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CAN FICK LAW-BASED MODELS ACCURATELY DESCRIBE MIGRATION WITHIN A COMPLETE FOOD PRODUCT LIFE CYCLE?

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ABSTRACT

The concept of migration from polymeric packaging materials to food and food simulants, under the environmental conditions expected during the food products' complete life cycle, is discussed here. The most approved models that cope migration as a diffusion-driven process, neglecting more complicated mass transport mechanisms, and environmental involvement that are occurring in parallel or simultaneously in the whole system, are considered and weighted

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against the extensiveness of their use. Having identified the areas of inadequacies of usage in validating migration during food process applications affecting food quality rather than safety, this work outlines and proposes specific and eventually more complete directions for working towards the modeling of the food – packaging interactions comprehensively involving the storage environment in terms of both conditions and constituents.

KEYWORDS

Food-packaging interactions; migration models; packaging; food quality control

PRACTICAL APPLICATIONS

Several papers indicate differences between experimental observations and theoretical predictions, while significant research effort estimates the parameters' values for achieving better agreement. Instead of considering diffusion process as being the single mechanism to describe the migration from packaging to foodstuffs, this work proposes to incorporate more complicated phenomena (sorption, surface reactions, etc.) to overcome the above-mentioned discrepancies. Potential future models, may then allow for a comprehensive quality control, compared to the presently acceptable safety reassurance.

Introduction

Among the most important physical-chemical interactions within a food-packaging-environment system, migration, sorption and permeation of substances through and from the various material phases, have gained high legal and therefore scientific concern, too.

Migration of chemical compounds from packaging material to food has been broadly attributed to a diffusion process, occurring due to the dissolution of the migrant in the food (see, for example, Brandsch et al., 2002, Arvanitoyannis and Bosnea, 2004).

The mathematical models developed on that process use the Fick's approach to describe mass transfer, they have to solve the elliptical differential equation for diffusion and spent significant effort in determining the parameters applied (e.g. the diffusion coefficient), on which base the differences among several models exist (see, for instance, Baner et al., 1996). Aspects of migration, such as partitioning, heterogeneous reactions, packaging-material morphology, shape/polarity of the migrant, etc., have not yet been considered in full within these models, although discrepancies in predictions and experimental observations have been revealed (Franz, 2007).

The main point of this note concerns the mathematical models on substances' migration from packaging material to foods under various storage conditions, on the side of the post legal limitations of acceptance of food safety, but rather on the overall food quality control assessment. For that, our opinion encounters the identification of the theoretical drawbacks of the approaches themselves behind the models and also an improvement via the inclusion of more relevant, though complex, transport phenomena. In this context, a critical discussion on the widely-accepted Fickian approach and its applicability and drawbacks, for identifying impending shortcomings towards a potential indication of a direction towards the forthcoming research on that topic, are presented herein.

Materials and Methods

Migration may be divided to several fundamental mass transport processes simultaneously evolving within an environment-packaging-food system, including diffusion, convection, and chemical reactions (see, for example, Del Nobile et al., 2003). Migration modeling engages a deterministic approach, usually considering the migration process to be controlled by migrant's diffusion through the packaging material, as described by Fick's second law (Pocas et al., 2008), relying on specific assumptions needed for assisting the model development and application, yet, not being necessarily extensively valid, in each and every case of substances' migration between various phases. Accordingly, based on Fick's first law, the diffusion coefficient of a compound in a particular matrix during a certain time period, through a control volume, should be proportional to the gradient of its concentration. The fundamental considerations for a Fick's law valid use, are actually dependent on the following specific assumptions:

1. The migrant was distributed homogeneously in either the packaging material or the food phase.
2. There was no boundary resistance in the transfer of the migrant between packaging and food phases.
3. There were no interactions between packaging and food.
4. No swelling phenomena occurred within the food-packaging system.
5. A specific partition coefficient between food and polymer might be assumed.
6. There has been no external supply of migrant during migration process, i.e. the sum of the total migrant amount in the food-packaging system is constant.

The above assumptions are made in order to achieve a solution for the resulting second order partial differential equation for the diffusive mass transport and include the consideration of the diffusion coefficient as in general being constant in either the food or the packaging material (see, for instance, Chan et al., 2015). Additionally, both the diffusion and the partition coefficients of the migrant should be known in order to practically apply this equation. Furthermore, it has been often assumed that the solubility of the migrant in the polymer is very high, which consequently results to a partition coefficient =1, avoiding any difficulties in estimating this coefficient for a given migrant - packaging material - food system (Brandsch et al, 2002).

Up today, two simplified though widely accepted and applied models are the Piringer's model (Piringer, 1994) and Limm & Hollified's model (Limm and Hollifield, 1996). The first one correlated the diffusion coefficients with the relative molecular mass of the migrant with a specific parameter along with the absolute temperature, while the later one proposed a similar approach but with limited use in other packaging materials beyond polymers.

Nevertheless, a number of studies have shown moderate to low accuracy of either model and quite frequently, an either under- or over-estimation of the migration results (see, for example, O' Brien et al., 2001, Pennarun et al., 2004, Franz, 2007). The apparent inadequacy of the Fickian approach in achieving such agreements, has been attributed to the values of the parameters, such as diffusivity, assigning a lot of effort in highly sufficient estimations. Within the above works, environment was included as being solely the migration defining factor, while its active role in the total food-packaging material-environment system has been neglected. In support of that, major "contaminants" may originate from the surrounding environment (e.g. oxygen) or may end up into the environment, such as flavors desorbed into packaging. Hence, independent of the food type, overall environment has a direct and independent impact on packaging materials at the packaging-environment interphase.

Results and Discussion

Certain theoretical concerns are raised regarding the approaches converge to the widely accepted consideration on the migrant mass transfer being diffusion driven, for then the process to be adequately described by Ficks laws. Up today, the main effort has been placed on identifying the diffusion coefficients and other parameters within the models in order to identify the application area for each and every model. At the same time the Fickian approach has been considered without much hesitation since models provide an over estimation of the migrants present in foods at the upper acceptance limits for food safety in terms of legal purposes.

In contrast, though, it seems apparently rather less likely for this consideration to be incorporated in more complicated phenomena, such as sorption of specific food contaminants by the packaging material, partitioning on the food-packaging interface, chemical reactions of packaging material or of some of its byproducts with the food content, etc., all of which possess a high potential within a real food-packaging system's life cycle. We may safely propose then, that the above assumptions cannot be valid, in a universal way. In support of that, we have identified cases where at least one of the above assumptions cannot be valid as, for example, the case that the assumption #1 could not be valid for packaging materials other than plastic polymers, or assumption #2 that might not be valid for sticking migrants, and so on.

Another significant drawback widely adopted by published literature, is regarding the system consideration that the environment is usually considered as the entity that just imposes the conditions (boundary/initial conditions as well as values of the parameters involved in the equations) without being part of the system. Consequently, environmental influences have not been directly engaged in the mass transport process, but only through the conditions and parameters, being therefore, somehow arbitrary. Hence, it is in need to rework and potentially restructure the traditionally accepted "packaging-food" system with a proposed reformed one now being "environment-packaging-food", which shall allow for a more detailed and quite more solid consideration of the totality of the transport phenomena through a complete system consideration.

Equations of parameters describing complex migration and the consideration of a more complex system are missing for the current references as it focuses on the migration acceptable limit for safe human consumption. This note does not wish to deal with the potential improvement of the legal requirements approach but rather to initiate a work direction for a food processing tool from a food quality point of view as affected by migration phenomena in agreement with a similar direction recognized in works discussing specific cases and presenting the peculiarities for certain food migration studies (see Del Nobile et al., 2003).

Conclusions

Main migration models discussed before may well enough predict the migration of known and already characterized migrants from commonly used plastic containers, while when the contact material contains a number of completely unknown compounds, these models may not be capable for accurately predicting the overall migration of each substance. Therefore, such models in their philosophy tend to inaccurately estimate migration, of a migrating additive potentially adversely impacting on the optimum product quality. In such cases a highly accurate prediction of the migration process must be in hand in order to reassure the optimum quality of a food within the complete supply chain environment.

Therefore, we be apt to conclude on the actual non-Fickian behavior of migrants on a universal scale and a consequent need for a mass transport process to be modeled via more complicated mathematical expressions, potentially containing non-linear terms, for a more complete expression of the migration phenomena, when working beyond legal requirements and towards a holistic food process quality control.

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