

**Phase envelopes of multicomponent mixtures: From the simple to the complex.**

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Phase behavior can be of interest in a lot of processes in the chemical engineering field. The petroleum and separation industries can be an example where this is of importance since an indispensable number of unit operations are related to phase equilibria, like a separator in a reservoir extraction field. In this kind of operation it is relevant to be able to predict how a fluid could behave under certain conditions (like a pressure and temperature specification) or to find the conditions where a desired state happens.

A widely used approach of determining phase equilibria properties is the well known flash algorithm, that provides phase separation balances at some specification but it is needed to know beforehand the working conditions and only provides information of a single point. It is possible to explore a wide region of specifications with multiple flash calculations, but this can be computationally very intensive. A better way of knowing the overall phase behavior of a mixture can be obtained from the calculation of the whole phase envelope.

An efficient algorithm to trace two-phase envelopes has been developed by Michelsen in the eighties and it is very used to this day. It is also discussed in detail in the book by Michelsen and Mollerup [1]. This method firstly finds an easy to converge point (for example, a low temperature bubble point) and uses the information given in that point to calculate the next one, this is repeated until the whole phase envelope is traced.

Complex multi component mixtures, like reservoir fluids, can be prone to present more complex behaviors than simple two phase equilibria, mostly as a cause of the high asymmetry of the systems due to the presence of not only hydrocarbons but also polar components like water, methanol and other additives, sometimes there is presence of high concentrations of CO2 or asphaltenes. The high asymmetry in a mixture can cause the existence of a three-phase equilibrium besides the usually expected two-phase one.

A method that extends the previously named algorithm by Michelsen to calculate three-phase phase envelopes where an incipient phase could be either a vapor or a liquid has been proposed by Cismondi [2].

In this work we explore how compositional variations can affect the phase behavior of complex mixtures, starting from simple hydrocarbons systems and then going to more complex ones, increasing the asymmetry of the system by the addition of other components, like water and carbon dioxide. And we show the influence of these different compounds in the appearance of a third phase and both similarities and differences in the topology of the whole systems.

***References***

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2. Cismondi, M. Phase Envelopes for Reservoir Fluids with Asphaltene Onset Lines: An Integral Computation Strategy for Complex Combinations of Two- and Three-Phase Behaviors. Energy and Fuels 2018, 32 (3), 2742–2748.