

Properties of PBS

Food contact properties

The requirements of European regulations in the field of food safety are the following:

- Basic components of the material are to be included in the positive list
- Substances with restrictions must be controlled (specific migration in intended conditions of use must be lower than specific migration limits) either by experimental tests, or with migration modelling
- The overall migration must be less than 10mg /dm² packaging
- The contact between the packaging and the food must not cause changes in product organoleptic characteristics
- Non intended added substances must be identified and further evaluation is needed for eventual critical substances

Basic components

Succinic acid and butanediol1-4 are in the positive list identified as monomers; PBS which results from the polycondensation of both building blocks meets the polymer composition requirements of regulation EU 10/2011 on plastic materials and food contact materials.

Experimental specific migration tests

As no restricted substances were used in the formulation of PBS in the SUCCIPACK project, no specific migration test was carried out; generally PBS does not need any low molecular weight substance addition to adapt its properties which are rather adapted by strategies of polymer blending or mineral filler addition.

The virtual situation of specific migration of restricted substances was studied by the approach of migration modelling.

Modelling of specific migration

The modelling of specific migration requires the use of simple diffusion models, which takes into account (i) a Fickian diffusion in the bulk material described by a constant diffusion coefficient D (ii) a partition at packaging food interface described by a partition coefficient K. The key issue is to have the adapted mathematical tool for the prediction of D. The most often model used for the prediction of D is the Piringer model. The parameters measured **for pure PBS** in the project are shown in the table below.

τ	Ap'^*
-827	4.5

Piringer equation parameters for PBS homopolymer

In the case of **soft copolymers such as PBSA**, the Piringer equation parameters of polypropylene could be used for the migration modelling (low migrant barrier properties of copolymers).

Sensory analysis

The sensory analyses were performed according to the ISO 13302 standard and Robinson test.

According to the results of sensory analysis with water, only the IBIOPBS gives an average score different from 0. In this case, it can lead to a modification of the flavour of the water by this material because the average score is greater than 1 (average=3.8).

From the results of sensory analysis with chocolate, for all samples, no significant change in the flavour of chocolate has been noted. The average score for all materials including the IBIOPBS is between 0 and 0.2.

These results generally show the influence of the type of food in contact with the material PBS. Indeed, the modification of the flavour is more pronounced for the IBIOPBS in the case of water.

Rather than attributing the defaults to the green origin of bioPBS, the sensory effect of this material was attributed to a higher monomer / oligomer content due to a higher sensitivity to hydrolysis.

Overall migration

The determination of overall migration of PBS packaging has been mainly studied on the basis of the use of ethanol water mixture food simulants.

Indeed other attempts of overall migration testing have led to severe issues:

- Migration in olive oil: to determine the migrant mass loss of a packaging after contact with olive oil, the normalized test proposes a procedure allowing to subtract the sorption of oil in the packaging to the packaging weight variation. This procedure works for most of packaging on the market but with PBS we observed a high oil sorption in the material; moreover the extraction procedure, even by modulating the time and the solvent type for the soxhlet extraction, was not efficient: the re-extraction of absorbed oil was not complete, leading to negative overall migration values. This issue was attributed both to the high level of oil sorption, and to a possible reactivity or high oil interaction with the material;
- Extraction by isooctane: this solvent preconized as substituting medium for fatty food simulant was observed as too aggressive (partial solubilisation and physical damage of all types of packaging).

The best way to access to the migration behavior of PBS was then to study ethanol water mixtures.

- Migration increases systematically with the ethanol content, as lipophilic contact increases probably both (i) the affinity of PBS oligomers to the food simulant (partition effect), (ii) and the diffusion coefficient by a plasticization effect.
- No effect of the acidity of food simulant was observed. This can be explained by a too short contact time (10 days) to induce PBS degradation. In shelf life conditions this could be an influencing factor (catalysis of PBS degradation for long contact time)
- The sensitivity to hydrolysis has a clear incidence on overall migration: higher migration was obtained on bioPBS or on samples stored more than 1 year in ambient humidity/temperature conditions.
- PBS PLA blends shows a reduced migration. During injection, a fraction of PLA migrates at the surface; PLA confers a functional barrier effect.

- Temperature and material thickness have classical effect on migration: migration at 40°C (simulating room temperature uses) can be higher than the regulation limit for thick PBS samples; at the contrary, migration at 20°C of thin PBS films is always under the regulation limit.

NIAS Screening

The identification of the migrants from different PBS packaging material was systematically studied. This approach allowed the determination of products systematically observed in PBS materials. These substances were classified in 3 families:

- Simple degradation reactions and recombinations from PBS oligomers and or from its monomers;
- Additional mechanisms leading, from the previous compounds, to cyclic compounds;
- Additives.

All these products (aliphatic esters and ethers, and common additives) are assumed not to be critical.

At the contrary some of the other compounds observed could be of potential critical structures (to be studied by toxicological tests); but none of them are observed systematically (from one type of sample to another). This shows that none of them can be considered as a systematic NIAS of PBS. Their presence is probably due to process or environmental pollution.

As a conclusion PBS materials have **no critical NIAS**. But real commercial formulation must be controlled; to differentiate the classical and anomalous NIAS, a specific annex was produced, giving the reference mass spectra of systematic NIAS.

Complete guidelines for migration testing are proposed in deliverable D3.5.