Development of Physicochemical Data for the Cannabis and Hemp Industries

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The extraction and processing of the components associated with medicinal cannabis and hemp extracts is rather daunting since cannabis plant materials can have in excess of 400 molecular compounds. Two molecular groups consisting of 12 major cannabinoids and 10-15 terpenoids components are of particular interest and the focus of using pressurized fluid extractions for their processing. A sequence of steps maybe employed in processing cannabis and its hemp analogue such as decarboxylation, extraction, dewaxing, solvent devolatilization, and several forms of distillation. Optimization of extraction and fractionation conditions is difficult due to the lack of fundamental solubility, phase equilibria, and kinetic-based data. Pressurized fluids such as carbon dioxide and butane coupled with conventional liquid solvents such as ethanol and water are routinely used to produce cannabis concentrates in which the pressurized fluid is used in both the sub- as well as the supercritical state (CO₂), or as a near critical fluid in the cases of neat propane or butane, dimethyl ether, tetrafluoroethane, or their mixtures thereof. Sources of useful data have been employed toward this end are available for essential oil components in liquefied- and supercritical- carbon dioxide as well as the meager literature data available at lower pressures pressures (<200 bar) for important cannabinoids such as cannabinol (CBD) and tetrahydrocannabinol (THC). Solubility parameter theory has also been employed to rationalize experimental extraction data by using group contribution calculations based on the molecular structure of the major cannabinoid and terpene components for both critical fluids and liquid solvent media - particularly with respect to their sequential use in extractions in both the near critical and supercritical state in CO₂. For the major cannabinoid components found in cannabis and hemp extracts, solubility parameter theory predicts solubility maximum occurring to occur at quite high extraction pressures equivalent to solubility parameters of 22-25 MPa^{1/2}, or equivalent to the solubility parameter of ethanol. Major terpenoid components such as beta-carophyllene - found in cannabis - can be fractionated from plant wax material optimally below 40°C and a CO₂ pressure of 90 bar. Many of the difficult-to-isolate terpenoid components show solubility minimum in CO₂ at 80-90 bar and 60°C (limonene and beta-carophyllene) and their solubility increases in both suband supercritical CO₂ with both increases/decreases in temperature, allowing the separation from wax components which exhibit a solubility maxima under these conditions. Separator conditions can be adjusted between 30-70 bar and 0-40°C to separate the essential oil components, i.e., the terpenes from the plant wax material.