Optimization, modelling and scaling-up of linalool supercritical extraction from lavender essential oil

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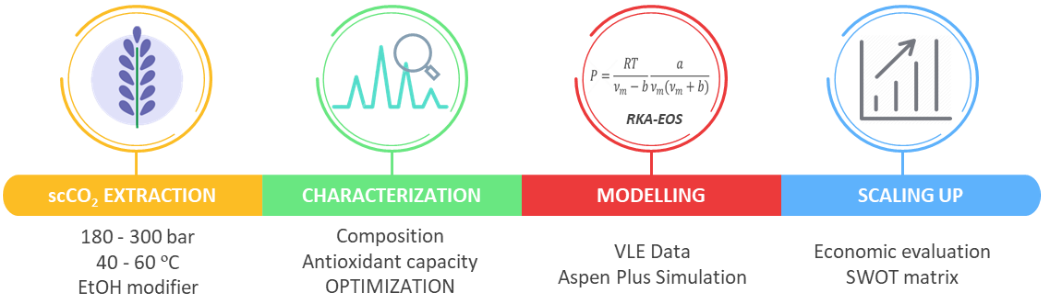

Nowadays, the increase in the demand of nutraceutical and pharmaceutical products of natural origin has led to the search of sources of bioactive products. Special interest has been paid to compounds with antioxidant and anti-inflammatory potential for the treatment of skin-related diseases like lavender essential oil that has been reported to these properties, which is attributed to one of its predominant compounds, linalool. In recent decades, extraction with supercritical fluids has proved to be one of the most interesting extraction methods because of its versatility and environmental friendliness, thus overcoming the disadvantages of traditional extraction techniques. Carbon dioxide (CO_2) is the most widely used supercritical fluid, as it is inert, non-toxic and allows extraction at lower temperatures and pressures.

The present work focuses on the supercritical extraction of lavender essential oil for its application in drugs and nutraceuticals. The influence of pressure and temperature on the extraction yield and antioxidant capacity was studied (Figure 1). The composition of the extracts was determined by gas chromatography/mass spectrometry (GC-MS) and high-performance liquid chromatography (HPLC), and the DPPH (2,2-diphenyl-1-picrilhidrazil) assay test was carried out in order to evaluate their antioxidant potential.

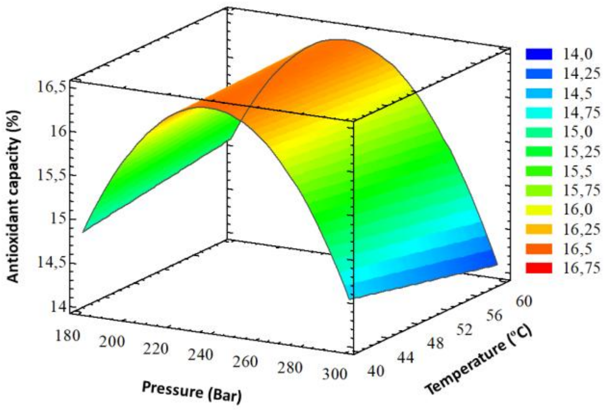

Figure 1. Influence of extraction pressure and temperature on antioxidant potential.

In addition to optimizing the extraction process of this compound, depending on the extraction yield and antioxidant potential of the extracts, it has been developed a model for the simulation of the equilibrium system formed by lavender essential oil and supercritical CO_2, using the Redlich-Kwong-Aspen equation of state thermodynamic model and the Aspen Plus commercial simulator. The essential oil was represented by its five main components by weight (linalool, linalyl acetate, camphor, nerol acetate, endoborneol and caryophyllene) and the modeling procedure involved estimating pure component vapor pressures and critical properties and computing a regression of phase equilibrium behavior. The interaction parameters for the RKA model were obtained from the regression of experimental phase equilibrium data for a binary system formed by each one oil component and supercritical CO_2 available in the literature. The distribution coefficients and solubilities calculated by this model showed good agreement both with our experimental data and bibliographic material. Finally, with the data obtained from this model the laboratory facility has been scaled up in order to assess the economic viability of this process.