✓ Examples of objective functions

$$O.F._{total} = O.F._{x,LL} + O.F._{x,LLL} + O.F._{y,LV} + \ldots$$

$$O.F._{x,L_1L_2} = \sum_{j=1}^{NTL}\sum_{q=1}^{2}\sum_{i=1}^{C}\left(x_{i,j}^{Lq,exp} - x_{i,j}^{Lq,cal}\right)^2 \quad \text{subject to:} \quad \left\{\sum_{j=1}^{NTL}\sum_{i=1}^{C}\left(a_{i,j}^{L1,cal} - a_{i,j}^{L2,cal}\right)^2 < \varepsilon \quad \ldots\right.$$

$$O.F._{x,L_1L_2L_3} = \sum_{k=1}^{3}\sum_{i=1}^{C}\left(x_{i}^{Lk,exp} - x_{i}^{Lk,cal}\right)^2 \quad \text{subject to:} \quad \left\{\sum_{p=1}^{2}\sum_{k>p}^{3}\sum_{i=1}^{C}\left(a_{i}^{Lp,cal} - a_{i}^{Lk,cal}\right)^2 < \varepsilon \quad \ldots\right.$$

$$O.F._{y,LV} = \begin{cases} \sum_{j=1}^{NTL}\sum_{i=1}^{C}\left(y_{i,j}^{exp} - y_{i,j}^{cal}\right)^2 \\ \sum_{j=1}^{NTL}\sum_{i=1}^{C}\left(T_{i,j}^{exp} - T_{i,j}^{cal}\right)^2 \\ \sum_{j=1}^{NTL}\sum_{i=1}^{C}\left(g_{i,j}^{ML,exp} - g_{i,j}^{ML,cal}\right)^2 \\ \sum_{j=1}^{NTL}\sum_{i=1}^{C}\left(\dfrac{\gamma_{i,j}^{exp} - \gamma_{i,j}^{cal}}{\gamma_{i,j}^{exp}}\right)^2 \quad \ldots \end{cases}$$

$$\text{subject to:} \quad \begin{cases} \sum_{j=1}^{NTL}\left(\sum_{i=1}^{C} y_{i,j}^{cal} - 1\right)^2 < \varepsilon \\ \sum_{j=1}^{NTL}\sum_{i=1}^{C-1}\left(\dfrac{\partial g_j^{M,V}}{\partial y_{i,j}^{cal}} - \dfrac{\partial g_j^{M,L}}{\partial x_{i,j}^{exp}}\right)^2 < \varepsilon \quad \ldots \end{cases}$$

j = Tie lines (1, …, NTL)
i = Components (1, …, C)
q = Liquid phases of a LLE tie lines (e.g. L_1L_2)
k,p = Liquid phases of a LLLE tie triangle (e.g.: L_1, L_2 and L_3)

Examples of data correlation analysis & procedures

1. Olaya et al. **Computing Liquid-Liquid Phase Equilibria: An exercise to understand the nature of false solutions and how to avoid them**. Chemical Engineering Education 2007, 41(3), 218-224. Institutional Repository RUA: http://hdl.handle.net/10045/14277.
2. Marcilla et al. **Pitfalls on computing liquid-liquid phase equilibria using the k-value method**. 11th Mediterranean Congress of Chemical Engineering. EXPOQUIMIA 2008. Institutional Repository RUA: http://hdl.handle.net/10045/26610.
3. Marcilla et al. **Simultaneous correlation of liquid-liquid, liquid-solid, and liquid-liquid-solid equilibrium data for water + organic solvent + salt ternary systems: hydrated solid phase formation**. Ind. Eng. Chem. Res. 2008, 47, 2100-2108 (http://dx.doi.org/10.1021/ie071290w).
4. Reyes-Labarta et al. **Solid-Liquid Equilibrium Thermodinamics: checking stability in multiphase systems using Gibbs Energy Function**. Ind. Eng. Chem. Res. 2001; 40: 902-907 (http://dx.doi.org/10.1021/ie000435v).
5. Marcilla et al. **Methods for Improving Models for Condensed Phase Equilibrium Calculations**. Fluid Phase Equilib. 2010, 296(1), 15-24 (http://hdl.handle.net/10045/13314).
6. Reyes-Labarta et al. **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 (http://hdl.handle.net/10045/24683).
7. Marcilla et al. **Gibbs energy based procedure for the correlation of type 3 systems including a three-liquid phase region**. Fluid Phase Equilib. 2008, 278, 87-95 (http://hdl.handle.net/10045/13315).
8. Olaya et al. **Modelling Liquid-Liquid Equilibria for Island type Ternary Systems**. Fluid Phase Equilib. 2008, 265, 184-191 (http://hdl.handle.net/10045/24681).
9. Marcilla et al. **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 (http://dx.doi.org/10.1021/ie1010383).
10. Marcilla et al. **Checking Liquid-Liquid Critical Point Conditions and their Application in Ternary Systems**. Industrial & Engineering Chemistry Research. 2012, 51(13), 5098-5102 (http://dx.doi.org/10.1021/ie202793r).
11. Marcilla et al. **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 (http://hdl.handle.net/10045/19865).

Examples of correlation data analysis & procedures

12. Olaya et al. **Vapor-Liquid Equilibria using the Gibbs Energy and the Common Tangent Plane Criterion**. Chemical Engineering Education. 2010, 44(3), 236-244. Institutional Repository RUA: http://hdl.handle.net/10045/24677.
13. Marcilla et al. **Gibbs energy of mixing function: topological analysis in azeotropic systems**. 27th European Symposium on Applied Thermodynamics ESAT 2014. Institutional Repository RUA: http://hdl.handle.net/10045/42249.
14. Reyes-Labarta et al. **Mapping Binary Liquid-Vapor or Liquid-Liquid-Vapor Equilibria Regions, including the Different Azeotropic Behaviours, as a Function of the NRTL Binary Parameters**. 13th Mediterranean Congress of Chemical Engineering. 2014. Institutional Repository RUA: http://hdl.handle.net/10045/42248.
15. Marcilla et al. **Refreshing the Relevance of Analyzing the Topology of the GM Function in the Phase Equilibrium Correlation Data**. Equifase 2015. X Iberoamerican Conference on Phase Equilibria and Fluid Properties For Process Design. Alicante (SPAIN), 28 June - 1 July, 2015. (Book of Abstracts: http://hdl.handle.net/10045/50110).
16. Marcilla et al. **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 (http://dx.doi.org/10.1016/j.fluid.2016.11.009). **GUI for the representation of GM surfaces and curves, including tie-lines. 2015-2018**: http://hdl.handle.net/10045/51725.
17. Rodríguez-Escontrela et al. **Correlation of Three-Liquid-Phase Equilibria involving Ionic Liquids**. Physical Chemistry Chemical Physics. 2016, 18, 21610-21617 (http://dx.doi.org/10.1039/C6CP03467E).
18. Marcilla et al. **Phase Equilibrium Correlation. Regarding the full consistency of the thermodynamics**. 10th World Congress of Chemical Engineering. Barcelona (SPAIN), 1t-5th October, 2017. RUA: http://hdl.handle.net/10045/70035.
19. Marcilla et al. **Influence of the temperature in the activity coefficient models used for the correlation of vapour-liquid equilibrium (VLE) data**. Fluid Phase Equilibria. April, 2018 (in press).
20. Marcilla et al. **Ensuring that Correlation Parameters for Liquid-Liquid Equilibrium Produce the Right Results (Guest Editorial)**. Journal of Chemical & Engineering Data. April, 2018 (in press).