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## Release of essential oil constituent from thermoplastic starch/layered silicate bionanocomposite film as a potential active packaging material

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### Abstract

In this present work, we study the release of essential oil constituents from thermoplastic starch/layered silicate (TPS/LS) bionanocomposite films used as antimicrobial proposed as a potential antimicrobial packaging material. A comprehensive application of design of experiments and multivariate calibration was used in order to study bionanocomposite formulation parameters that influence the release profile of carvacrol (CRV). Three formulation parameters (type of nanoclay, concentration of nanoclay and concentration of plasticizer) were simultaneously calibrated with three experimental responses (mechanical properties, thermal stability, and CRV release profile) by using D-optimal design and partial least squares (PLS) regression. The validated PLS model ( $R^2 = 0.9272$ ) showed that packaging properties as Young's modulus and thermal resistance are positively correlated with concentration of nanoclay and negatively correlated with concentration of plasticizer in the formulation due to an increase in the intercalated/exfoliated structures, which was corroborated by XRD and TEM images. CRV release is controlled by complexes interactions among these formulation variables. Higher amount of nanoclay is correlated with higher intercalation/exfoliation due to the formation of intricate structure of the matrix that could hinder the migration of CRV by formation of tortuous pathways that increase CRV half-life ( $\theta_{1/2}$ ). Also, non-polar interaction between CRV and the hydrocarbon chains of nanoclay organomodifiers increases  $\theta_{1/2}$ . Thus, by knowing the formulation characteristics of this packaging material it is possible to predict the release of the active compound, so this could provide information that allows to design an efficient active packaging material with optimal antimicrobial release profiles according its use.

**Keywords:** thermoplastic starch; bionanocomposites; carvacrol; D-optimal design; partial least squares regression; chemometrics

### Abbreviations:

$\theta_{1/2}$  half-life

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