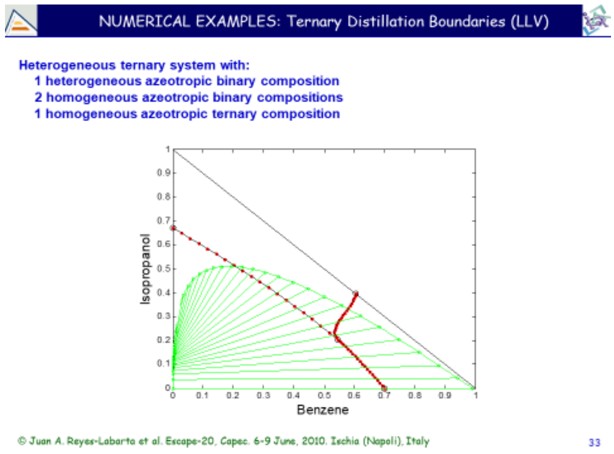

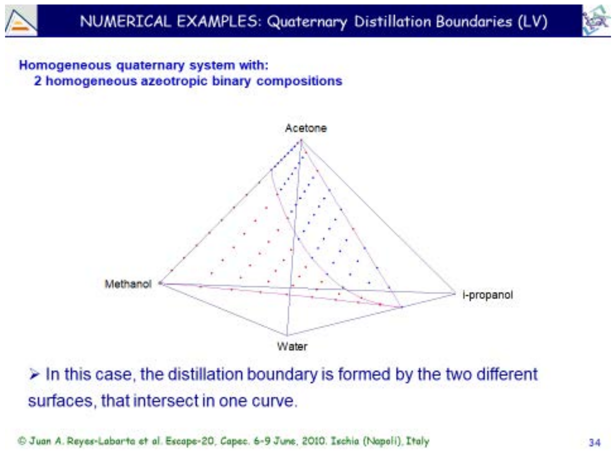

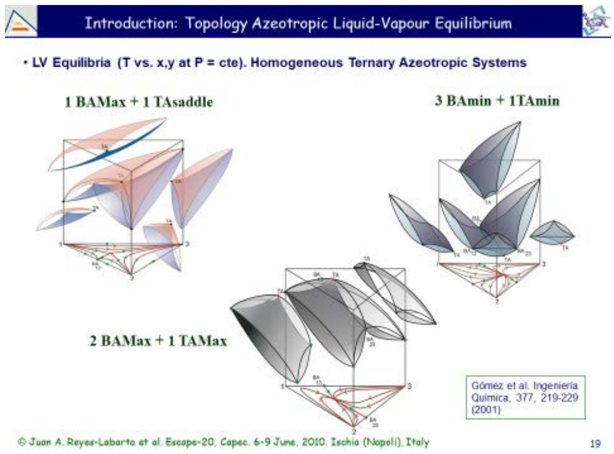

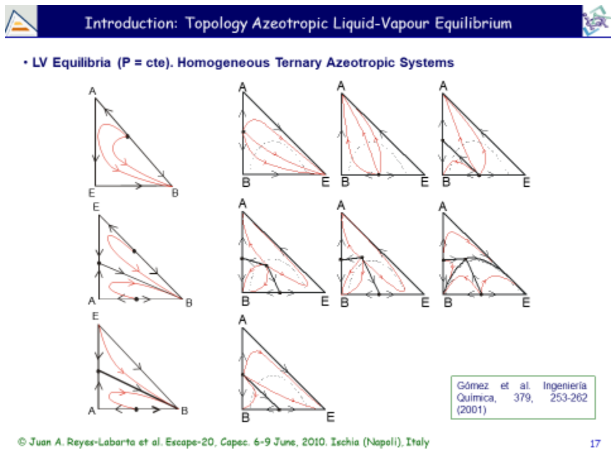

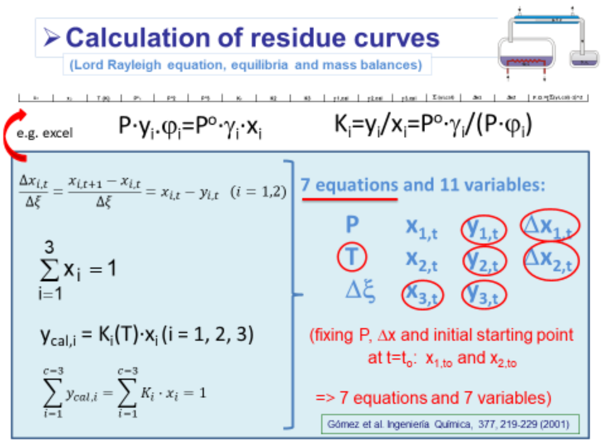

- **Graphical User Interface (GUI) GMcal_TieLinesVL:**

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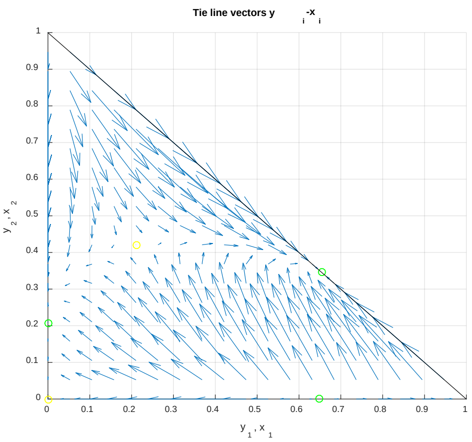
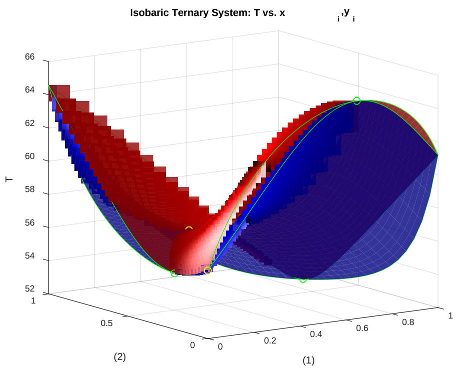
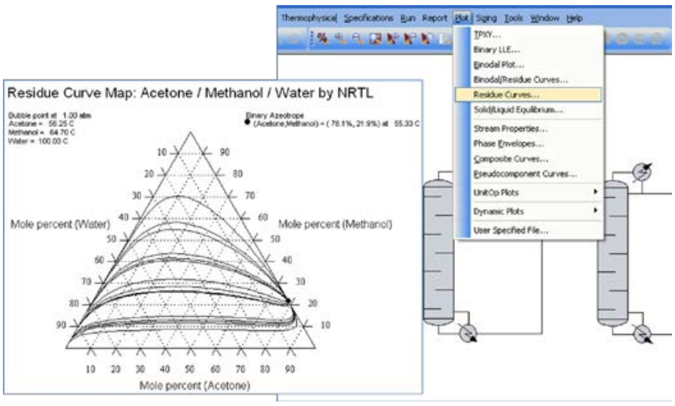
At this point just to comment that the MatLab Graphical User Interfaces (GUI) GMcal_TieLinesVL [5] developed to systematically check the consistency of VLE data and correlation results, allows representing calculated VL tie line maps and calculated Txy equilibrium surfaces (including binary subsystems), and to check the possible existence of different distillation regions and boundaries [1-2]. Additionally, this GUI allows the analysis of experimental and calculated (isobaric or isothermal) vapor-liquid (or vapor-liquid-liquid) equilibrium data for binary and ternary systems, in the sense presented in the bibliography [6-7], to detect the necessity of considering larger dependences (of temperature or pressure, respectively) in the binary interaction parameters of the model used (e.g. NRTL model) and also to check the consistency of VLE data correlation results through the topological information contained in the Gibbs energy of mixing function. This analysis allows researchers involved in the correlation of experimental vapor-liquid equilibrium data, to visualize experimental data's behavior and also the consistency and quality of the results obtained in the correlation process.





Additional just to comment that some chemical engineering process simulation software such as CHEMCAD ®ChemStations™, also allows the representation of calculated Residue Curve Maps.



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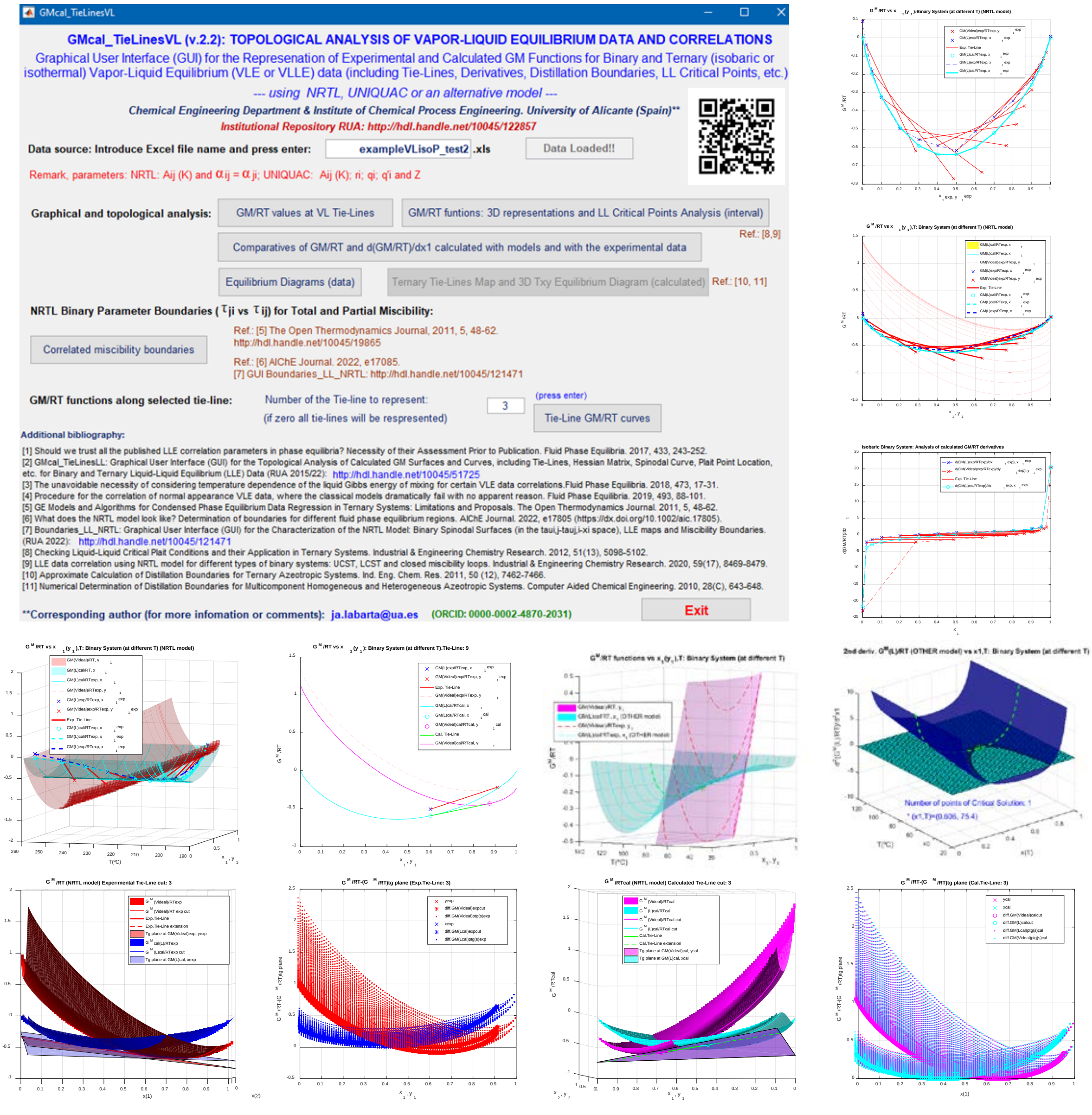

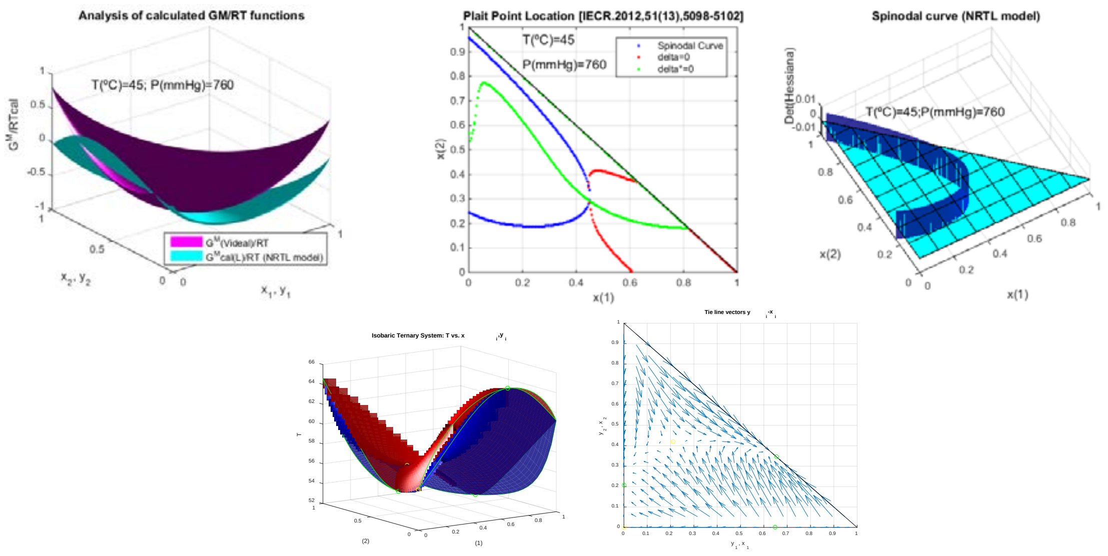

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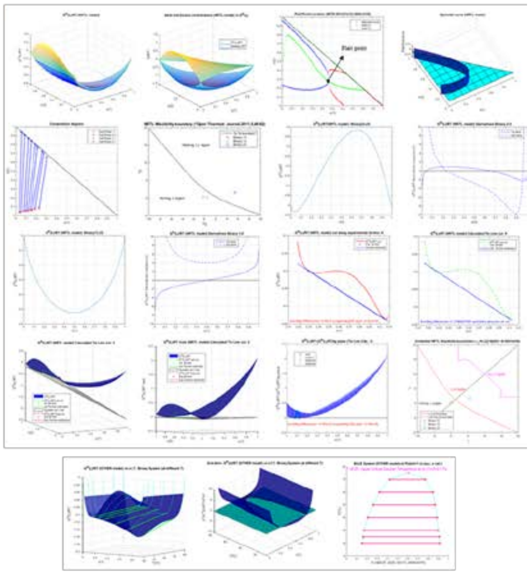

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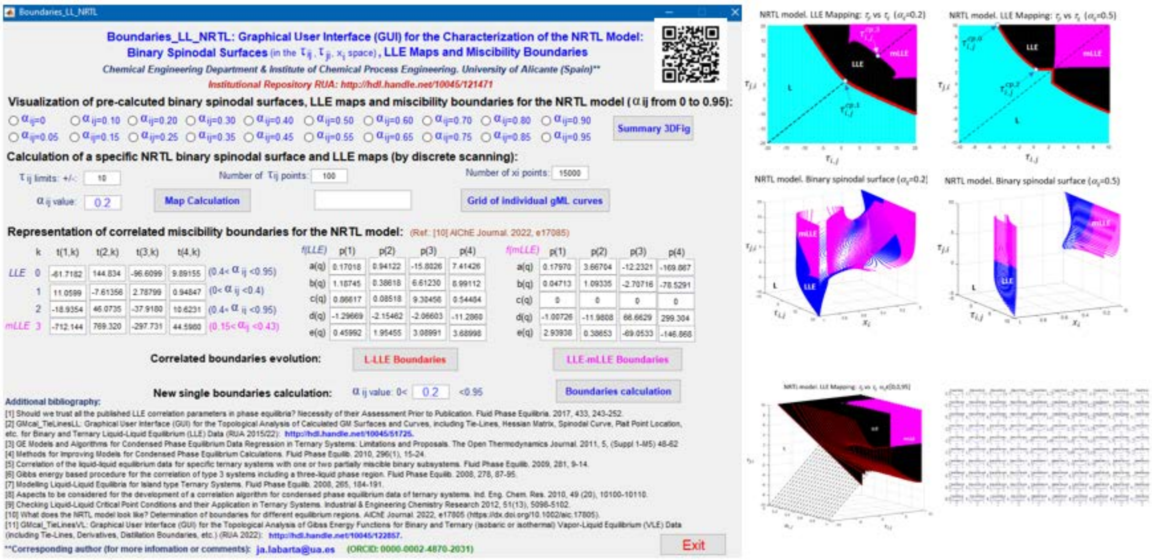

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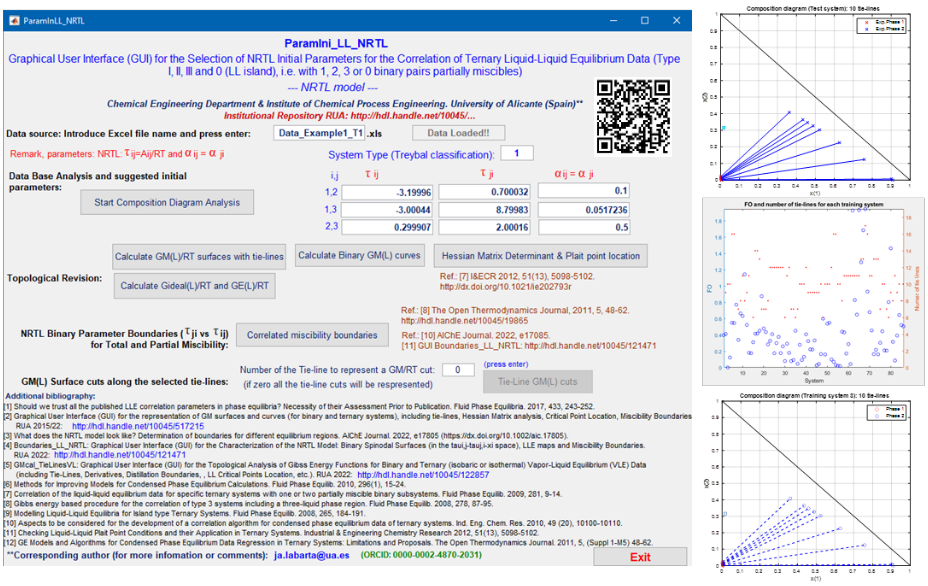

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