Modeling of the structure and transport properties of hybrid membranes with nanotechnology-based barrier promoters for food packaging

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Summary

Food industry has been largely developed in the last fifty years and still grows creating new products and markets all around the world. As a result, packaging industry has also been developed to assure the best quality and extended life time of the product. In addition, worldwide litter accumulation has also increased and, thus, there is a vast demand for new packaging materials that can be easily recycled or are biodegradable. Strong research efforts have been dedicated to improve the properties of the materials used for food packaging by reducing their permeability to O_2 and H_2O in order to increase the product lifetime. Moreover, by creating different kinds of sensors, e.g. temperature and pH sensors, and adding them to the packaging materials, 'smart' food packaging is introduced, which will be able to inform the consumer and the seller/distributor whether the product is safe for consumption.

In this work, polymer membranes containing nanoparticles that act as barriers to gas penetration are considered and the relation between the internal structure of the hybrid membrane and barrier performance is elucidated by computer aided reconstruction of the membrane and by permeability calculations. Moreover, the potential mechanisms and kinetics of nanoparticles migration in the polymer composite and their subsequent entrance in the food are examined to investigate the safety of the new packaging material.

For this purpose an algorithm for the reconstruction of the hybrid membrane has been developed that takes into account the nanobarrier volume, shape, size and orientation inside the polymeric matrix. The algorithm can also take into consideration the formation of a third phase between the nanobarriers and the polymer phase that can be formed because of affinity issues between the polymer and the barriers and in some cases even increase the membrane permeability. Several different potential membrane structures have been reconstructed for different

nanobarrier concentrations and their effective diffusivities were calculated. The results elucidate the effect of the nanobarrier volume fraction, size, shape and orientation on the permeability reduction. The outcome of these calculations has been compared with Effective Medium Theory (EMT) calculations and polymer crystallinity issues have also been addressed.

A diffusion-type model has also been developed to investigate the dynamics of the nanoparticle diffusion and migration within the membrane. The model can incorporate data from the reconstructed hybrid membrane for the nanoparticle size, shape and distribution with data on the migration rates of the nanoparticles in the polymer matrix and towards the food from theory and experiments. Migration calculations have been performed for various nanoparticle diffusivities, regarding different relevant environmental conditions and considering several types of food/nanobarrier affinity, resulting in different transfer rates of the nanoparticles from the membrane to the food. Polymer crystallinity effect on the migration has also been investigated considering various volume fractions of the crystalline phase and amorphous/ crystalline polymer structures. EMT calculations have also been performed for the effective diffusivities of the nanoparticles in the interior of the polymer matrix.

The results obtained from this study indicate the importance of the right selection of the type, shape and amount of the nanoparticles that can be used to have pronounced barrier effects, the potential of their migration from the packaging to the food, as well as the role of the formation of a crystalline phase in the polymer matrix in the membrane permeability and nanoparticle migration. The insight that is gained can be used to guide the design of new hybrid membranes, saving significant experimental time and resources.