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Testing the Applicability of the Safe-by-Design Concept: A Theoretical Case Study Using Polymer Nanoclay Composites for Coffee Capsules

Supporting Information

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S1. Similar concepts to the Safe-by-Design approach

In 1996, Wang et al. [1] described "Design for Safety" as a systematic approach from the field of engineering that combines the expertise of engineers and scientists to analyze entire systems through all phases of the life cycle. Within this approach areas with particularly high risks are to be identified and the probabilities of occurrence and the extent or severity of effects minimized. The first step towards minimizing potential hazards is inherently safe design. The four main methods of this concept are "minimize", "substitute", "simplify" and "moderate" [2]. This means reducing or replacing hazardous substances with less hazardous ones, simplifying design instead of adding additional measures and reducing possible effects. Nevertheless, inherent safety cannot always be achieved, especially if functionality is counteracted with safety.

The idea of designing processes and products that have intrinsically low hazards instead of coping with hazards through protective systems has also established itself in the field of chemistry. Behind the "Green Chemistry" framework lie environmental considerations. There are different conceptualizations of what the term "Green Chemistry" covers, but it always revolves around the minimization of hazardous substances and environmental pollution. In 2006, the United States Environmental Protection Agency (EPA) formulated twelve principles for the "Green Chemistry Framework", which cover the design, distribution and use of processes and products. Great importance is placed on the early integration of safety-relevant aspects into the development of new technologies [3].

In the area of quality management, the "Quality by Design" (QbD) concept should also be mentioned. The aim is to enable more targeted defect-identification and more efficient defect-reduction by carrying out several quality tests during the product development process. It describes a systematic approach in which all critical process parameters regarding safety, efficacy and quality are recorded and controlled during production with the support of real-time measurements [4]. The concept has long been well-received in various branches of industry, such as aerospace, automotive and medical technology, as well as in the biotechnology and pharmaceutical industries [5]. A comprehensive knowledge of material properties, development and manufacturing processes is essential in order to identify and evaluate risks. The QbD concept was introduced to the pharmaceutical industry between 2009 and 2012 by means of internationally valid guidelines.

S2. Environmental impacts of the coffee capsule

A life cycle analysis (LCA) covering the entire life cycle of coffee capsules revealed that the environmental impacts depend primarily on the coffee contained and its cultivation conditions [6]. However, the LCA results, which are expressed as carbon footprint or global warming potential (GWP), are also significantly influenced by the composite materials used and their subsequent recycling and disposal options. As long as the used aluminum capsules are not collected separately and recycled, plastic capsules result in a comparably lower GWP if the polymer composite materials are thermally treated, and thus energetically recycled during waste incineration [6]. It must be stressed that polymer-based coffee capsules will be disposed as municipal solid wastes and will – in the Austrian case – end up in waste incineration plants [7].

In general, multi-layer packaging decreases the quality of recycling materials (re-granulates) and packaging made of mono-material structures would increase recyclability. It can be assumed that single-layer plastic packaging can ensure the same performance as multi-material solutions and that such mono-material structures can be recovered as recyclates without loss of efficiency. Consequently, such a single-layer material would also result in a decrease of the GWP within LCA studies, as the polymer could be re-granulated and re-processed into new food grade materials, similar to PET bottles. In summary, nanoclay-containing polymer nanocomposites would be promising mono-layer FCMs that show improved recyclability [8,9]. We therefore concluded that nanoclay- and polymer-based coffee capsules present a promising case study example to test the applicability of the SbD concept. In addition, polymer nanocomposites used as FCMs represent a challenging case study, for which comprehensive risk assessment is crucial regarding the authorization by the EFSA and respective national authorities in the European member states. If a producer intends to place montmorillonite (nanoclay) on the European market as an FCM, exposure assessments – in addition to hazard assessments (toxicity studies) – are mandatory according to REACH. Therefore, a material flow analysis was applied to predict potential exposure pathways and emission hotspots of nanoclays.

S3. Material flow analysis

The nanoclay-specific material flow analysis for the identification of exposure hotspots is based on expert knowledge and literature. The estimated nanoclay quantities for plastic coffee capsules refer to 40,397 t of coffee total market volume in Austria for 2016. Of this, "single portions" (capsules and pads) took a market share of 15% [10]. Consequently, this corresponds to an Austrian-wide total market volume of approx. 6,060 t for 2016. According to the estimation of the industry partner, capsules (excluding pads) have a market share of 85% to a maximum of 95% of the single-serving market and thus a total of approx. 5,150 and 5,760 t of coffee in the form of capsules (made of plastic and aluminum composite materials) are sold in Austria. To be able to calculate the number of coffee capsules based on the total consumption of 5,150 and 5,760 t, the coffee content itself (excluding packaging material) per unit was weighed (n = 34). Coffee capsules from different capsule suppliers, such as Tchibo, Nestlé, laCOOP, Gourmeso and others, were used. Figure S1 shows that the weighing resulted in a median value of the coffee content per capsule (excluding packaging material) of approx. 6.2 g. If the Austrian coffee consumption for capsules is now divided by the median, an Austria-wide consumption of around 842 and 941 million capsules ("MIN" and "MAX" scenario, respectively) is obtained.

In order to be able to draw conclusions about material consumption throughout Austria, the empty weight (without coffee content) of 70 plastic capsules from different manufacturers was weighed. In order to better reflect the different capsule systems and the fluctuation ranges of the empty capsule weights, the so-called 1st quartile (25%) of 6.0 g was used for the "MIN" scenario and the 3rd quartile (75%) of 7.0 g for the "MAX" scenario. This in turn results in an Austria-wide total annual consumption of approx. 942 to 2,589 t of plastic coffee capsules. A market volume of approx. 10% to a maximum of 20% is assumed for plastic coffee capsules. These considerations result in a quantitative market share of 94 t or 518 t of potentially nanomaterial-containing coffee capsules. In the present study, it was assumed that only nanoclay and no other nanomaterial is used as a food contact material, since in 2017 nanoclay was already approved as an FCM. Finally, in order to determine the MFA input of nanoclay per se, literature values regarding the weight fraction of nanoclay in coffee capsules were used. Gazsó et al. [11] summarized that about 5% by weight of nanoclay in FCM made of plastics or in coffee capsules would be sufficient to ensure an efficient gas barrier. If this weight percentage is multiplied by the lower limit of the Austrian-wide coffee capsule or packaging material consumption of approx. 94 t, this results in a nanoclay consumption of approx. 5 t nanoclay per year for the "MIN" scenario. For the "MAX" scenario, a weight share of 12% was assumed, as this corresponds to the maximum permissible share in polyolefins according to the "Union list" (Regulation (EU) No. 10/2011, Annex I, as of May 2017). This results in a theoretical nanoclay consumption of approx. 62 t per year for Austria in the "MAX" scenario.

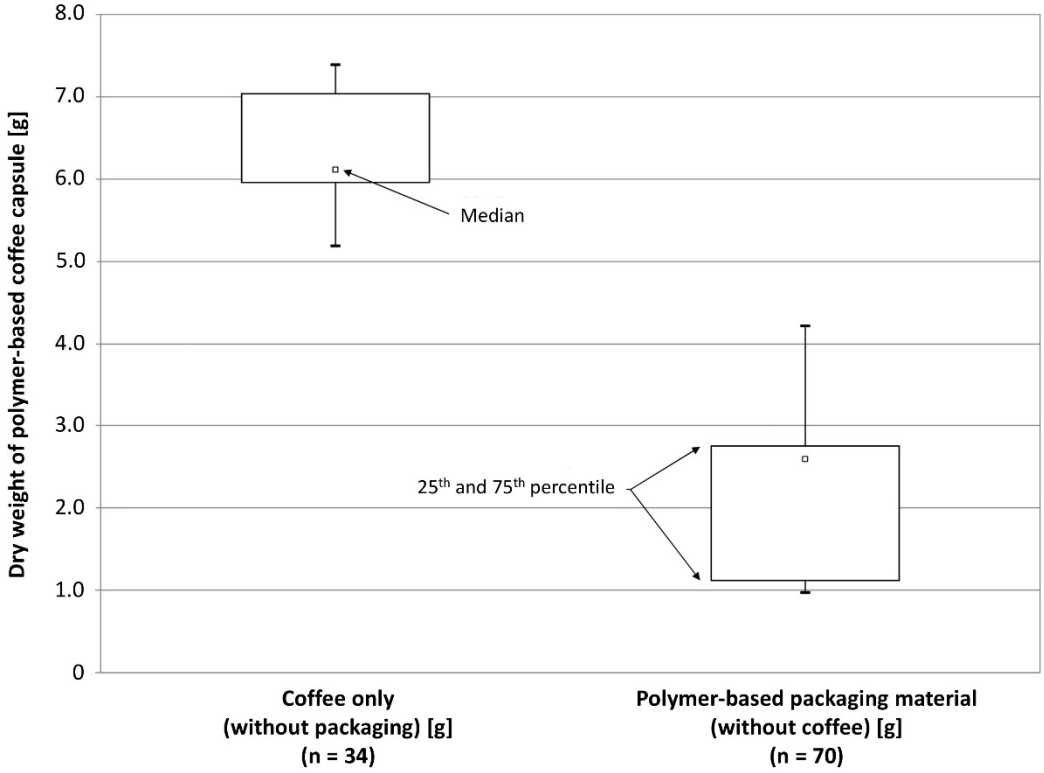

Figure S1. Boxplot diagram of the dry weights of weighed empty coffee capsules and the coffee content (n = 70 and 34 respectively). The 1st and 3rd quartile – 25% and 75% of the data values are less than or equal to these characteristic values – served as the basis for extrapolating the lower and upper limits of Austrian-wide coffee capsule consumption in tonnes per year.

S4. Guided expert interview

The following 23 questions were sent to the plastic manufacturer (compounder) in advance by email in order to be able to prepare sufficiently for the personal interview.

Concerning production:

1. *Have you already gained practical experience in processing nanoclay?*
2. *Which companies already offer nanoclays and how expensive are they? Which physicochemical parameters – in best case nanospecific – do they enclose?*
3. *What quantities are introduced into the polymer?*
4. *How difficult was it to process nanoclay during compounding and extrusion?*
5. *Do you additionally modify the nanoclays to increase dispersibility? Do you assume or know if the nanoclay platelets are exfoliated after extrusion?*
6. *Why are nanocomposites not yet state of the art for the production of gas-impermeable food packaging?*

Concerning safety and the environment:

7. *What quantities of waste are generated during production? How is this waste then disposed of?*
8. *Do you have any concerns processing nanoclays in your products?*
9. *Do you know what exactly happens to nanoclay when it is released into the environment?*
10. *What are the exclusion reasons for processing nanomaterials in your masterbatches?*
11. *Is there an increased dust load during processing of nanoclay powders? If so, what additional measures are taken to protect workers?*
12. *Are you generally sufficiently informed about the possible health effects of nanoclay and other nanomaterials?*
13. *What advantages do you see here?*
14. *What disadvantages do you see here?*
15. *What information must be passed on to the coffee capsule manufacturers? Are you directly affected by the EFSA authorization?*

Concerning SbD implementation in the company:

16. *You heard about the safe-by-design concept for the first time during this research project. Would you voluntarily apply this concept in your company?*
17. *Where do you see the biggest obstacles to actually applying the SbD concept?*
18. *Who are the so-called gatekeepers in your company?*
19. *Would you also consider other people outside your company as gatekeepers?*
20. *Would you hire an external consultant to apply the SbD concept?*
21. *Would you share important nanoformula information with external people? If not, under what conditions would you share this information?*
22. *Is this concept interesting despite not yet been standardized – e.g. at ISO or CEN level?*
23. *Do you have any suggestions for improving the implementation of the SbD concept in the future?*

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