UNDERSTANDING THE BARRIER PROPERTIES OF CLAY-BASED FOOD PACKAGING. A CONTRIBUTION FROM COMPUTATIONAL MODELLING

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Non-swelling clays have been used in traditional paper coating technologies for many years because these exert the least effect on the rheological properties of a formulate coating. However, recent work [1] has demonstrated that combining swelling clays, particularly the smectites, with starch and plasticisers to form a sustainable coating, results in water vapour transmission rates (WVTR) that are competitive with oilderived barrier coatings. Coatings with high barriers to gases, vapours and flavours find their major application in food packaging materials [1]. Taking into account the amount of food currently wasted every year, packaging that keeps it fresh for a longer time has an important role to play in reducing the amount of energy consumed during the food production and transport cycle.

The simultaneous presence of both starch and plasticiser in the clay gallery is critical in order to achieve the lowest possible WVTR values, though only some clays are able to incorporate starch into the gallery. Current experimental techniques are lacking in performance for investigation intercalated layered materials and give little information due to static and dynamic disorder. Because of these limitations, interest in the use of computational methods [2] for studying these layered solids has increased in order that observed physical and chemical properties may be rationalised and predicted, thus providing sustainable paper coatings, which are competitive with oil-derived barrier coatings.

We have employed computer simulation techniques – Molecular Dynamics (MD) to extend understanding of the roles played by the clay, water, starch and plasticiser in these sustainable coatings. The impact on the barrier properties is assessed as well. MD models were validated with experimental observations. Later, the influence of the magnitude of the clay layer charge and its distribution on the hydration dynamics of smectite clay minerals and its barrier properties.

Keywords: barrier packaging, bio-polymer, simulation, clay-polymer nanocomposites, food-safety

References.

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