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Equilibria of ternary system Acetic Acid—Water—CO₂ under subcritical conditions

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Carbon dioxide has been subject of research in the past decades, with special attention targeting different uses of this “greenhouse” gas as raw material, technological fluid, building block or as a carbon supply for fuels, turning it from a pollutant to a green resource. Albeit likely it will be returned to the atmosphere (as part of the carbon cycle), CO₂ is an inexpensive and clean source with numerous industrial applications in diverse fields: from chemical processes to biotechnological purposes (Aresta 2010).

Many of these studies have been focused on supercritical CO₂, due to its broad potential uses in a very wide range of applications. However, those conditions, especially the levels of high pressure required at larger scale, involve certain equipment limitations. An alternative to overcome those restrictions is to use subcritical carbon dioxide.

In order to understand the different systems to be tackled within the bio-process design comprising subcritical CO₂, and therefore to improve its applicability, it becomes necessary to investigate the behaviour of such gas at different conditions. Some bioprocesses which require CO₂ might also involve the presence of other substances in the medium, such as acetic acid in fermentations (Straathof 2014; Cabrera-Rodríguez 2017).

Thus, from a biotechnological perspective, it is highly interesting to research on the system CO₂—H₂O with different concentrations of acetic acid (HAc). Based on previous studies (Rumpf *et al.* 1998; Bamberger *et al.* 2000), this project aims to investigate the vapour/liquid equilibria (VLE) of the ternary system HAc—H₂O—CO₂ at different subcritical conditions. A proposed computer model could be validated with experimental data, leading to a certain degree of adjustment due to specific factors, such as the binary interaction parameter k_{ij} , used in the model based on the Peng-Robinson EoS coupled with the mixing rules, or in the calculation of the cross second virial coefficients (Prausnitz *et al.* 1986).