Title Experimental study of chemical kinetics and simulation of 5-O-caffeoylquinic acid oxidation during manufacturing of mate (*Ilex paraguariensis*)

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Abstract

A set of experiments was carried out to investigate the chemical oxidation of 5-O-caffeoylquinic acid (5-CQA) in the temperature range of 96–188 °C. A batch cylindrical reactor made of glass and operated at isothermal conditions was used in the experiments. The decay of 5-CQA concentrations was monitored with a spectrophotometer at 323 nm by involving a coefficient of molar absorptivity equal to $2.7 \times 10^4 \pm 0.3 \times 10^4$ M^{-1} cm^{-1} for 5-CQA. A simplified kinetic model suggested by assuming an irreversible homogeneous pseudo-first order reaction was able to describe the effect of reaction time on 5-CQA concentrations. The influence of temperature on reaction rates was correctly reproduced with the Arrhenius expression with an activation energy and a natural logarithm of the frequency factor close to 42185 ± 7399 J mol^{-1} and 3 ± 2, respectively. The reliability of the entire experimental and modelling procedure was confirmed by comparisons between calculated and experimental dimensionless 5-CQA concentrations reported in the literature. Uncertainty analysis was performed to check the consistency of the estimated parameters and experimental data. Simulations indicate high rates of oxidation 5-CQA in the mate industry at temperatures and residence times typically found in the stages of enzymatic deactivation and drying.