Microscopic model mass transfer of contaminants from recycled paper and board into foodstuffs

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Goals

Food packaging made of recycled cellulosic materials is a systematic source of aliphatic and aromatic mineral oils (MOA). Almost all MOA are potentially carcinogenic and transferable significantly to foods. Underlying mechanisms according to the dispersion of MOA on fibers and their volatility are poorly described. This study reports one of the first mechanistic descriptions based on microscopic chemical imaging down to the fibers' scale. The observations are used to propose a microscopic mass transfer model incorporating the properties of the fibrous network. Homogenized diffusivities are compared with experimental ones for validation.

Methods

Model blotting papers were impregnated with various aromatic surrogates dispersed in good and bad solvents of cellulose fibers to reproduce the typical contamination profiles met in recycled papers. The 3D fibrous network was reconstructed in microcomputed X-ray tomography. The dispersion of solutes was directly imaged on fibers by combining Raman spectral imaging and laser scanning confocal microscopy. Apparent diffusivities were experimentally measured with the help of a modified Roe method involving a stack of paper sheets, including two formulated sources.

Results

The main observations were translated into mechanisms and a mass transfer model. Three factors limit the transfer across the paper sheet: the fugacity of the considered surrogate on the fiber, surface diffusion, and the distance between fibers. Highly volatile substances can cross several layers before being re-adsorbed on fibers. Low volatile aromatic compounds that are highly precipitated travel much shorter distances. Impregnating fibers with such MOA by evaporating a poorly wetting solvent reduces their mass transfer dramatically. These effects were experimentally measurable with the Roe method and offered an easy path to validate our microscopic model. The proposed model combines a mutual diffusion model in the gas phase and an "evaporation-condensation" model for the interactions with the fibers. The model is homogenized by assuming a periodic elementary representative volume. Predicted diffusivities were shown to be in satisfactory agreement with experimental macroscopic values.

Conclusions

The effects of fiber packing were captured by the microscopic model. They enable the design of optimal density and tortuosity to grant sufficient barrier properties at the scale of food packaging.