Supercritical fluids: from clustering effect in mixtures to gas-like and liquid like demarcation lines.

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Some processes related to energy and environmental topics involve asymmetric supercritical fluid systems. These systems are formed by the addition of light elements which are typically in a gaseous state at standard conditions and heavy components in small amounts. The resulting mixture is brought to a monophasic state above the critical point of the light element, which is considered as the solvent. In such supercritical conditions, the solute can be extremely well solvated, resulting in a clustering effect. This is the case when a gas, such as CO2, is injected to improve oil production of or to store the injected gas in situ, during the hydro-conversion of vegetable oils for biofuel production or when using supercritical fluids to extract specific components from a solid or a liquid carrier. Designing such processes requires the consideration of thermophysical properties (phase equilibria, PVT properties, viscosity, etc.). However, few measurements of such properties have been conducted on these systems. Furthermore, modeling these systems remains problematic due to the asymmetry between the species of interest and the thermodynamic conditions that are close to the critical point. The aim of the present work is to show how molecular simulations may help to characterize asymmetric supercritical mixtures and ultimately improve the modeling of these complex systems.