Rectification process of essential oils: modeling and simulation.

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The fractionation process of essential oils on industrial scale receives little attention from the scientific community because of its complexity and application quite limited. Since the essential oil is a mixture of thermolabile compounds and has little known physical properties, studies on the subject are scarce. Thus, this work seeks to define thermodynamic correlations that describe the properties necessary for the calculation of chemical equilibrium as well as the definition of a dynamic model to describe the essential oil batch distillation process. The determination of physical properties is the crucial step when it comes to essential oils rectification processes, due to the reduced experimental data available, which leads to the use of predictive models. A consistent model that suits this requirement is the combination of group contribution methods with the corresponding states theory (CSGC), which uses only the groups within the molecule and its normal boiling point for the calculation of the vapor pressure of the substance. For the activity coefficient, COSMO-SAC technique is used. The batch distillation process is widely studied and numerous models have been developed, mainly for the separation of well-known mixtures, as petroleum fractions. This work also aims to validate a dynamic model proposed by Domench e Enjalbert (1), which consists of the system mass balance and its equilibrium relationships, in order to describe the separation of essential oil constituents. The model also has a few fundamental considerations like the constant plate holdup and negligible vapor holdup, which generate constant internal flow and eliminate the need to use hydrodynamic correlations. The vaporization rate is determined in relation to the enthalpy of vaporization and the feed composition in the reboiler. The temperature profile is calculated as a result of thermodynamic equilibrium. Simulations were performed in the equation-oriented simulator EMSO. *Eucalyptus citriodora* Hook and *E. globules* Labill essential oils were chosen due to their large production and economical potential. *E. globulus* oil has an initial composition of eucalyptol (83 %) and α-pinene (4 %), among others (2). The simulation provided four fractions: the first main-cut has a purity of 99.5 % of α-pinene, as the second one has 99 % of eucalyptol. Each batch has a 35 % recovery of the initial feed and the remainder is intended for a recycle batch with the same starting oil composition. *E. citriodora* simulation provided an 80 % recovery of the initial feed with 95.0 % of citronellal and a minor cut with 99.6 % of (-)-isopulegol. Its initial composition has 71.8 % of citronellal and 11.6 % of (-)-isopulegol (2). The simulations were carried on a 20 stages column, with constant pressure of 133 Pa, leading to a temperature range from 345 K to 373 K for the *E. globulus* oil and 330 K - 420 K for the *E. citriodora* oil.

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