

## Determination of the vapor pressure of *Piper hispidinervum* C. DC. essential oil by thermogravimetric analysis.

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The genus *Piper* (Piperaceae) has more than 700 species distributed in tropical and subtropical regions. Many of these, including *Piper hispidinervum*, have high commercial value due to its essential oil. This essential oil have presented antifungal activity against phytopathogenic fungi, as well as insecticidal, nematicidal and ixodicidal activities (1). These essential oil compounds are easily degraded when exposed to high temperature or in contact with ultraviolet light, thus compromising their biological activity. Thus, the micro or nanoencapsulation of essential oils is currently being investigated in order to promote protection against degradation and controlled release. In this context, the essential oil vapor pressure data are not only fundamental to the design of the equipment, when one intends to concentrate the major components by distillation, but also for the understanding of the evaporation and diffusion process from different matrices. The thermogravimetric analysis (TG–DTA) has been a useful tool for determining vapor pressure because it is a short test and requires small samples, through a modified Langmuir equation. There are several studies using the TG–DTA technique for vapor pressure determination, including essential oils (2, 3). According to Hazra et al., (2002) the method for calculating the vapor pressure curve for a single-component system can be used to construct the vapor pressure curve for the essential oil (multicomponent system) if the composition and the average molar mass of this essential oil is known. In this study, the GC/MS technique was used to determine the molar mass of the *P. hispidinervum* essential oil. The result obtained was  $158.3 \text{ g mol}^{-1}$ . The samples were analyzed in a thermogravimetric system (TA Instruments STD Q600). The method consists in a  $10 \text{ }^\circ\text{C min}^{-1}$  heating rate, in nitrogen atmosphere at  $50 \text{ mL min}^{-1}$ . In order to obtain thermogravimetric curves all compounds were subjected to a temperature range of ambient up to  $300 \text{ }^\circ\text{C}$ . The initial samples mass ranged from 20 to 60 mg, which were placed in an alumina crucible with a cross-sectional area of  $0.28 \text{ cm}^2$ . In this work, limonene and eucalyptol were chosen as the calibration compounds, and the Langmuir constant value was obtained as  $1.572 \pm 0.025 \times 10^6 \text{ Pa kg}^{-0.5} \text{ mol}^{-0.5} \text{ s}^{-1} \text{ K}^{-0.5}$ . All the compounds and the essential oil presented a process of zero order kinetics, which can be attributed to the evaporation. The vapor pressure curve for the *P. hispidinervum* essential oil, for 303 K up to 478 K was built and semi-empirical models parameters were determined. The fitted Antoine constants are  $A = 15.60$ ,  $B = 1353.56$  and  $C = -194.28$ , with a good representation, but without any physical significance. For this purpose, the parameters of Clarke and Glew equation were fitted at the reference temperature and pressure ( $\theta = 298.15 \text{ K}$  and  $p_0 = 10^5 \text{ Pa}$ ), obtaining  $\Delta G_\theta^0 = 16290.97 \text{ J mol}^{-1}$ ,  $\Delta H_\theta^0 = 41996.41 \text{ J mol}^{-1}$  and  $\Delta C_{p,\theta}^0 = -39.84 \text{ J K}^{-1} \text{ mol}^{-1}$ , which are in agreement to other essential oils components submitted to the same methodology (3,4).

1. Andrés, M.F., et al., Food Chem. Toxicol, 2017.
2. Phang, P.; Dollimore, D.; Evans, S.J., Thermochim Acta, 2002, **392**, 119-125.
3. Hazra, A.; Dollimore, D.; Kenneth, A., Thermochim Acta, 2002, **392**, 221-229.
4. Štejfá, V., et al., J. Chem. Thermodyn., 2013, **60**, 117-125.

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