PITTCON2020 – extended abstract

Session "*Understanding Food Packaging Materials: Challenges in the Analysis of Packaging Components and Migrants in Food***"**

Migration modeling related to food contact materials: present and future

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Predictive methodologies to evaluate the migration from food contact materials offer numerous advantages compared to experimental testing. The results can be obtained in real-time without delay and without consideration of detection or quantification limits. They do not require any analytical standards and can be applied in routine to unknown compounds, such as breakdown products, cross-contamination, and non-intentionally added substances (NIAS). They can accommodate real conditions instead of accelerated ones, and they can be used in forensic analysis to track the causes of unattended contaminations. The main benefits of migration modeling are, however elsewhere; it can be applied at virtually no cost and without requiring the finished product to be available. It can be, therefore, integrated at the early stages of packaging design, polymer formulation, additive design, process optimization, and combined along with other preventive approaches, such as ecodesign and life-cycle assessment. In essence, modeling is holistic and could virtually cover many aspects of product shelf-life, environmental impacts, and safety issues to reach a global optimum. The results can be expressed either in deterministic or probabilistic manners.

Though the arguments sound cogent, applying migration modeling suffers several complications and limitations: recognition by authorities, confidence and validity of the conclusions. After presenting a brief history of the early developments of migration modeling in the US and the UE, the presentation will bring an overview of the state of the art, and of the new perspectives offered by multiscale modeling from atoms to consumer exposure. Migration modeling is well accepted in the US and the EU for compliance testing, but under some conditions, that guarantee that the entire process can be reviewed and tested. The **first principle** ("*conservatism*") is that modeling and related calculations should overestimate the real migration. The **second principle** ("*reliability*") implies that the foreseen mass transfer pathways and substances obey to well-described mechanisms (diffusion, sorption/desorption, permeation), accepted conditions (e.g., uniform distribution) and proper integration in commercial or free software. The **third principle** ("*consistency*") is that the transport and thermodynamic properties (e.g., diffusivities and partition coefficients) are known or guessed in a way they fulfill the requirements of the first principle. The **fourth principle** ("*parsimony*") states that sophisticated and refined scenarios should be considered only when simpler ones cannot demonstrate compliance. The fifth and finally **last principle** ("*proportionality*") is that the non-compliance cannot be demonstrated by calculation. In other words, the authorities cannot oppose their own migration modeling to justify a product recall, but they can use it to orient their own survey.

Two-thirds of food packaging are tested for compliance by modeling in Europe. With the increasing demand of recycled materials and safe-by-design materials for food contact, migration modeling has become an essential tool to validate various critical points along the chain of value: the rate of recycled materials, functional barriers, effects of aging, etc. Concurrent engineering and computer-aided design are highly beneficial for the consumer and the environment, but they require more refined tools than the coarse ones used for compliance testing. Databases of composition and properties are essential and span all applications of materials, specifically regulated or not. Molecular theories and atomistic calculations are the new grail are attracting new research efforts. Rapid deformulation techniques, using ^{1}H NMR, FTIR-ATR, thermal desorption-GC-MS direct infusion mass spectroscopy combined with proper chemiometric tools, feed migration hypothetical scenarios[1,2]. Prioritizing methods (e.g. Failure Mode Effects and Criticality Analysis) select the most relevant substance candidates, critical steps or components[14]. There are currently nevertheless no standards, and the expandable frameworks are scarce and mainly proprietary. Several milestones have been, however, reached in recent years and many situations can be simulated with advanced migration modeling just by sketching the molecules, the packaging and the flow chart of the supply chain. With the always growing power of computers, algorithms can even change elements of the 3D design[16] along with its formulation to reach various targets: improved safety and shelf-life, minimum waste, and environmental impact. We developed recently such a detailed workflow so-called [E]valuation[3-8], [D]ecision[9-12], and [S]olving[13-16]. Safety, ecodesign, and processability are combined within the same multicriteria optimization loop looking for the best compromises between contradictory criteria . The objects generated *in silico* can be finally printed in 3D or integrated into virtual or augmented reality scenes for rapid prototyping and evaluation. Better design and prevention are at our fingertips. Encapsulating the physicochemical knowledge in models and computers will harmonize the practices between stakeholders and free resources to tackle emerging issues: contamination by secondary and ternary packaging, cross-contamination between packaging components, interactions with food, non-specifically regulated material, etc. Large-scale education and training initiatives are imperative to make the entire ecosystem applicable, socially acceptable, and economically viable. Several universities are currently collaborating in the EU to create the first massive open online courses on migration modeling and packaging issues.

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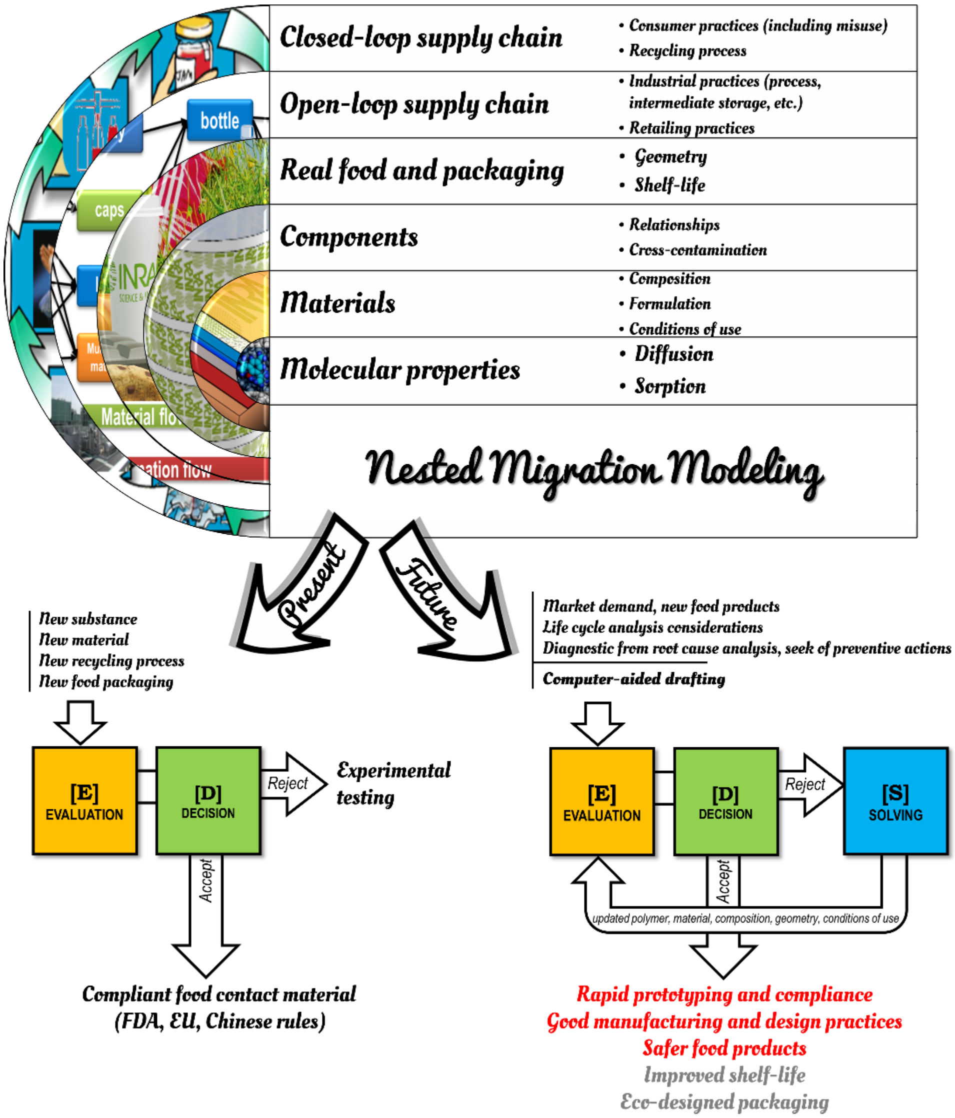

Figure 1. Illustration of the possibilities of the current and future evolution of advanced migration modeling.