# Diffusion behaviour of the acetaldehyde scavenger 2-aminobenzamide in polyethylene terephthalate for beverage bottles

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## Introduction

Polyethylene terephthalate (PET) is widely used as packaging material for natural mineral water bottles. However, trace levels of acetaldehyde, a PET related substance, can migrate into the water during the shelf life time and might influence the taste of the PET bottled water. 2-Aminobenzamide is typically used during PET bottle production as a scavenging agent for acetaldehyde.
The aim of this study was the determination of the migration kinetics of 2-aminobenzamide into natural mineral water as well as into 20% ethanol. From the migration kinetics, the diffusion coefficients of 2-aminobenzamide in PET should be derived.

## Method

PET bottles were spiked with 2-aminobenzamide in a concentration of 198±3 mg/kg. The doped PET bottles were filled with carbonated mineral water and 20% ethanol. Subsequently the bottles were stored at 23 °C and 40 °C, respectively. In regular terms up to 60 d (23 °C) and 40 d (40 °C) three bottles of each kinetic point were drawn. After storage aliquots of the carbonated mineral water were analysed towards their 2-aminobenzamide concentration by use of HPLC/MS. Column: Synergi polar RP 150x3 mm. Eluent A: 0.5% Formic acid (aqueous), Eluent B: Methanol, flow: 0.6 ml/min. Injection volume: 5 µl, column oven temperature: 45 °C. Ion source APCI positive, SRM, parent ion 137 Dalton, daughter ion 120 Dalton.

## Results

The experimental kinetic migration data show a linear correlation between the migration and the square root of time, which is expected from diffusion theory (Figure 1). Therefore, it can be concluded that the migration of 2-aminobenzamide follows Fickian laws of diffusion in the performed experiments. From the migration kinetics, the diffusion coefficients of 2-aminobenzamide in PET at 23 °C and 40 °C were determined to be 4.2 $10^{-16}$ $cm^2/s$ and 4.2 $10^{-15}$ $cm^2/s$, respectively. The diffusion coefficient for 20% ethanol at 40 °C was determined to be 7.7 $10^{-15}$ $cm^2/s$, which indicates that 20% ethanol is causing some swelling of the PET polymer at 40 °C (Figure 1). From a comparison of migration values between 23 °C and 40 °C, acceleration factors of 9.7 for water as contact medium and 18.1 for 20% ethanol as simulant can be derived for definition of appropriate accelerated test conditions at 40 °C corresponding to storage at 23 °C. The European Union regulatory acceleration testing based on 80 kJ/mol as conservative activation energy overestimates the experimentally determined acceleration rates by only a factor of 1.6 and 3.1, respectively.

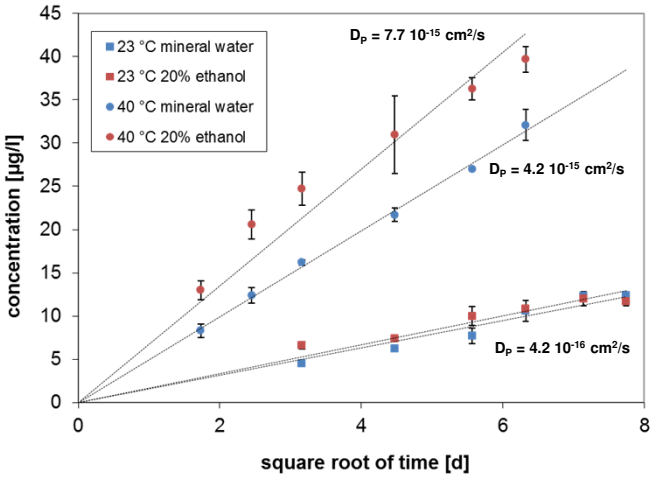


**Figure 1: Migration kinetic of 2-aminobenzamide in mineral water and 20% ethanol at 23 °C and 40 °C (bottle wall concentration 198 ±3 mg/kg)**

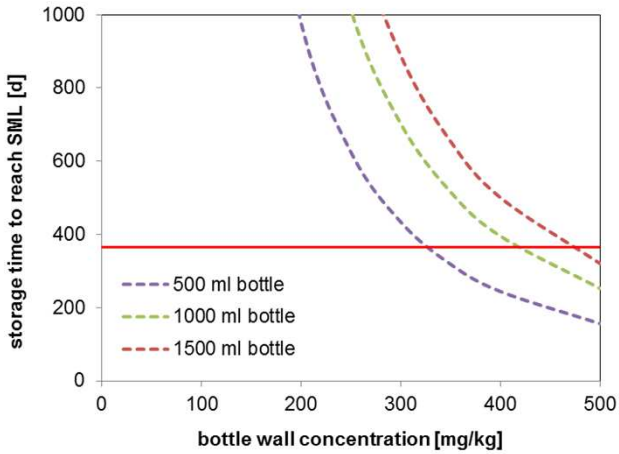


**Figure 2: Storage time to reach the SML at 23 °C as a function of the 2-aminobenzamide bottle wall concentration (calculated with $D_P$ = 4.2 $10^{-16}$ $cm^2/s$, partition coefficient K = 1, bottle wall thickness l = 300 µm), red line 365 d.**

The determined diffusion coefficients can be used for the prediction of the migration of 2-aminobenzamide in water and EU food simulant C as well as for foods which do not cause swelling effects in the PET polymer. The predicted migration into mineral water at 23 °C into 500 ml, 1000 ml and 1500 ml bottles is shown in Figure 2. From such correlations the maximum bottle wall concentration for 2-aminobenzamide for a given storage time (e.g. 365 d) can be derived. For example, the specific migration limit (SML) of 2-aminobenzamide of 50 µg/l in a 500 ml PET bottle at 23 °C with a bottle wall concentration of 200 mg/kg is reached after 975 d of storage. Under the same conditions the SML is reached after 165 d if the bottle wall concentration is 500 mg/kg. The bottle wall concentration can be therefore used as routine control parameter during PET bottle manufacturing.

## Conclusions

The experimentally derived diffusion coefficients obtained with water can be used to calculate migration of 2-aminobenzamide into PET-bottled water under any realistic long-term storage conditions. Therefore a fast and economic way of compliance testing can be performed based on (i) measurement of the free 2-aminobenzamide concentration in the bottle wall and (ii) calculation of the migration for room temperature (or similar) for any long-term storage. In this way, the bottle wall concentration of 2-aminobenzamide can be taken as an easily measurable compliance check parameter against the EU legal SML value of 50 µg/l for 2-aminoanthranilamide.

## Acknowledgements

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## References

[1] R. Franz, M. Gmeiner, A. Gruner, D. Kemmer, F. Welle. Diffusion behaviour of the acetaldehyde scavenger 2-aminobenzamide in polyethylene terephthalate for beverage bottles. Food Additives and Contaminants 2016, 33(2), 364-372.

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