A mathematical model to predict the release of encapsulated food active compounds from viscoelastic matrices

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In the food industry, encapsulation is used to protect and deliver active compounds (probiotics, essential oils, vitamins, etc.), which are sensitive to normal processing, storage, transportation, and digestion conditions. An adequate encapsulation of these active compounds can prevent their degradation, increasing their stability and bioavailability and ensuring their controlled release at the right time and site. In this regard, mathematical modelling of release kinetics could be a useful tool for the development and/or optimization of encapsulation systems, since it would help to minimize the number of experiments, experimental time, and costs. The objective of this work was to obtain and validate a mechanistic mathematical model to predict the release kinetic of encapsulated food active compounds.

The system consisted of a particle surrounded by liquid, composed of an active (dissolved and non-dissolved), water (present in the matrix and the surrounding liquid), and an encapsulating matrix. The model assumed that the water of the surrounding liquid can diffuse into the particle, causing the dissolution of the non-dissolved active, the diffusion of the dissolved active, the degradation of the matrix (erosion), and the development of stresses in the matrix (swelling). Characteristic dimensionless parameters related to the described phenomena were obtained. Model validation was carried out to evaluate the descriptive capacity of the experimental data of the in vitro release of astaxanthin encapsulated in calcium alginate beads.

A mean absolute percentage error less than 10% was obtained. The validation step was complemented with the experimental determination of model parameters related to the molecular weight of encapsulating matrix, the diffusion coefficient of water in the matrix, and the depolymerization kinetics of the matrix in simulated intestinal conditions. These values were used for estimating characteristic dimensionless parameters and specific values of the studied system.

The results showed that the proposed model can describe the release kinetics of active encapsulated compounds and it could be used to design and optimize food encapsulation systems.