A spatial dependent 3D model to predict the composition of the headspace of microperforated packages for respiring products

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Modified Atmosphere packaging (MAP) is a widely applied technology for preserving the quality and safety of fresh and fresh-cut fruits and vegetables. It is based on achieving the most suitable gas composition for the product inside the package, and for certain high respiring products this is possible only by using microperforated packages. The application of mathematical models to the in-package gas composition is very useful for the optimal design of MAP, so different models have been evolving last years, incorporating new features to enhance precision in calculations. However, most models neglect the spatial dependence of the gas composition in the headspace and the convective flow through microperforations. Computational fluid dynamics (CFD) models applied to microperforated packages have enabled a more comprehensive investigation of gas exchange phenomena. The aim of this study was to develop and validate a spatial dependent 3D multiphysics model capable of adequately describing the gas composition in the headspace of microperforated packages during the storage of respiring products. The model, implemented in COMSOL Multiphysics® software, considers fully coupled transient convective and diffusive mass transfer and momentum transport through the microperforations, using the Maxwell Stefan and Navier-Stokes equations for compressible Newtonian flow. The model was validated in fresh-cut peach stored in microperforated packages, considering different microperforation sizes (from 90x50 µm to 210x130µm) and peaches cultivars (Andross, Calante and Catherine). The respiration rate, expressed as consumption of O_2, was considered to potentially vary with O_2 concentration, while the production of CO_2 was considered to follow a linear relationship with the O_2 concentration. The developed model matches the experimental evolution of the gas composition inside the packages, allowing to visualize the gas concentration profiles around the perforations and the entry of external air into the package to compensate the pressure drop caused by product respiration.

Keywords: *Gas exchange; Mathematical model; Microperforated package; Modified Atmosphere packaging (MAP); Respiration kinetics.*