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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 or to find the conditions where a desired state happens.

The P-T flash is probably the most useful and frequently used phase equilibrium calculation in industry. It provides quantitative and qualitative information for a phase separation at a single specification of pressure and temperature. It is also possible to explore a wide region of specifications by performing a series of flash calculations for varying T-P conditions, which in fact has become a widely used approach for determining regions of complex phase diagrams with multiple-phase regions. However, this can be computationally very expensive. A better way of predicting the overall picture for the phase behavior of a mixture can be naturally based on the explicit calculation of the whole phase envelope, including not only two-phase but also three-phase boundaries when necessary.

An efficient algorithm to trace two-phase envelopes was developed by Michelsen is very much 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 and uses the information given in that point to calculate the next one, this being 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, heavy compounds like asphaltenes or, sometimes, high concentrations of CO2. These types of asymmetry in a mixture can cause the existence of three-phase equilibrium besides the usually expected two-phase one.

A method that extends the previously named algorithm by Michelsen to calculate three-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 hydrocarbon 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. We also show the influence of these different compounds in the appearance of a third phase and both similarities and differences in the topology of the complete envelopes.

References

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