In the past, many strategies have been proposed to solve liquid-liquid equilibrium (LLE). Nevertheless, some papers and process simulation software packages still show inconsistent procedures for LLE regressions that lead to apparent solutions which are not true tie-lines. This study illustrates some of the pitfalls of the LLE data correlation and proposes some ideas to overcome them.

**The activity objective function (O.F.(a))** is evaluated close to the LLE solution (Figure 1). A variety of false tie-lines can be obtained that correspond with very low values of the activity objective function although, obviously, the true tie-line is unique. The activity function provides a poor definition of the objective function minimum (O.F.(a)<10^-12 in Figure 2), because the gM surface for this system is very flat. The activity function is obtained (necessary condition). The common tangent line contribution to the objective function is:

\[
\text{O.F.(a)} = \sum \left( a_i - a^* \right)^2 = 0
\]  

Next, a combination of the activity and the minor common tangent condition (O.F.(t) in Figure 2) based on Iglesias-Silva et al. [2] is used, and a sharper minimum for the objective function value is obtained. The common tangent line contribution to the objective function is:

\[
\text{O.F.(t)} = \frac{\left( \frac{\partial g_{ax}}{\partial x_a M} \right)_I + \left( \frac{\partial g_{ax}}{\partial x_a M} \right)_II}{\left( \frac{\partial g_{ax}}{\partial x_a M} \right)_I - \left( \frac{\partial g_{ax}}{\partial x_a M} \right)_II} \left[ \left( \frac{\partial g_{ax}}{\partial x_a M} \right)_I - \left( \frac{\partial g_{ax}}{\partial x_a M} \right)_II \right] \cdot \frac{x_a^I - x_a^II}{x_a^I - x_a^II} 
\]

**Finally, we present a modification of the vector method** [3] developed by Eubank et al. [4]. The original work used the vector method combined with the maximum area criterion as equilibrium condition (later proved to be only applicable for binary systems [5]).

Our algorithm, that is applicable to the ternary systems, uses the minor common tangent equilibrium condition (O.F.(t)) [2]:

- An α-angle range for each ternary global mixture M (Figure 3) is defined.
- For a sheaf of straight lines passing through M, the two common tangent points (I, II) to the gM function in the corresponding sectional plane are obtained (necessary condition).
- Among all pairs of calculated compositions, the “true” tie-line corresponds to the O.F.(a) equal to zero (sufficient condition) which corresponds to the minimum value for the Gibbs energy of mixing (gM).

The O.F.(a) is evaluated for each α-angle at the two common tangent points. Those values (suggested method O.F.(a)) are compared to the other previous approaches (Figure 2) showing that a sharper minimum is obtained.

**When the activity condition is combined with the common tangent line criterion, either simultaneously (eq 2) or sequentially (vector method), a more efficient equilibrium calculation can be carried out, avoiding false solutions with very low values of the O.F.(a)).**

**The suggested method improves the convergence of the optimization.**