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Dimethylcarbonate as a new green solvent for fragrant extracts: extraction and recovery processes

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Dimethylcarbonate (DMC) is widely used as an organic synthesis reagent. Alkylcarbonates are also used as solvents in some applications like inks or paintings. DMC is now recognized as safe and a “green” solvent [1] and publications or patents propose its renewable sourcing, and safe production [2]. Our purpose was to use it on fragrant raw material, instead of using traditional solvent like hexane and derivatives. This is challenging as DMC boiling point is much higher and less volatile than hexane isomers distillation fractions. Many plant organs (seeds, leaves, fruits) or exsudates (gum) were extracted with DMC and analysed [3].

Recovery process by using batch distillation of DMC from a mixture of six reference compounds found in essential oils and considered as volatile is investigated with the help of experiments and simulation with Prosim BatchColumn [4]. Thermodynamic properties are described with the Modified UNIFAC model accounting for non ideality in the mixture. Preliminary calculations have been used to determine the operating pressure, so as to avoid possible azeotropes between the mixture compounds and the solvent. The batch distillation process simulator is used to find the most suitable operating parameters: number of trays, reflux ratio and boiling rate. Lab and pilot scale experiments are used to validate the simulation results. Up to 95% of DMC can be recovered with a purity greater than 99%, with a loss of the most volatile essential oil model molecule limited to 12%. As a conclusion DMC is a very interesting solvent for fragrances and flavours, and could be registered as a food grade extraction solvent.

References

[1] Prat Denis, Andy Wells, Hayler John, and al, CHEM21 selection guide of classical-and less classical-solvents, *Green Chem*, 18, 288-296, **2016**.

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[3] Lavoine-Hanneguelle Sophie, Method for extracting an odorous extract by an alternative solvent to conventional solvents, patent No: US 9,434,908B2, sep. 6, **2016**

[4] Prosim, Batchcolumn Manual, **2015**

<http://www.prosim.net/en/software-batchcolumn-9.php>