Temperature dependency of partition coefficients $K_{P/F}$ between polymer and food

Annika Seiler, Roland Franz

Fraunhofer Institute for Process Engineering and Packaging (IVV), Giggenhauser Straße 35, 85354 Freising, Germany,
email: annika.seiler@ivv.fraunhofer.de

facet
flavourings | additives | contact materials
exposure task

Introduction

Migration of a substance from a polymer reaches at equilibrium a thermodynamic controlled upper limit that is quantifiable by the partition coefficient $K_{P/F}$ between polymer (P) and food (F). This ratio depends on the migrants solubility in both phases (food and polymer) and is largely influenced by the food properties (Figure 1)[1],[2]. Since migration modeling must enable prediction of migrant concentrations for any time-temperature condition of a packed food knowledge of the temperature influence on $K_{P/F}$ as a key parameter of the migration model is essential.

Method

Within the FACET project a convenient method for the determination of partition coefficients $K_{P/F}$ for migrants between polymer was developed. This method was used within FACET to perform a systematic study to investigate the temperature effect on $K_{P/F}$ between LDPE and various model foods for 17 selected model migrants. In this study contact temperatures in the range from 5°C up to 60°C were applied being aware that in a number of cases the higher temperature would not be applicable to the packed foods in the real market situation.

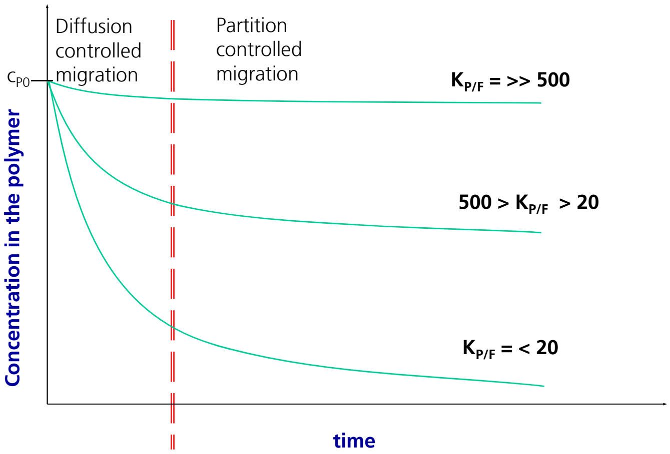

Figure 1: Influence of food properties on the partition coefficient

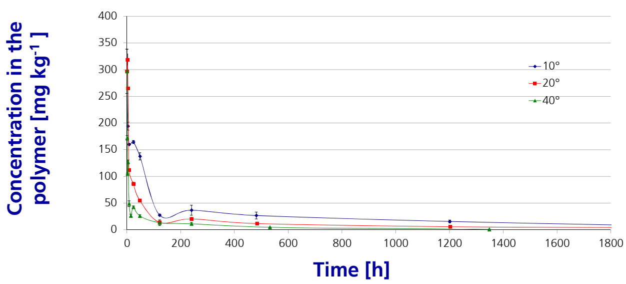

Figure 2: Migration of styrene from LDPE into soft cheese at different temperatures

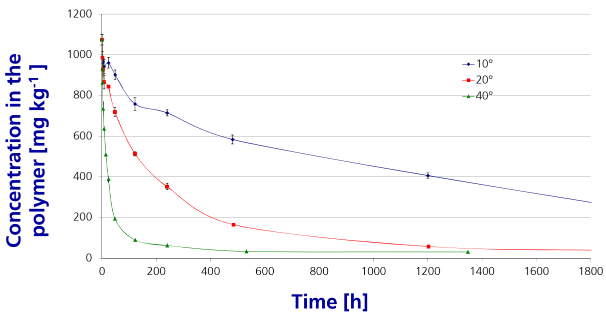

Figure 3: Migration of ATBC from LDPE into soft cheese at different temperatures

Results

As shown in Figure 2 and 3, for small migrants as styrene equilibrium is reached after few hours also at lower temperatures. In contrast, to reach equilibrium for bigger molecules e.g. as ATBC, needs up to several days at lower temperatures. However from the obtained results no significant temperature dependency of $K_{P/F}$ was observed.

Only in cases where the physical food characteristics changes e.g. oiling-off, for instance dough, or when melting as in the case of chocolate a clear temperature dependency can be observed (Figure 4 and 5).

In case of chocolate, the temperature dependency is based on the different diffusion properties of the chocolate at 20 °C where chocolate is solid and at 40 °C and 60 °C where chocolate is viscose. We assume that in all cases the partition comes down to the same level but at 20 °C equilibrium will be reached after several years. Therefore, the higher values were used to reach the equilibrium at appropriate times.

In conclusion, the large temperature independency of $K_{P/F}$ facilitates further correlations such as described in the poster "Seiler et al. Correlation of the solubility behavior for migrants of foods with ethanol-water mixtures and via log $K_{P/F}$ versus log $P_{O/W}$ relationships" where through a correlation of log $P_{O/W}$ with log $K_{P/F}$ solubility based assignments of foods to ethanol-in-water concentrations are made. In this way migration modeling can be simplified.

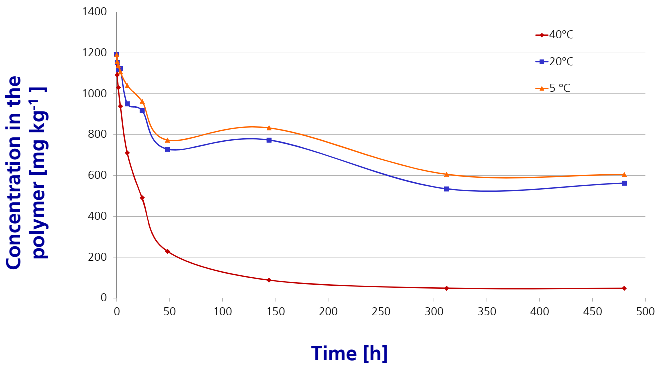

Figure 4: Migration of Irganox 1076 from LDPE into dough at different temperatures

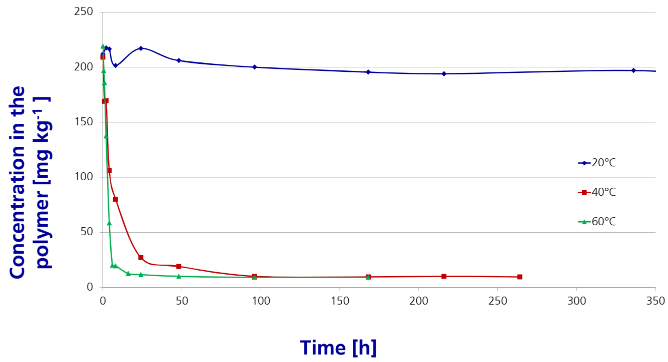

Figure 5: Migration of Chimasorb 81 from LDPE into chocolate at different temperatures

Reference

[1] FOODMIGROSURE project, contract number QLK-CT2002-2390

[2] Brandsch, J. et al. Migration modeling as a tool for quality assurance of food packaging, Food Addit Contam. 2002;19 Suppl:29-41

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