Equilibria of Aqueous Solutions of Disodium Terephthalate, Terephthalic Acid, and Compressed Carbon Dioxide for Separations

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Alkali depolymerization of polyester for polymer upcycling is a well-established polymer depolymerization pathway. Particularly, the decomposition of polyethylene terephthalate (PET) with sodium hydroxide has been shown to be highly productive and selective towards disodium terephthalate (Na_2TPA). Traditionally, the original monomer, terephthalic acid (TPA), is then recovered from aqueous disodium terephthalate solutions using acid-induced precipitation with solutions of strong acids, such as hydrochloric acid or sulfuric acid. As a potential sustainable alternative to strong acids, we are investigating the use of CO2-induced precipitation of terephthalic acid from aqueous disodium terephthalate solutions.

CO_2-induced precipitation involves both phase and chemical equilibria. We have attempted to measure solid-liquid-vapor equilibria at various temperatures, pressures, and loadings of Na_2TPA. The amount of terephthalic acid that can be recovered from aqueous disodium terephthalate solutions seems to be limited in some part by a buffering effect caused by the presence of the co-product, sodium bicarbonate. However, recovery efficiencies close to 90% can be achieved depending on the conditions. FTIR, NMR, and ICP analysis were used for the solution phase and precipitated TPA. Modeling using equations of state and activity coefficient models was attempted.