

Recommendation

Guideline for the Mathematical Estimate of the Migration of Individual Substances from Organic Material in Drinking Water (Modelling Guideline)¹

Last Update: 7 October 2008

Federal Environment Agency (UBA)

¹ The obligations under Directive 98/34/EC of the European Parliament and of the Council of 22 June 1998 laying down a procedure for the provision of information in the field of technical standards and regulations (OJ L 204 21.7.1998, p. 37), last amended by Directive 2006/96/EC of 20 November 2006 (OJ L 363 20.12.2006, p. 81) are observed.

1 Introduction

The mathematical estimate of migration can be used in place of experimental proof to verify the requirements of KTW, Coating or Lubricant Guidelines for the migration of individual substances.

Organic material, such as plastics, which comes into contact with drinking water, can release substances into the water (mass transfer or migration). This lowers the concentration of substances in the organic material and increases it in water (mass transport). The stage that determines the speed of the mass transfer is the diffusion of the substance in organic material. The transfer of substances from organic material in drinking water can be measured in a laboratory (performance of the migration test and analysis of the test water on formulation-specific individual substances with a migration restriction) under standard conditions (surface-volume ratio, number of change cycles, time, temperature) or can be calculated by simulation using diffusion models (modelling). Annex 1 illustrates the involvement of simulation in assessing organic material in contact with drinking water.

2 Special features of the model

The assessment of material in contact with foodstuffs and drinking water requires a high degree of hygienic safety. As a result, the simulation of a model requires that a direct comparison with migration values defined by testing automatically provide higher migration values (overestimate).

This objective is relatively simple to implement for the direct contact of organic material with foodstuffs, since only one migration cycle is calculated. Material constants are used to simulate migration, which on the one hand result in an accelerated mass transport in the calculation (higher diffusion coefficients) and on the other hand allow a higher transition in the foodstuffs on balance (degraded distribution coefficients).

In contrast, several migration cycles must be defined for the assessment of organic materials, which come into contact with drinking water. This takes into account the exchange of the drinking water in pipes or the installation. In the guidelines of the Federal Environment Agency the assessment is based on the 3rd test period for the cold water test and the 7th test period for the warm and hot water test. An overestimate of the calculation for the first test period can result in an underestimate of the calculation for the last test period when comparing directly with the real migration behaviour.

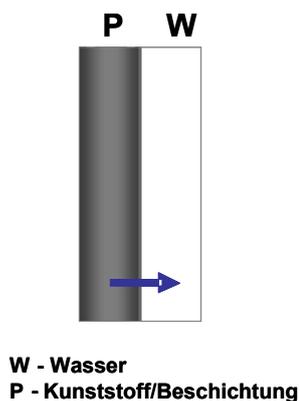
On closer inspection this underestimate can only occur, if a considerable overestimate is made and if in the first 24-hour stagnation period (pre-treatment of the test object in the migration test) more than 20% at 23°C or more than 10% at 60°C and 85°C of the material contained in the organic material is released into the drinking water. These scenarios are easy to identify from the simulation. When assessing the mass transfer, the first simulated test period should be taken into account.

Annex 2 contains examples of the mathematical estimate for the migration of an additive. In these examples, the calculated migration is compared if the requirements of Directive 2002/72/EC or the coefficients calculated specifically for drinking water are taken into account.

3 Model assumptions

The mass transfer (migration) from organic materials in drinking water is restricted by the mass transport in the organic material. The mass transport and thus the mass transfer can be estimated using Fick's Second Law (differential mass balance).

Modelling Guideline



$$\frac{\partial c}{\partial t} = D \cdot \frac{\partial^2 c}{\partial x^2}$$

c - Konzentration
t - Zeit
x - Abstand
D - Diffusionskoeffizient

Figure 1 Diffusion model and differential mass balance

Wasser	Water
Kunststoff/Beschichtung	Plastic/coating
Konzentration	Concentration
Zeit	Time
Abstand	Distance
Diffusionskoeffizient	Diffusion coefficient

The following assumptions are made for the model:

- Mass transfer is restricted by the mass transport (diffusion) in the organic material
- No chemical reactions occur (no hydrolysis of the migrants, no formation of migrants in the material)
- Uniform distribution of the migrating substance in water
- The material or the layers in the material lie parallel to one another (one-dimensional problem)
- The necessary material constants and parameters can be found in Annex 1 of the Practical Guide [3].

The following starting and boundary conditions are assumed:

- Before the start of the first migration cycle, the migrating substance is distributed uniformly in the polymer $c_{p,0}$.
- The equilibrium described with the distribution coefficients (see below) is reached automatically at the interfaces of the various layers or at the boundary layer between the water and the polymer.

A distinction must be made between monolayer and multilayer materials. If an organic material (consisting of a polymer) comes into direct contact with drinking water, this describes the system of two material constants, the diffusion coefficients of the migrant in the organic material and the distribution coefficient of the migrant between the organic material and the drinking water.

If an organic multilayer material with n layers comes into direct contact with drinking water, this describes the system of multiple material constants. These are n diffusion coefficients of the migrant in the n layers of the material and the n distribution coefficients of the migrant between the adjacent layers of the material or the contact layer and the drinking water.

The solution of the differential mass balance contains variables, which are necessary to calculate the migration of the substance in the water:

- The geometric variables (layer thickness, contact surface, volume) as well as time and temperature are chosen according to the experimental method in the guideline. This allows a direct comparison of the calculated and the tested migration values. The

Modelling Guideline

geometric variables for the test object and the conditions for the migration test are known.

- The initial concentration of the individual substance $c_{P,0}$ in the organic material must be known (e.g. for polymers the residual monomer content, additive content, etc.) or must be determined analytically. Standard test methods are normally available for this. Assuming that the migrant does not change during the manufacture and treatment process, the required quantity of the formulation, e.g. for an additive, can also be used.
- Modelling requires the diffusion coefficient and the distribution coefficient. In general, however, these material constants are not known and so have to be estimated using scientifically recognised methods.

4 Estimate of material constants

4.1 Diffusion coefficient

The diffusion coefficient is a time-based variable, which expresses how quickly the substance is transported in the organic material and how quickly it is released into the drinking water. The dependence of the diffusion coefficient on temperature can be expressed as follows:

$$D = D_0 \cdot e^{\frac{-E_A}{RT}}$$

D_0 - Präexponentielle Faktor

E_A - Aktivierungsenergie [J]

R - Gaskonstante [8,314 J/molK]

T - Temperatur [K]

Figure 2 Mathematical expression of the diffusion coefficient according to Arrhenius

Präexponentieller Faktor	Pre-exponential factor
Aktivierungsenergie [J]	Activation energy [J]
Gaskonstante [8,314 J/molK]	Gas constant [8,314 J/molK]
Temperatur [K]	Temperature [K]

4.2 Distribution coefficient

The distribution coefficient $K_{P,W}$ is a thermodynamic equilibrium variable, which expresses the maximum material concentration that is released in drinking water when the system reaches equilibrium. It is calculated from the ratio of the concentration of the material in polymer $c_{P,\infty}$ and the concentration of the material in water $c_{W,\infty}$.

$$K_{P,W} = \frac{c_{P,\infty}}{c_{W,\infty}}$$

c - Konzentration

P - Kunststoff

W - Wasser

Figure 3 Mathematical expression of the distribution coefficient

Konzentration	Concentration
Kunststoff	Plastic
Wasser	Water

Diffusion coefficients can be estimated using the following validated methods [1]:

Modelling Guideline

- (a) Arrhenius $D_P = f(D_0, E_A, T)$
 (b) Piringer (A_P values) $D_P = f(A_P', \tau, M_r, T)$

D_P - Diffusionskoeffizienten
 D_0 - preexponentieller Faktor (Arrhenius)
 E_A - Aktivierungsenergie Arrhenius
 T - Temperatur [K]
 A_P' - polymerspezifische Materialkonstante (Piringer)
 τ - polymerspezifische Temperaturkonstante (Piringer)
 M_r - relatives Molekulargewicht

Diffusionskoeffizienten	Diffusion coefficients
preexponentieller Faktor (Arrhenius)	Pre-exponential factor (Arrhenius)
Aktivierungsenergie (Arrhenius)	Activation energy (Arrhenius)
Temperatur [K]	Temperature [K]
polymerspezifische Materialkonstante (Piringer)	Polymer-specific material constants (Piringer)
polymerspezifische Temperaturkonstante (Piringer)	Polymer-specific temperature constants (Piringer)
relatives Molekulargewicht	Relative molecular weight

There is no validated method for estimating distribution coefficients. However, it is still possible to estimate a distribution coefficient based on solubility in water:

- (1) Solubility S_w $K_{P,W} = f(S_w)$
 (2) "worst case" $K_{P,W} = 1$

If the solubility of the substance is not known, the "worst case" distribution coefficient $K_{P,W} = 1$ must be used.

If the substance is insoluble, the distribution coefficient $K_{P,W} = 1000$ can be used.

4.3 Validation of estimated material constants

Validated A_P' values and tau values for the most common plastics are already listed in Annex 1 of the Practical Guide [3] and can be applied when simulating migration from organic materials in direct contact with drinking water.

A subgroup of KTW-AG (see Annex 3) is to publish recommendations concerning the validation of material constants for polymers, which are so far not listed in Annex 1 of the Practical Guide.

The material constant A_P' for polymers specific to drinking water can be found in Annex 5.

5 Modelling results

Several software solutions are available commercially for the application of modelling.

In place of an analysis report with test results in accordance with KTW guideline Annex 1, a corresponding report must be prepared, which contains the entered data and the simulated concentrations of the test water for the individual migration periods.

These are compared with the maximum permissible migration rates $M_{\text{Individual substance, max}}$ in accordance with 4.2 of the KTW guideline.

6 Validation of the diffusion model

A model can be classed as validated if it reflects the real system with sufficient accuracy. Diffusion models are best validated by a direct comparison between the time-dependent migration values determined in the tests and the migration values simulated under identical boundary conditions. This is described in detail in Annex B of Annex 1 of the Practical Guide [3].

7 Validation of the software used

Assuming that an organic material consists of a single layer (monolayer), that drinking water has a limited volume and that migration follows Fick's Second Law, there is a range of analytical solutions that can be used to calculate the temporal course of migration from the organic material into drinking water for the differential equation in Figure 1. One of these solutions [3] was used to calculate migrations from polymer commodities in Annex 1 of the Practical Guide under EU Directive 2002/72/EC.

If an organic material consists of several layers (multilayer), the differential equation can be solved numerically [4] Chapter 7-9, [5]. A numerical method is a (relatively complex) algorithm developed by an expert, which solves, e.g. the equation for a multilayer organic material in contact with a limited liquid substance. During this process, each layer is divided into a number of points as in a network. A suitable numerical method can calculate the time-dependent migration in drinking water or the concentration profile of the migrant in organic material or in drinking water.

In principle, there is no difference between the results of an analytical solution or a numerical solution of the equation in Figure 1. However, an analytical formula such as the formula given in the aforementioned Annex 1 of the Practical Guide is much easier for users to understand and apply than a numerical method developed by an expert. The latter is thus presented as a "closed" algorithm in which the users are unable to directly follow the calculations. This naturally raises the question of how users can be sure that this type of "closed" algorithm delivers the correct results.

The accuracy of the migration calculations for a numerical method can in some cases be proven directly, but can also be checked indirectly based on certain criteria:

- 1) If a calculation of the migration is possible using an analytical formula, these results must be compared with the results achieved with the numerical method being verified. This must be carried out for non-stationary time-dependent migration as well as for equilibrium in the organic material drinking water system.
- 2) The results calculated using a numerical method must accurately reflect the input conditions and parameters at any point during the migration, e.g. concentration flows at the interfaces between the individual layers of the organic material or at the interface surface between the organic material and the drinking water.
- 3) The total quantity of the tested substance in the organic material drinking water system must remain the same at any point during the numerical calculation (mass preservation in the system).

Annex 4 details an example for validation using these criteria.

References:

- [1] T. Begley, L. Castle, A. Feigenbaum, R. Franz, K. Hinrichs, T. Lickley, P. Mercea, M. Milana, A. O'Brien, S. Rebre, R. Rijk, O. Piringier; "Evaluation of migration models that might be used in support of regulations for food-contact plastics."; Food Additives and Contaminants, January 2005; 22(1): 73-90
- [2] Crank, J. *Mathematics of Diffusion*, 2nd Edition, 1975, Clarendon Press, Oxford University Press.
- [3] *Withdrawn by the EU Commission: Practical Guide of the EU Commission in Annex 1, Mathematical Models*, download available from

Modelling Guideline

http://crl-fcm.jrc.it/files/PRACTICAL%20GUIDE%20_2003.04.15__annex%201%20modelling.pdf

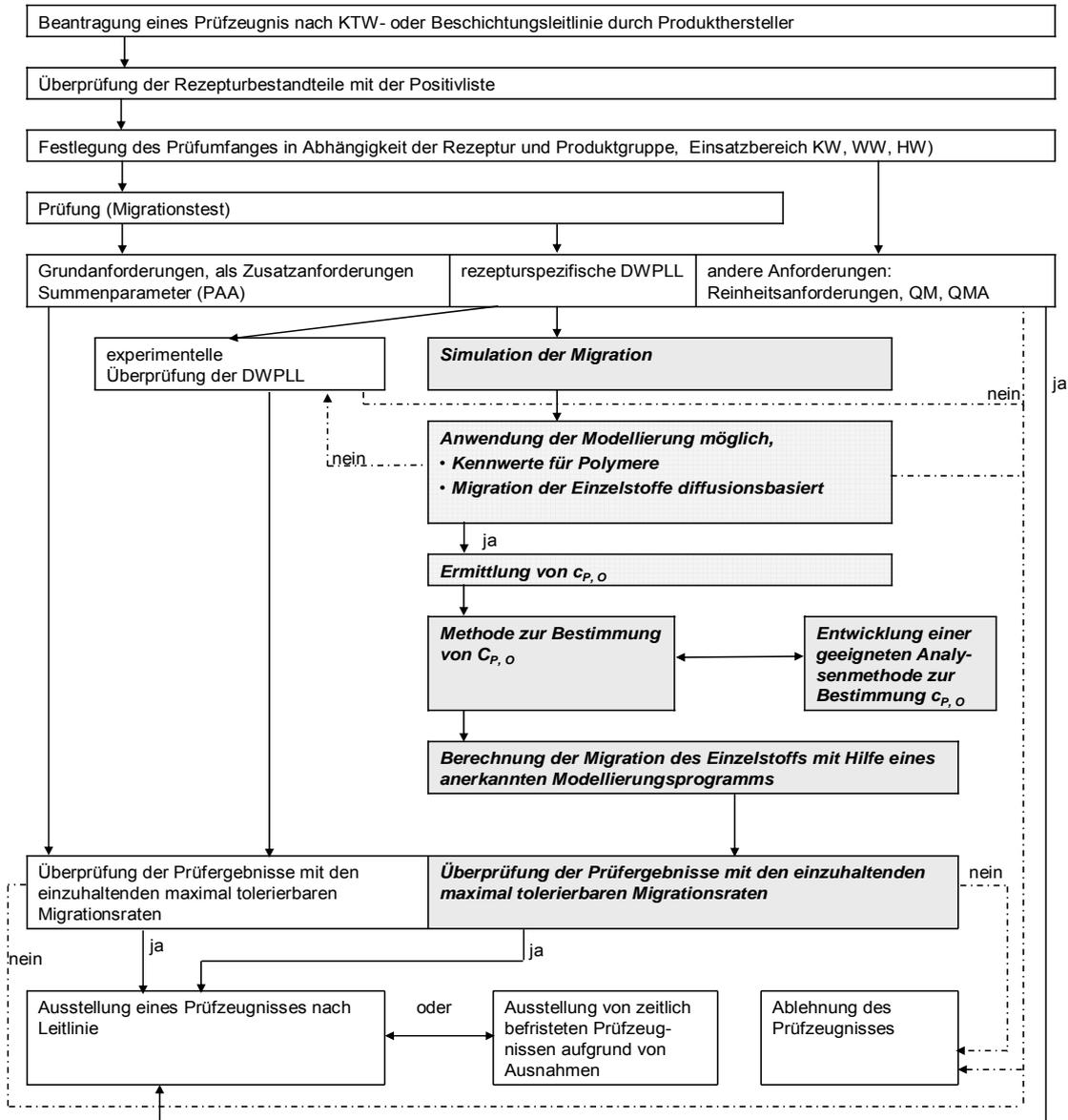
In future: C. Simoneau, ed., "Estimation of specific migration by generally recognised diffusion models in support of EU Directive 2002/72/EC", JRC Scientific and Technical Reports, 2008

[4] Piringer, O.G, and Baner, A.B., *Plastic Packaging. Interactions with Food and Pharmaceuticals*, 2nd Edition, 2008, WILEY-VCH Verlag GmbH & Co.KgaA.

[5] B. RODUIT, C.H. BERGEAT, S. CAVIN, C. FRAGNIERE, & V. DUDLER, " Application of Finite Element Analysis (FEA) for the simulation of release of additives from multilayer polymeric packaging structures.", *Food Additives and Contaminants*, October 2005; 22(10): 945–955

[6] JRC Scientific and technical Reports, 2008, "Technical guidance document to determine diffusion coefficients of migrants to update the A_p value of a food contact plastic for migration evaluation by mathematical modelling"

Annex 1: Flow sheet for the use of modelling to obtain a test certificate in accordance with KTW, coating or lubricant guidelines



Modelling Guideline

Beantragung eines Prüfzeugnis nach KTW- oder Beschichtungsleitlinie durch Produkthersteller	Application for a test certificate in accordance with KTW or coating guidelines by the product manufacturer
Überprüfung der Rezepturbestandteile mit der Positivliste	Verification of formulation components with the white list
Festlegung des Prüfumfanges in Abhängigkeit der Rezeptur und Produktgruppe, Einsatzbereich KW, WW, HW)	Definition of the scope of testing depending on the formulation and product group, application KW, WW, HW
Prüfung (Migrationstest)	Migration test
Grundanforderungen, als Zusatzanforderungen Summenparameter (PAA)	Basic requirements, as additional requirements sum parameters (PAA)
rezepturspezifische DWPLL	Formulation-specific DWPLL
andere Anforderungen: Reinheitsanforderungen, QM, QMA	Other requirements: Purity requirements, QM, QMA
experimentelle Überprüfung der DWPLL	Examination of DWPLL
Simulation der Migration	Simulation of the migration
nein	No
ja	Yes
Anwendung der Modellierung möglich,	Application of modelling possible,
<ul style="list-style-type: none"> • Kennwerte für Polymere • Migration der Einzelstoffe diffusionsbasiert 	<ul style="list-style-type: none"> • Parameters for polymers • Migration of individual substances based on diffusion
Ermittlung von $c_{p,o}$	Determination of $c_{p,o}$
Methode zur Bestimmung von $C_{p,o}$	Method for determining $C_{p,o}$
Entwicklung einer geeigneten Analy-senmethode zur Bestimmung $c_{p,o}$	Development of a suitable testing method for determining $c_{p,o}$
Berechnung der Migration des Einzelstoffs mit Hilfe eines anerkannten Modellierungsprogramms	Calculation of the migration of the individual substance using a recognised modelling programme
Überprüfung der Prüfergebnisse mit den einzuhaltenden maximal tolerierbaren Migrationsraten	Verification of test results with the maximum permissible migration rates
Überprüfung der Prüfergebnisse mit den einzuhaltenden maximal tolerierbaren Migrationsraten	Verification of test results with the maximum permissible migration rates
Ausstellung eines Prüfzeugnisses nach Leitlinie	Issue of a test certificate in accordance with the guideline
oder	or
Ausstellung von zeitlich befristeten Prüfzeug-nissen aufgrund von Ausnahmen	Issue of time-restricted test certificates based on exceptions
Ablehnung des Prüfzeugnisses	Rejection of the test certificate

Annex 2: Examples for the mathematical estimate of the migration of an additive

In the following examples a polyethylene pipe of density 0.95 g/cm³, wall thickness 5 mm, internal diameter 40 mm is chosen with a typical stabiliser PM REF No. 59120 and a molecular weight M=637. The SML value of the tested substance is 45 mg/l (pap).

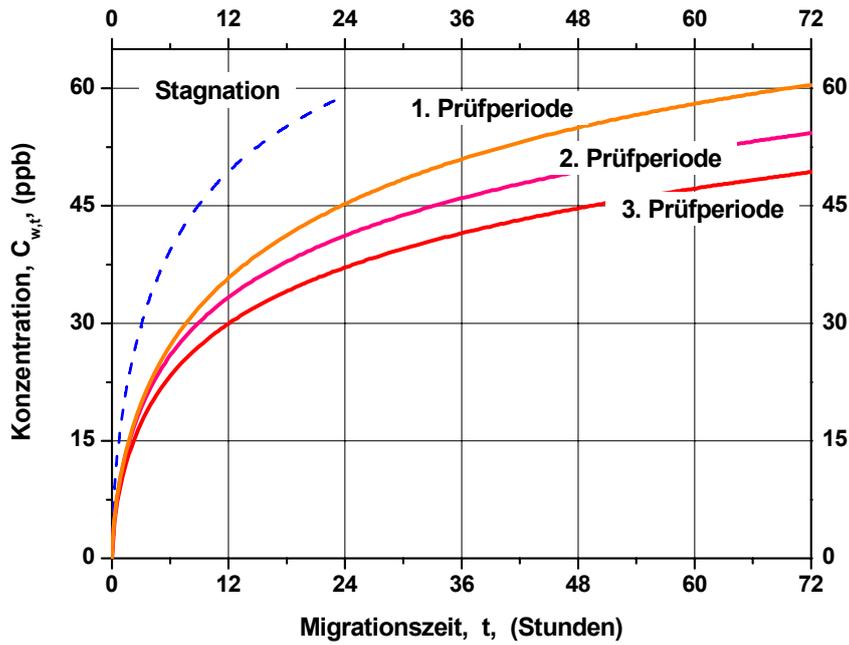
Migrant: $c_{p,o} = 100$ ppm
 Contact medium: Drinking water, density = 1.0 g/cm³
 Migration conditions: 24 hour stagnation at T = 23°C (pre-treatment)
 1st test period, 72 hours at T = 23 °C
 2nd test period, 72 hours at T = 23 °C
 3rd test period, 72 hours at T = 23 °C

Example 1. Cold water test with material constants in accordance with [3]

Diffusion coefficient: $D_{\text{polymer}} \sim 1.8 \times 10^{-11} \text{ cm}^2/\text{s}$, ($A'_p = 14.5$ and $\tau = 1577$)
 $D_{\text{water}} \sim 1 \times 10^{-4} \text{ cm}^2/\text{s}$

Distribution coefficient: $K_{p/w} = 1000$ (not soluble)

Modelling Guideline



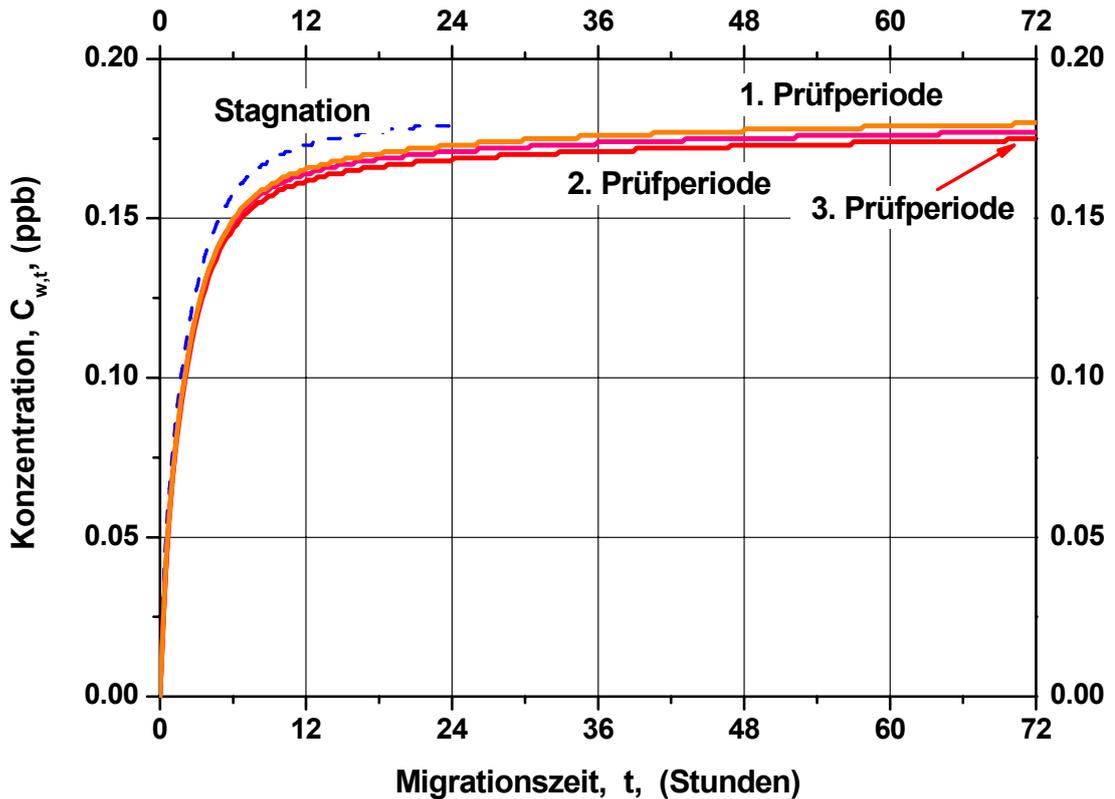
Konzentration, $C_{w,t}$, (ppb)	Concentration, $C_{w,t}$, (ppb)
Stagnation	Stagnation
Prüfperiode	Test period
Migrationszeit, t, (Stunden)	Migration time, t, (hours)

The mass balance requires that 99.6% of the migrant is still preserved in the polymer at the end of the 3rd test period. This prevents the calculated concentrations of the 3rd test period from being underestimated.

**Example 2.
testing**

Cold water test with material constants determined by

Diffusion coefficient: $D_{\text{polymer}} \sim 5.6 \times 10^{-15} \text{cm}^2/\text{s}$, ($A'_p = 6.5$ and $\tau = 1600$, determined by testing)
 $D_{\text{water}} \sim 1 \times 10^{-4} \text{cm}^2/\text{s}$
 Distribution coefficient: $K_{p/w} = 500,000$ (not soluble, determined by testing)



Konzentration, $C_{w,t}$, (ppb)	Concentration, $C_{w,t}$, (ppb)
Stagnation	Stagnation
Prüfperiode	Test period
Migrationszeit, t , (Stunden)	Migration time, t , (hours)

The mass balance requires that 99.998% of the migrant is still preserved in the polymer at the end of the 3rd test period. This prevents the calculated concentrations of the 3rd test period from being underestimated.

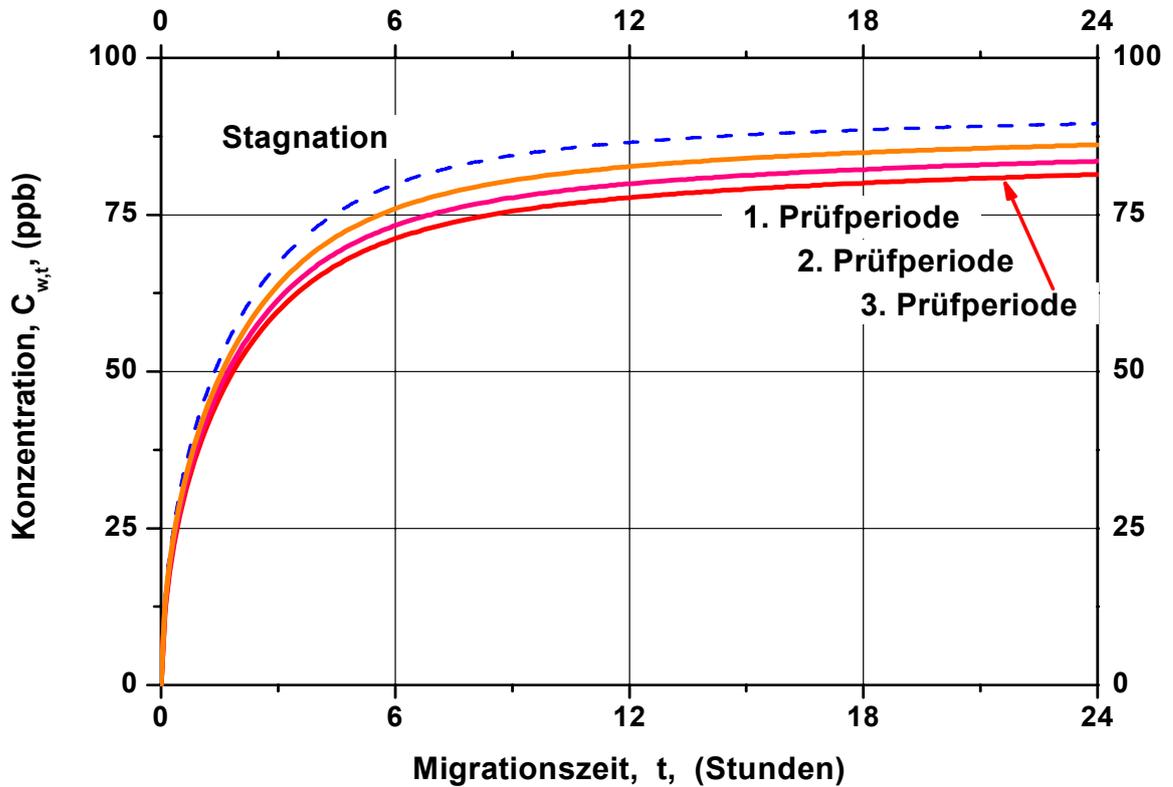
Modelling Guideline

Example 3. Warm water test with material constants in accordance with [3]

Migration conditions: 24 hour stagnation at $T = 60^\circ\text{C}$
 1st test period, 24 hours at $T = 60^\circ\text{C}$
 2nd test period, 24 hours at $T = 60^\circ\text{C}$
 3rd test period, 24 hours at $T = 60^\circ\text{C}$

Diffusion coefficient: $D_{\text{polymer}} \sim 1.3 \times 10^{-9} \text{cm}^2/\text{s}$, ($A \cdot p = 14.5$ and $\tau = 1577$)
 $D_{\text{water}} \sim 1 \times 10^{-4} \text{cm}^2/\text{s}$

Distribution coefficient: $K_{p/w} = 1000$ (not soluble)



Konzentration, $C_{w,t}$, (ppb)	Concentration, $C_{w,t}$, (ppb)
Stagnation	Stagnation
Prüfperiode	Test period
Migrationszeit, t , (Stunden)	Migration time, t , (hours)

The mass balance requires that 99.4% of the migrant is still preserved in the polymer at the end of the 3rd test period. This prevents the calculated concentrations of the 3rd test period from being underestimated.

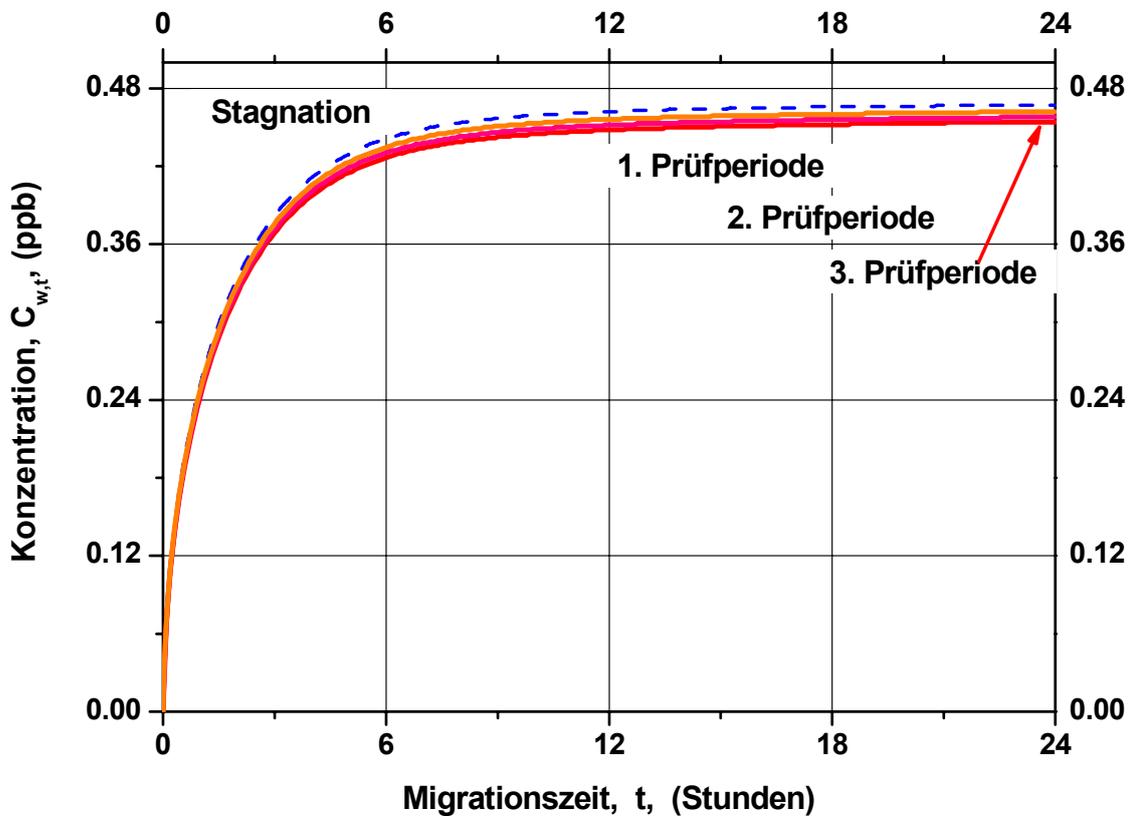
Example 4. Warm water test with material constants determined by testing

Migration conditions: 24 hour stagnation at T = 60°C
 1st test period, 24 hours at T = 60 °C
 2nd test period, 24 hours at T = 60 °C
 3rd test period, 24 hours at T = 60 °C

Diffusion coefficient: $D_{\text{polymer}} \sim 3.9 \times 10^{-13} \text{cm}^2/\text{s}$, ($A'_p = 6.5$ and $\tau = 1600$, determined by testing)

$D_{\text{water}} \sim 1 \times 10^{-4} \text{cm}^2/\text{s}$

Distribution coefficient: $K_{p/w} = 200,000$ (not soluble, determined by testing)



Konzentration, $C_{w,t}$ (ppb)	Concentration, $C_{w,t}$ (ppb)
Stagnation	Stagnation
Prüfperiode	Test period
Migrationszeit, t , (Stunden)	Migration time, t , (hours)

The mass balance requires that 99.996% of the migrant is still preserved in the polymer at the end of the 3rd test period. This prevents the calculated concentrations of the 3rd test period from being underestimated.

Annex 3: Validation of new material constants for polymers for mathematic modelling

1. A subgroup of KTW-AG validates material constants for polymers, which have so far not been published in Annex 1 of the Practical Guide. This group includes representatives from the Federal Environment Agency, BfR, trade and industry and accredited test laboratory.
2. The application must submit documents detailing the experiment and modelling in accordance with this guideline and [3] to validate new material constants.
3. The members of the subgroup prepare an assessment of the application for submission and approval by KTW AG.
4. The material constants are published in Annex 5.

Annex 4: Criteria for the accuracy of migration calculations for multilayer materials

Migration from planar or cylindrical monolayer structures in a stationary medium (drinking water) with limited volumes can be calculated analytically or using numerical algorithms.

The procedure takes into account both the diffusion of the migrant in the monolayer as well as its distribution at the interface with the water.

Migration from planar or cylindrical multilayer structures in a stationary medium (drinking water) with limited volumes can only be calculated using numerical algorithms. This procedure takes into account both the diffusion of the migrant in each layer of the system as well as the distribution of the migrant at the interface between the layers and with the water. The accuracy of migration calculations according to the numerical method for "planar or cylindrical test objects" – multilayer films or coatings or multilayer pipes – must be verified according to the following criteria:

- 1) If migration from the planar or cylindrical monolayers of an organic material in drinking water is calculated using an analytical formula and using a numerical method for planar or cylindrical test objects, the relative maximum deviations between the numerical and analytical results should be less than 0.5% or 1.00% (if at least 5% of the total quantity of the material being tested migrates and the discretisation is at least 200 points/layer). (See figure Example A)
- 2) The mass balance should demonstrate relative maximum deviations of less than 0.5% or 1.0% after calculation using an analytical formula and using a numerical method for planar and cylindrical test objects.
- 3) Assuming that in a planar or cylindrical multilayer organic material there is no distribution of the migrant at the interfaces between the layers (this means no concentration step or distribution coefficient $K = 1$), the calculation using the numerical algorithm should demonstrate a relative maximum deviation in concentration continuity at the interfaces of less than 0.5% or 1.0%.
- 4) In planar and cylindrical multilayer test objects in which a distribution of the migrant occurs at the interfaces between the layers, the calculations using the numerical algorithm for planar and cylindrical test objects should demonstrate a relative maximum deviation of the concentration steps at the interfaces of less than 0.5% or 1.0% (if at least 10% of the total migration time input is exceeded).
- 5) The numerical algorithm for calculating the migration from planar and cylindrical test objects must ensure that at any point during the migration the mass balances of the migrant can be calculated in all layers of an organic material drinking water system. The calculated results should deviate from the initial value of the migrant mass in the organic material drinking water system by no more than 0.5% or 1.0% (if at least 5% of the total migration time is exceeded).

If the aforementioned criteria are met, the numerical method can be used to estimate the migration from planar or cylindrical monolayer and multilayer organic materials in contact with drinking water. The relative and absolute uncertainty of such an algorithm would be less than the uncertainty of analytical methods used to determine migration by testing.

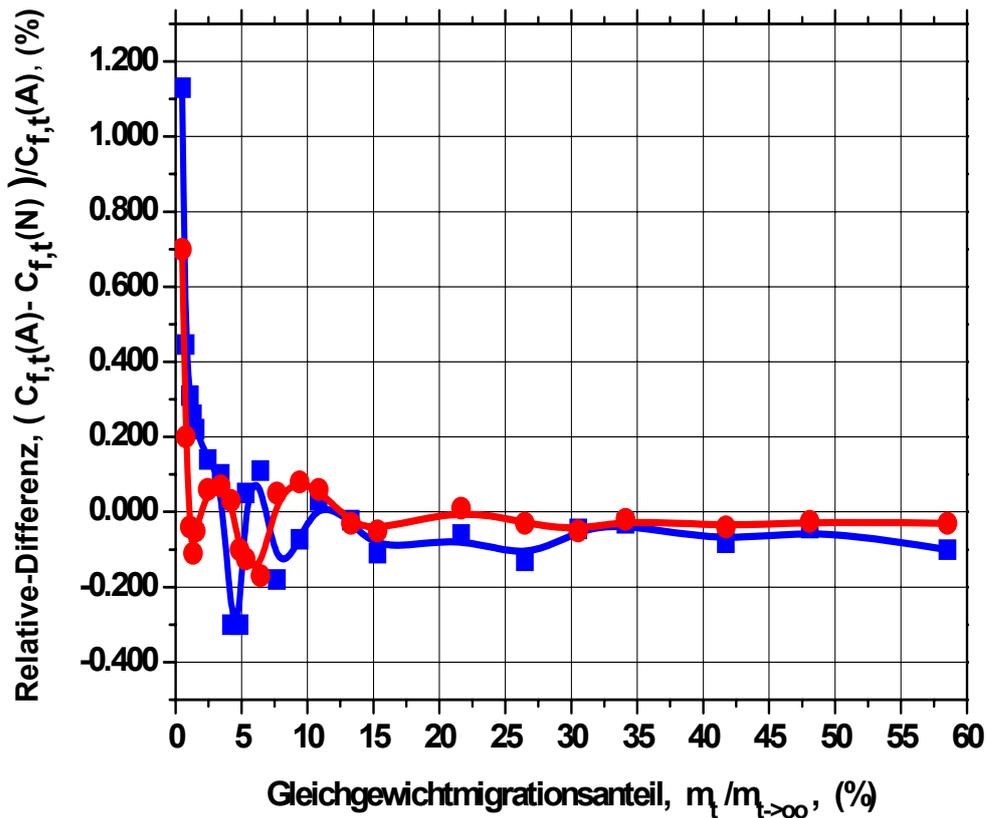
Example A

Application of the first criterion: Comparison of concentration calculations with analytical formulas, $C_{f,t}(A)$, and with numerical methods, $C_{f,t}(N)$:

Migration from a planar monolayer in a liquid medium was calculated using MIGRATEST Lite (analytically) and MIGRATEST EXP (numerically) and the outcome is shown in the following figure.

The low level oscillations in the beginning are due to the analytical solution, since this is not an exact solution of the differential equation, but consists of an expansion in series containing transcendental equations. This low percentage variation is not significant for calculating migration to assess the material.

Organic material:	Polymer with a coating thickness = 500 μm , density = 1.0 g/cm^3 and the surface = 6 dm^2
Drinking water as a liquid:	Density = 1.0 g/cm^3 , volume = 1000 cm^3
Migrant:	Organic substance with $M_w = 300 \text{ g/mol}$, $c_{p,o} = 1000 \text{ mg/kg}$
Diffusion coefficients:	$D_p = 5 \times 10^{-12} \text{ cm}^2/\text{s}$ $D_f > 1 \times 10^{-4} \text{ cm}^2/\text{s}$
Distribution coefficient:	$K_{p/f} = 1$ (blue dots), $K_{p/f} = 1000$ (red dots)
Maximum migration time:	$t = 1500$ days



Modelling Guideline

Relative-Differenz, $(C_{f,t}(A) - (C_{f,t}(N)) / C_{f,t}(A), \%$	Relative difference, $(C_{f,t}(A) - (C_{f,t}(N)) / C_{f,t}(A), \%$
Gleichgewichtmigrationsanteil, $m_t / m_{t \rightarrow \infty}, (\%$	Proportion of equilibrium migration, $m_t / m_{t \rightarrow \infty}, (\%$

Example B

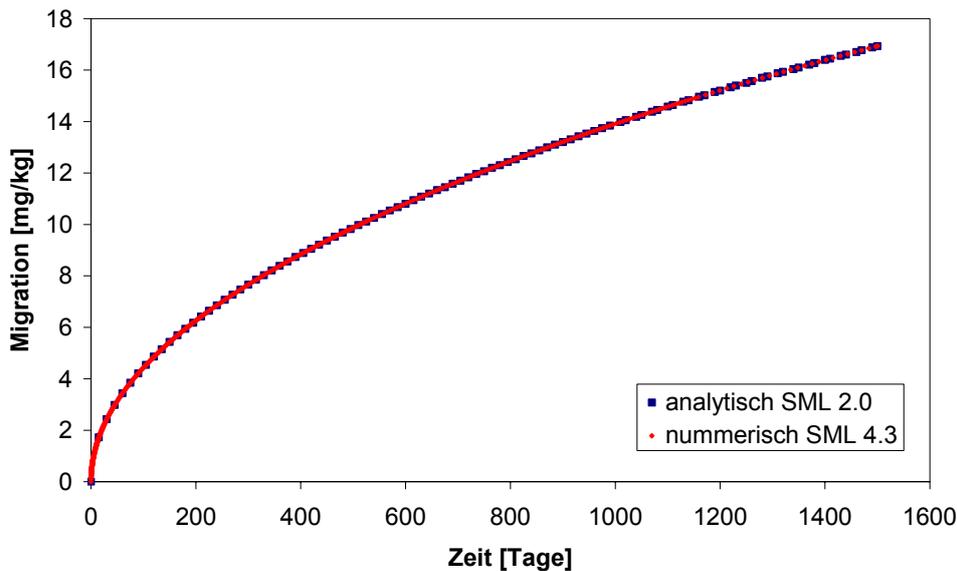
Application of the first criterion: Comparison of concentration calculations with analytical formulas, $C_{f,t}(A)$, and with numerical methods, $C_{f,t}(N)$:

Migration from a planar monolayer in a liquid medium was calculated using the software SML 2.0 (analytically) and the software SML 4.3 (numerically) and the outcome is shown in the following figures.

Low level oscillations are due to the analytical solution. The software SML 2.0 (analytical) outputs a value accurate to two decimal places and must be interpolated. This low percentage variation is not significant for calculating migration to assess the material.

Organic material:	Polymer with a coating thickness = 500 μm , density = 1.0 g/cm^3 and the surface = 6 dm^2
Drinking water as a liquid:	Density = 1.0 g/cm^3 , volume = 1000 cm^3
Migrant:	Organic substance with $M_w = 300 \text{ g/mol}$, $c_{p,o} = 1000 \text{ mg/kg}$
Diffusion coefficients:	$D_p = 5 \times 10^{-12} \text{ cm}^2/\text{s}$ $D_f > 1 \times 10^{-4} \text{ cm}^2/\text{s}$
Distribution coefficient:	$K_{p/f} = 1$, $K_{p/f} = 1000$
Maximum migration time:	$t = 1500 \text{ days}$

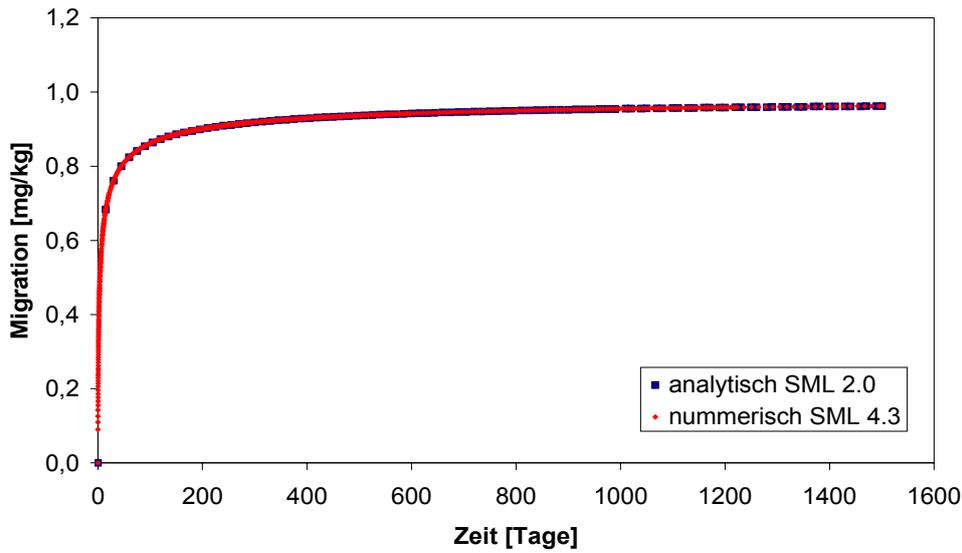
$K = 1$



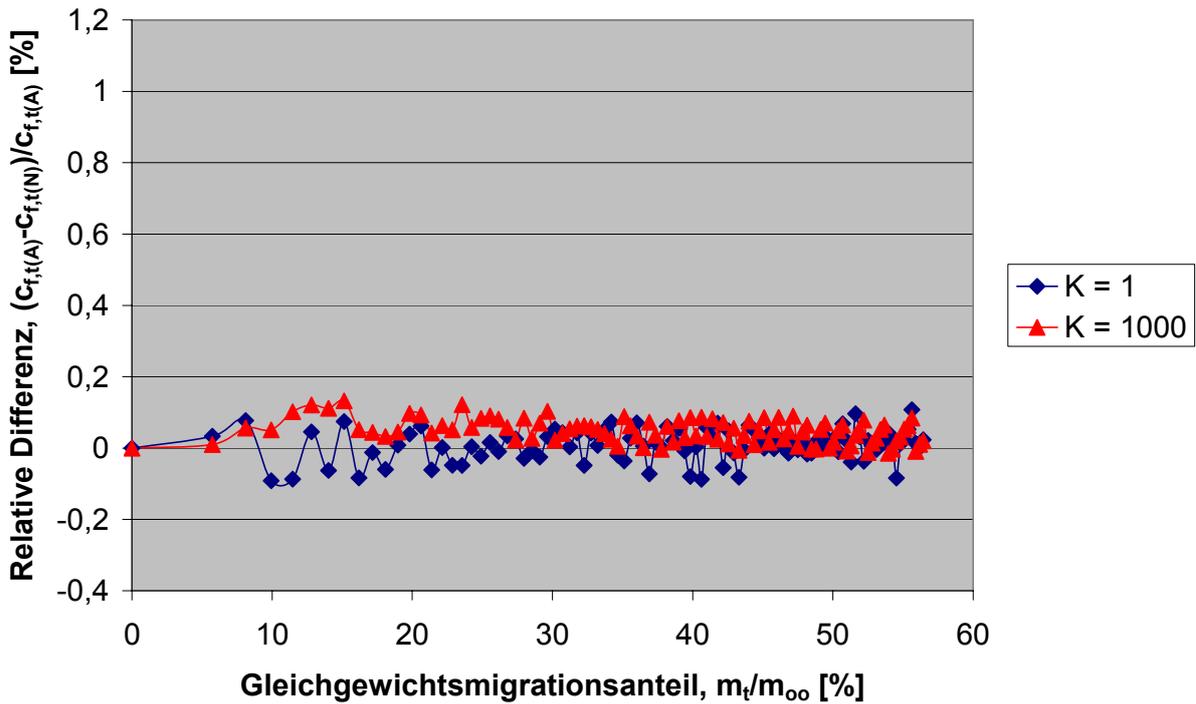
Migration [mg/kg]	Migration [mg/kg]
analytisch SML 2.0	Analytical SML 2.0
numerisch SML 4.3	Numerical SML 4.3
Zeit [Tage]	Time [days]

Modelling Guideline

K = 1000



Migration [mg/kg]	Migration [mg/kg]
analytisch SML 2.0	Analytical SML 2.0
numerisch SML 4.3	Numerical SML 4.3
Zeit [Tage]	Time [days]



Relative Differenz, $(c_{f,t(A)} - c_{f,t(N)}) / c_{f,t(A)} [%]$	Relative difference, $(c_{f,t(A)} - c_{f,t(N)}) / c_{f,t(A)} [%]$
Gleichgewichtsmigrationsanteil, $m_t / m_{oo} [%]$	Proportion of equilibrium migration, $m_t / m_{t \rightarrow oo}$ (%)

Annex 5: Material constants that can also be used for polymers in contact with drinking water within the framework of KTW, coating or lubricant guidelines

Version: 7.10.2008

Polymers	Material constant A_p^*
Epoxy resin	7.0