3D Mass Diffusion in Nanocomposite Systems: Finite Element Simulation and Phenomenological Modeling

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The optimization of polymer barrier properties is currently of crucial importance for a wide range of applications going from packaging to building or even energy applications. To meet the requirements of these applications, polymer matrices are often combined with impermeable (nano) fillers. Different nanofiller natures, shapes and contents have been experimentally used and a large range of barrier materials has been obtained. In the meantime, several numerical approaches have been developed to model gas diffusion properties of nanocomposite materials. However, these approaches most often only considered bidimensional systems. Nowadays, finite element modelling (FEM) approaches are being used increasingly as they allow the description of the materials in 3 dimensions.

The aim of our work is to develop and validate a new finite element model allowing predicting the gas diffusion properties of nanocomposites for different nanofiller shapes, contents and dispersion states. In this approach, the mathematical formulation describing the mass transfer is based on Fick's partial differential equation and the model is solved numerically using the commercial package COMSOL Multiphysics. The results obtained from our Finite Element modelling approach are discussed with respect to the literature data. The governing factors of the transport are identified allowing to develop an analytical equation that can be used to describe mass transport for a wide range of nanocomposite systems.