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# Evaluating use stage exposure to food contact materials in a LCA framework

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## 1. Abstract

*We present novel methods to incorporate exposure to chemicals within food contact materials (FCM) (e.g. packaging) into life cycle impact assessment (LCIA). Chemical migration into food is modeled as a function of contact temperature, time, and various chemical, FCM, and food properties. In order to reduce computing time and complexity, a double exponential curve was fit ($R^2 \approx 1$) to an exposure model which otherwise requires numeric solutions. The model is modified to evaluate the product intake fraction, PiF, which is a new metric that accounts for exposure to mass of chemicals embodied in a product in a way compatible with intake fraction, iF, a metric traditionally used in LCIA. The model predicts PiF increases with temperature and for compounds with lower octanol-water partition coefficients within more permeable materials which are in contact with foods with high ethanol equivalencies (fatty foods).*

## 2. Introduction

Various life cycle assessment (LCA) studies evaluating food contact materials (FCMs), like baby food packaging containers, have found advantages to plastic over glass [1]. Life cycle impact assessment (LCIA) includes human toxicity impacts from exposure to chemicals released throughout product life cycles, but excludes use stage exposures to chemicals migrating from FCM into food. Generally, regulatory risk assessments aim to ensure human exposure to potentially harmful chemicals in food is below certain thresholds of 'safety' and rely on submitted industry data or migration modeling of supposed worst-case scenarios [2]. Such efforts help limit dietary exposure, but actual human intake and levels of some phthalates within food nonetheless approach or exceed regulatory thresholds—with indication of FCMs as the chemicals source [3]. Furthermore, regulatory thresholds for toxic substances are continuously subject to change for various reasons and differ between countries [4, 5]. Unlike risk assessment the primary goal of LCIA is not to ensure individual consumer safety with respects to toxicity thresholds, but to indicate products with minimal potential for population-scale impact, and thus LCIA methods rely on linear dose-response relationships (not thresholds) derived from toxicity studies and combine these with average population-scale (not worst-case individual) exposure. Accordingly, LCIA is a promising risk-minimization and product-optimization approach for FCM; however, methods to include exposure to FCM in LCIA are currently lacking although they likely exceed other life cycle exposures [3]. Our goal is to provide LCIA-compatible methods to close this research gap.

## 3. Methods

To be compatible with the scope of LCIA, which defines a reference flow (e.g. a mass of packaging required to contain a volume of food), we built the FCM exposure model to estimate the newly defined product intake fraction, PiF ($kg_{intake}/kg_{in\ product}$) [6]. This method quantifies PiF as the chemical-specific mass taken in by users of the FCM product per kilo of chemical in the FCM—where ingestion is assumed to be the

dominating route, and food waste, inhalation, dermal contact, and exposure to environmental emissions are assumed negligible.

| | **Parameter** | | **Parameter** | | **Parameter** |
|---|---|---|---|---|---|
| a | octanol-water partition coefficient, $K_{ow}$ | b | root of tan $q_n = -\alpha q_n$ | c | volume of FCM |
| a | molecular weight, MW | c | initial concentration (migrant) | c | density of FCM |
| b | diffusion coefficient (migrant) | c | temperature | c | thickness of FCM |
| b | diffusion parameter (polymer) | c | time of contact | c | density of food |
| b | ethanol equivalency of food, E-eq | c | activation energy (polymer) | c | mass of food |
| b | package-food partition coefficient, $K_{P,F}$ | c | contact area | c | volume of food |

*Table 1: Required parameters for migration model, and their classification a, b, or c*

We adapted a numeric migration model commonly used in regulatory risk assessment and compliance testing [7, 8, 10], by deriving an analytical solution and providing average/realistic diffusion and partition coefficients for use in LCIA, instead of the default values used by risk assessors. Specifically, the model is for chemicals in plastic packaging (see [8]) relying on 19 input parameters (Table 1) which we classified as a) *available* in open-source platforms (e.g. molecular weight), b) *estimable* (e.g. by a linear regression), and c) *default assumptions* given by regulatory documents [8] which can be updated by the LCA practitioner. The model was programmed in MATLAB® and we developed approximation strategies when needed, e.g. the plastic-food partition coefficient ($K_{P,F}$) is a function of ethanol-equivalency (e.g. food fat content) and the octanol-water partition coefficient ($K_{ow}$) of the chemical migrant [9]. We also extracted data from [8] to calculate average polymer-specific diffusion parameters. Further, we investigated fitting a double exponential to the model: $PiF(kg_{intake}/kg_{in\ product}) = a*\exp(b*t) + c*\exp(d*t)$ which could then be programmed in a spreadsheet where computing time and required input parameters are reduced.

Hypothetical migrants across $K_{ow}$ and at two molecular weights (MW) within polyethylene terephthalate (PET) were modeled at 5°C for 10 days. PiF was also modeled for diethylhexyl phthalate (DEHP) in PET and high-density polyethylene (HDPE) as FCMs for milk, clear drinks, and dough (spanning ethanol equivalencies), at 125°C for in-bottle pasteurization.

**4. Results and Discussion**

We used a regulatory risk assessment FCM migration model, and derived a nearly identical but analytically computational solution, solved for the LCIA-compatible PiF metric, and estimated average (not worst-case) diffusion and partition coefficients. Our results and work by [7,8,9,10] identify $K_{P,F}$ as an important parameter. We developed a linear approximation for $K_{P,F}$ for all ethanol equivalencies (E-eq) i.e. content of organic phase, such as fat within foods, from data available in [9] for only three E-eq. More data may be needed for an improved approximation, e.g. as provided in background calculations in FACET [10]. When regulators apply the migration model [8] parameters classified as b) *estimatable*, are often set to a fixed value. Although stated in regulatory documents that package-food partition coefficient, $K_{P,F}=1$ is a fixed "worst-case," we found evidence $K_{P,F}<1$ may occur experimentally [9], and that conveniently, when $K_{P,F}=1$

dependent parameters are also fixed, simplifying the calculation. For various plastic-food combinations we found often $K_{P,F}$ >1, which supports the need to better approximate $K_{P,F}$ for model application in LCIA as well as for realistic exposure estimates [10].

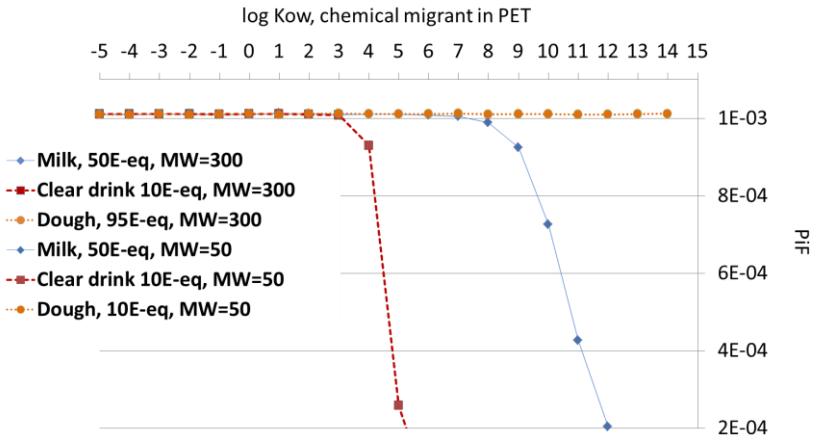


*Figure 1: PiF model results across $K_{ow}$ for hypothetical migrants at MW=300 and 50 g/mol, for foods with various ethanol equivalencies (E-eq).*

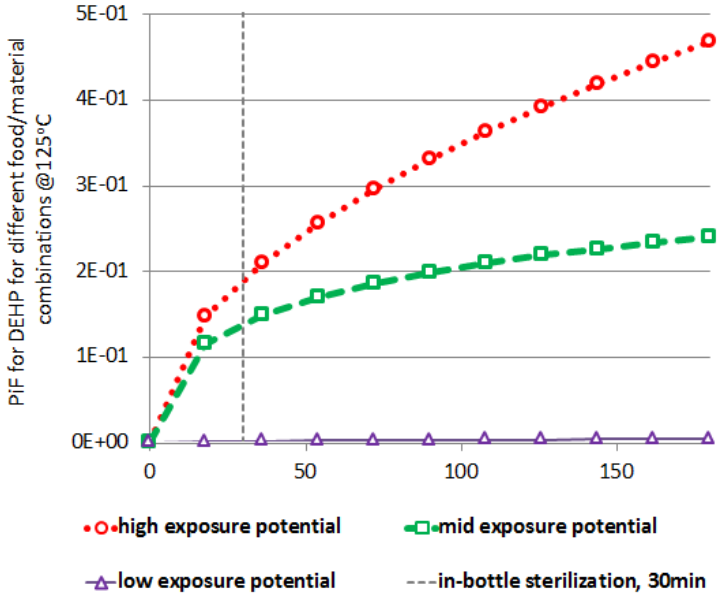


*Figure 2: Example of the PiF model results for DEHP, where exposure potential was found to be high for DEHP in HDPE for foods with 90%E-eq, mid for HPDE for foods with 50%E-eq, and low for DEHP in PET with all food types as well as HPDE with 10%E-eq.*

Further, via MATLAB® we fit and parameterized a double exponential curve ($R^2 \approx 1$), where for example parameter c=1-a, and a, b, d are functions of easily obtainable input parameters. In this manor, the difficult to obtain input parameters, e.g. iterative solutions of transcendental equations, were no longer needed and computational time was decreased.

Preliminary results, e.g. for PET demonstrate that when contact temperature, T= 5°C, PiF<$10^{-3}$ $kg_{intake}/kg_{in\ product}$ and is largely influenced by $K_{P,F}$ which is a function of $K_{ow}$ of the migrant and E-eq of the contacted (packaged) food. This reflects that chemicals tend to remain partitioned in plastic when in contact with foods with low ethanol-equivalencies (e.g. clear drinks), but increasingly partition into foods with higher ethanol

equivalencies (e.g. milk and dough) (Figure 1). A migrant's MW was unimportant for the T=5$^{o}$C scenarios (Figure 1), but has a major influence at T=125$^{o}$C for in-bottle pasteurization (results not shown) because of the influence of the diffusion coefficient. For high temperatures, PiF can approach 20% for contact times of 30 minutes (Figure 2) for foods with high ethanol equivalencies (e.g. >90%) when the model was run for DEHP within FCM made of HDPE (which is typically not legally allowed, however may occur at low levels via recycling processes and/or contamination). As our model is based on a regulatory model, the trends we observed with respect to chemical, food, material, and scenario properties are also considered by risk assessors, e.g. reduction factors for certain fatty foods are applied assuming that modeling with a high E-eq greatly overestimates exposure [2].

## 5. Conclusion

We developed a modeling strategy that adapts and parameterizes a numerical FCM migration model normally used to ensure risk-based regulatory compliance, to be operational in LCIA by analytically estimating an average/realistic PiF. While risk assessment based on supposed worst-case scenarios is required to evaluate FCM safety compliance, including FCM migration modeling in LCIA has a different goal of comparative risk minimization which accounts for impact trade-offs due to the entire FCM life cycle. Including use stage exposures to FCM in LCIA—which judging by preliminary calculation of PiFs has the potential for exposure exceeding environmentally mediated exposures by orders of magnitude—may help minimize exposure to chemicals within FCM, which is especially important for those which already exceed regulatory statutes, like DEHP, and may be due to recycling or other processes along the products' life cycles.

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