

Review to “*Geometry of Double Retrograde Vaporization Prediction*” by G. Libotte et al.

26th December 2017

General opinion of the reviewer

The work has a very good quality and the theme is flesh and interesting to analyse. In addition, the methodology is applicable for any equilibrium calculation and therefore, authors could considerer to change the title to reach a wider audience. I see a solid work but in some moment it become hard to follow. Having said this, I only limit myself to making some corrections on the structure of the work to provide other vision to help to improve the understanding of the work.

General comments on the structure

The work is very flesh and innovative. Always it is a issue to solve complex problems concerning to equilibria and therefore this kind of work are always a contribution. The work by G. Libotte has a solid mathematical foundation and calculations shown in the examples and in the body of the work are correct.

Sometime the work is hard to follow; even for an expert eye, due to the later, I shall give to authors some suggestion and guidelines in order to make the work most accessible to general public. I will do my comments as an enumeration below:

- In the first place, I am surprised that the work is much more general than a simple treatment of the double retrograde vaporisation, the same methodology presented by the authors is able to compute any equilibrium system and even the authors show the computation of critical lines for binary mixtures. For this reason, authors could think in a better and most general title in order to their work be most visible on the journal.
- The **1D example** could be extremely illustrative and a guide for the rest of the work if the narration was accompanied by a figure showing the polynomial function in its jumping points, \mathcal{J}_i .
- I think that when the authors begin to show the main problem of the work, *i.e.* to solve thermodynamic equilibrium with their method, they should show their function and mathematical structures, this can simplify considerably a quick understanding by readers. In additional, an example showing the seed vector for the numerical problems shall be very helpful.
- Authors could considerer to move the paragraphs from **Page 4 line 17** to the main section of the work. The cited text is very specific for the introduction and it is far from the specific work. In my opinion the impact of the understanding of the work in higher if the cited text is in the right place. The text in the introductory section can be replaced by a brief one.

Comments on some specific issues

- **Page 1 line 34:** “...of binary mixtures **and** characterized by...”

- **Page 2 line 30:** authors say “*we must mention that the composition of the vapor phase is arbitrarily chosen, in order to produce the thermodynamic phenomenon*” I think that this asseveration is not clear.
- **Page 2 line 36:** the references for Chen’s works must be cited when the mixtures are named.
- **Page 3 line 29:** “*to be used as good initial estimates*”?
- **Page 3 line 53:** What the authors means with “*global perspective*” maybe the adjective *utter* or proper is better in this case.
- **Page 4 line 27:** “*as can be seen in Fig. 1 at $T = 307.4$ K.*”
- **Page 6 line 18:** “*and y_i represents the mole fraction of the vapor phase*”
- **Page 16 line 44:** authors say “*Thus, it is clear that there is no obvious relationship between the thermodynamic critical curve and the loci singularities of the Jacobian matrix*”. This is a interesting point that authors can take advantage and to show an example at constant temperature, where both features are displayed.
- **Page 24 line 48:** authors says “*Since the critical curves have a direct influence of the process of obtaining pre-images*”, the cited quote must be explained in more detail.
- **In Fig. 1:** the vertical line could be labeled with the specific mole fraction as mentioned in the text.
- **In Fig. 2:** authors could plot the vapour pressure curves of the pure compounds, so that the equilibrium area be demarcated. The position of the critical point of each compound must be labeled in the figure.
- **In Fig. 3;** the caption must be improved. The caption must refer to the temperature of the calculation. An in addition, it is always welcome to label in the plot specific point as the intersects and cite them in the text.
- **In Fig. 4:** Fig. 4a is a detail of Fig. 3 therefore it must preserve the same colours and lines.
- **In Fig. 7:** this figure needs a general caption.
- Throughout the length of the text and plot axis the units must be in roman fonts.

Reviewer(s)' Comments to Author:

Reviewer: 1

Comments to the Author

Comments and suggestions are in the attached file.

Reviewer: 2

Comments to the Author

Authors have reported a mathematical analysis of the calculation of dew points in thermodynamic systems with double retrograde phenomenon. Two cases of study have been described in detail. Theoretical and numerical implications of the approach proposed have been discussed properly. Therefore, I consider that this paper is suitable for the IECR. There are few corrections to be performed:

- Please review the english in all the document, there are few grammatical errors.
- Phase stability of solutions identified has not been verified. Please comment and discuss this point in your corrected manuscript.

I suggest the acceptance of this paper after a minor revision.