## Phase Behavior of Fatty Acids, Fatty Acid Methyl Esters, and Carbon Dioxide Mixtures and Simulation of the Non-Catalytic Transesterification Process for Biodiesel Production

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Biodiesel is a promising renewable and sustainable fuel that can replace fossil fuels in some applications. Among the different techniques used to produce biodiesel, the transesterification process is preferred. The conventional transesterification process is based on acid-base catalysis, but this technique has many drawbacks including a requirement for high-purity feedstocks, and costly pre-treatment and downstream processes. An alternative process, using a supercritical alcohol (preferably methanol) without a catalyst, may offer advantages. This process can utilize a wide range of potential feedstocks (especially wastes), shows high production efficiency, and requires only simple post-processing. However, this technique requires conditions of high temperature and high pressure that increase the utility costs and may restrict the economic feasibility and sustainability of the process. The addition of co-solvents, such as CO2, may help improve the process. However, in order to assess this, a better understanding of the phase behavior of relevant mixtures is required. Accordingly, in this work, we report phase equilibrium measurements on different representative mixtures, SAFT-y Mie modelling, and a process simulation for the technology using gPROMS. The experiments were carried out with a high-pressure quasi-static-analytical apparatus at temperatures from (323.15 to 423.15) K and at pressures up to the critical pressure at each temperature. Vaporliquid equilibrium (VLE) data obtained have been compared with the predictions of SAFT-y Mie in which the functional group parameters were fitted to pure-component and binary-mixture data. We determined interaction parameters for the other functional groups available in the biodiesel process using our VLE and reliable literature data. Finally, the biodiesel production process has been simulated in gPROMS with a view to determining the optimal process conditions.