molecules

Supplementary data

Impact of partitioning in short-term food contact applications focused on polymers in support of migration modelling and exposure risk assessment

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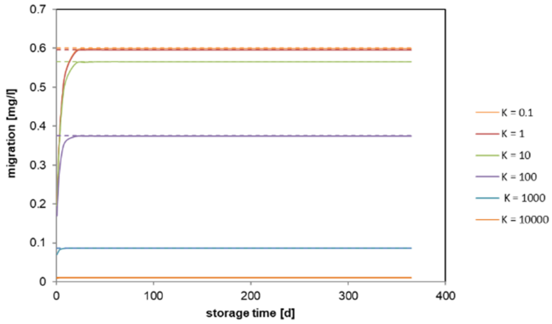
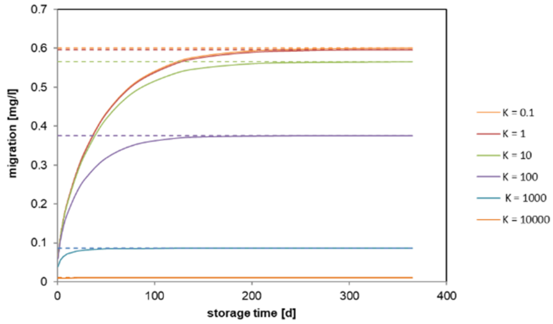
1. Generic Diffusion Coefficient Approach

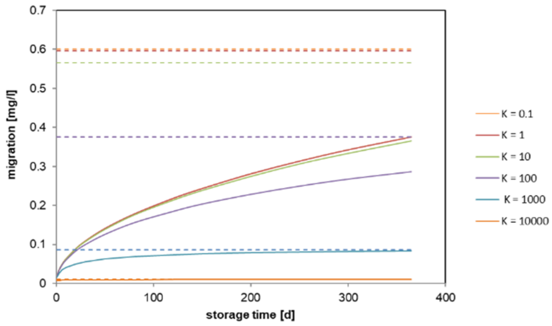
Figure S1 to Figure S3 shows the predicted migration in dependence of diffusion coefficients D_P ranging from 10^{-10} cm²/s to 10^{-15} cm²/s and partition coefficients ranges $K_{P,F}$ = 0.1 to 10000 for several thicknesses of the packaging material (100 µm, 200 µm and 1000 µm) with an initial concentration $c_{P,0}$ = 100 mg/kg in the material. The surface volume ratio was set V = 1000 ml and A = 600 cm².



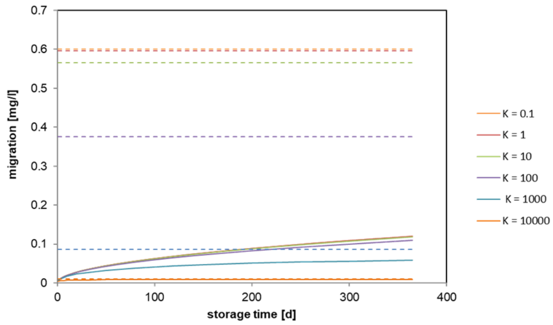
(**a**)



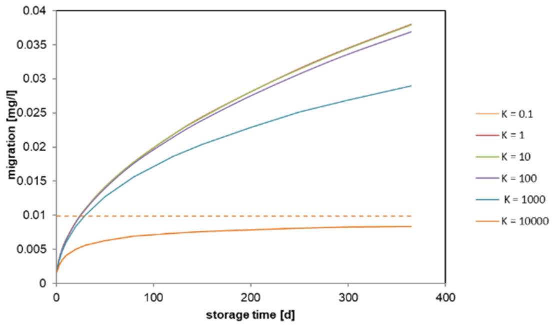
(**b**)



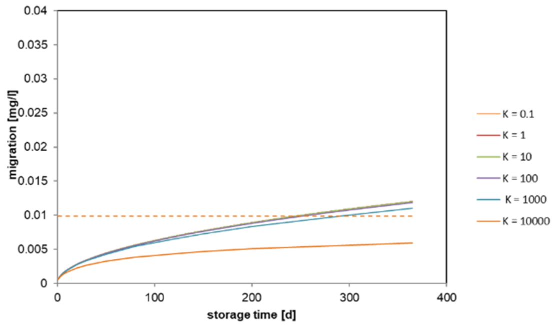
(**c**)



(**d**)

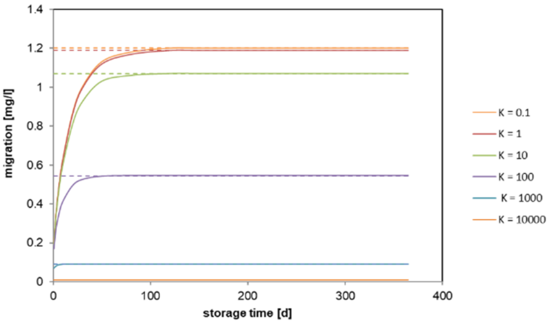


(**e**)

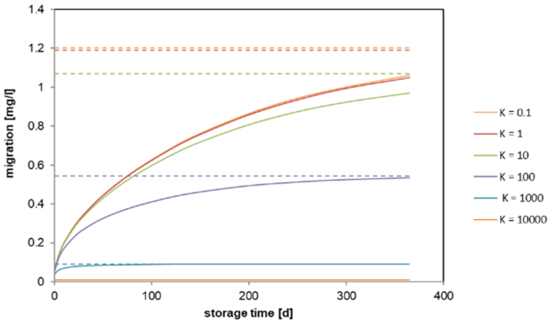


(**f**)

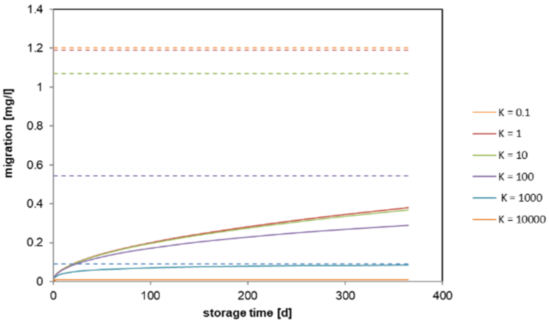
Figure S1. Calculated migration into food considering different partition coefficients: (a) diffusion coefficient DP = 1 × 10^{-10} cm^2/s, (b) DP = 1 × 10^{-11} cm^2/s, (c) DP = 1 × 10^{-12} cm^2/s, (d) DP = 1 × 10^{-13} cm^2/s, (e) DP = 1 × 10^{-14} cm^2/s and (f) DP = 1 × 10^{-15} cm^2/s. Calculated for a layer thickness of d = 100 μm, cP,0 = 100 mg/kg, V = 1000 mL, A = 600 cm^2. Note: (e) and (f) different scale on y-axis.



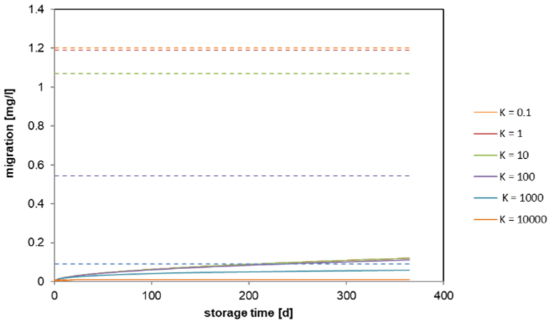
(**a**)



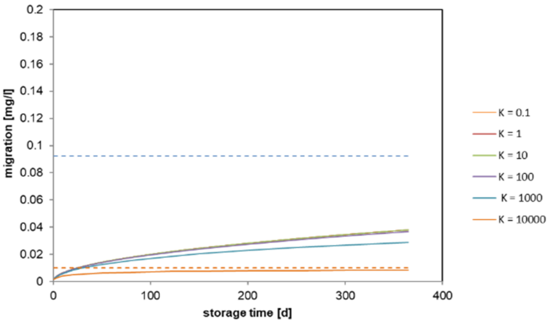
(**b**)



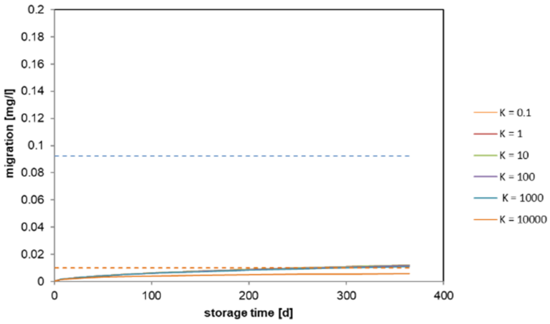
(**c**)



(**d**)



(**e**)



(**f**)

Figure S2. Calculated migration into food considering different partition coefficients: (a) diffusion coefficient DP = 1 × 10^{-10} cm^2/s, (b) DP = 1 × 10^{-11} cm^2/s, (c) DP = 1 × 10^{-12} cm^2/s, (d) DP = 1 × 10^{-13} cm^2/s, (e) DP = 1 × 10^{-14} cm^2/s and (f) DP = 1 × 10^{-15} cm^2/s. Calculated for a layer thickness of d = 200 μm, cP,0 = 100 mg/kg, V = 1000 mL, A = 600 cm^2. Note: (e) and (f) different scale on y-axis.

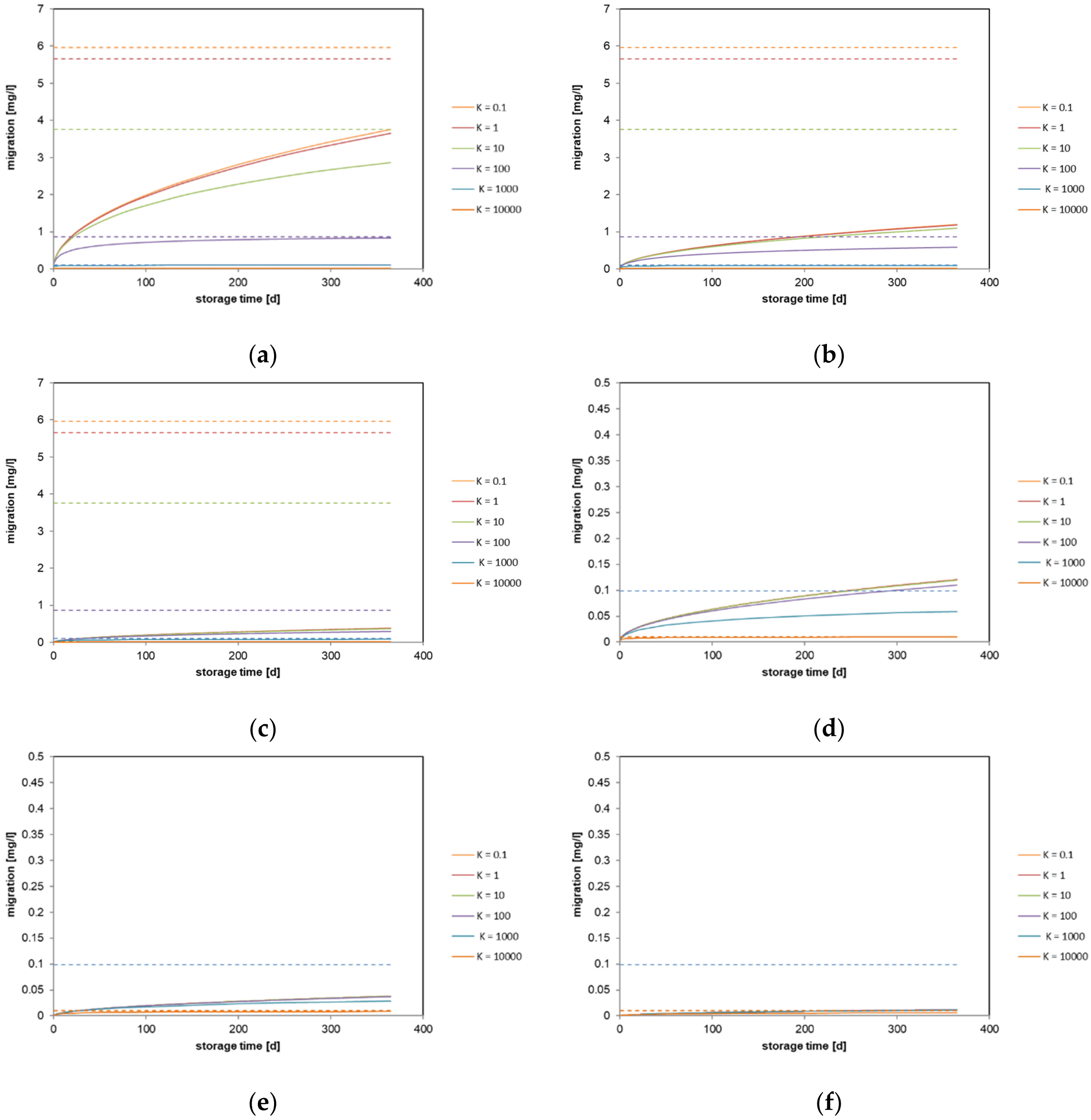


Figure S3. Calculated migration into food considering different partition coefficients: (a) diffusion coefficient DP = 1×10^{-10} cm^2/s, (b) DP = 1×10^{-11} cm^2/s, (c) DP = 1×10^{-12} cm^2/s, (d) DP = 1×10^{-13} cm^2/s, (e) DP = 1×10^{-14} cm^2/s and (f) DP = 1×10^{-15} cm^2/s. Calculated for a layer thickness of d = 1000 μm, cP,0 = 100 mg/kg, V = 1000 mL, A = 600 cm^2. Note: (e) and (f) different scale on y-axis.