German Environment Agency

RECOMMENDATION

Guideline for the mathematical estimate of the migration of individual substances from organic material in drinking water (Modelling Guideline)[1,2]

Last updated: 3. December 2024

English translation – only the German document version is binding

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[1] Notified in accordance with Directive (EU) 2015/1535 of the European Parliament and of the Council of 9 September 2015 laying down a procedure for the provision of information in the field of technical regulations and of rules on Information Society services (OJ L 241, 17.9.2015, p. 1).

[2] Notified under 2024/0424/DE

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Contents

List of Variables

D_W	Diffusion coefficient of a substance in water in m^2/s
D_{Pk}	Diffusion coefficient of a substance in the polymer layer Pk in m^2/s, where k is the index of the polymer layer with $1 \leq k \leq n$ and n is the total number of polymer layers
c_W	Concentration of a substance in water in µg/l
c_{Pk}	Local concentration of a substance in the polymer layers Pk in µg/kg
t	Time in d
c_{eq}	Concentration in partition equilibrium
$c_{Pk,0}$	Mean initial concentration of a substance in the polymer layer Pk in µg/kg *Note: Designated as* c_0 *in the KTW evaluation criteria.*
MTC_{tap}	Maximum tolerable concentration of a substance at the tap in µg/l
c_{tap}	maximum concentration expected at the tap in µg/l
$c_{calculated}$	calculated concentration of a substance in migration water during a migration period (analogous to the measured concentration $c_{measured}$)
F_c	Conversion factor in d/dm (see KTW evaluation criteria)
$K_{P/P}$ or $K_{P/W}$	Partition coefficient between two polymer layers or between a polymer and the water layer
P_k	Polymer layer
O/V	Ratio of wetted surface to water volume in dm^{-1}

1 Introduction (regulatory framework)

The mathematical estimate of the migration (modelling) can be used to verify the requirements of the KTW evaluation criteria for the migration of individual substances instead of experimental evidence (formulation-specific individual substance requirements).

The following requirements must be met:

- implementation only with scientifically recognised models
- systematically higher migration levels in the assessment-relevant migration period (overestimation)
- traceability
- use of numerical methods.

2 Application of modelling

The assessment of materials in contact with drinking water requires a high level of hygienic safety. For this reason, a model is required for the simulation that, when compared directly with experimentally determined migration levels, provides at least comparable or systematically higher migration levels (overestimation).

Organic materials, e.g. plastics, that are in contact with drinking water can release substances to drinking water (mass transfer or migration). The concentration of the substances decreases in organic material and increases in drinking water (mass transfer). The rate-determining step of the mass transfer is the diffusion of the substances in the organic material. The transfer of substances from organic materials into drinking water can be measured under standardised conditions (surface/volume ratio, amount of change cycles, time, temperature) in the laboratory (performance of migration test and analysis of the test water on formulation-specific individual substances with a migration restriction in accordance with DIN EN 12873-1/-2) or calculated by simulation based on diffusion models (modelling). In Appendix 1, the involvement of simulation in assessing organic materials in contact with drinking water is illustrated.

For testing organic materials that come into contact with drinking water in accordance with DIN EN 12783-1/2, several migration cycles are to be determined. This is intended to take into account the exchange of drinking water in pipes or installation. In the simulation, all migration periods up to the relevant migration period must be calculated for the migrant of interest (see Table 1 and Table 2). During preliminary treatment according to DIN EN 128731/-2, only the 24-hour stagnation is taken into account in the simulation. Rinsing before and after stagnation can be neglected.

In the KTW evaluation criteria, the 3rd test period for the cold water test and the 7th test period for the warm and hot water test or, in the case of the extended test duration, the 9th test period for the cold water test and the 22nd test period for the warm and hot water test are to be used for the assessment.

Like the measured concentration, the calculated concentration is to be converted into the standardised tap concentration c_{tap} (see KTW evaluation criteria). The c_{tap} of the assessment-relevant migration period should not exceed the maximum tolerable concentration (MTC_{tap}).

In the event of non-compliance after 10 days of contact time, the test may be extended to 31 days. The migration waters to be considered in the cold/warm and hot water test are highlighted in Table 1 (cold water test) and Table 2 (warm and hot water test). The extension of the test can also be modelled.

For the assessment of multilayered products, the requirements of the KTW evaluation criteria should be implemented (see Chapter 5.7 of the KTW evaluation criteria).

Table 1: Migration cycles for the extended cold-water test

Week	Migration cycle	Total contact time in days	Contact time per migration in days
1	0 (preliminary treatment)	1	1
1	1	4	3
2	2	7	3

Week	Migration cycle	Total contact time in days	Contact time per migration in days
2	3	10	3
3	4	14	4
3	5	17	3
4	6	21	4
4	7	24	3
5	8	28	4
5	**9**	**31**	**3**

Table 1: Migration cycles of the extended warm or hot water test

Week	Migration cycle	Total contact time in days	Contact time per migration in days
1	0 (preliminary treatment)	1	1
1	1	2	1
1	2	3	1
1	3	4	1
2	4	7	3
2	5	8	1
2	6	9	1
2	**7**	**10**	**1**
2	8	11	1
3	9	14	3
3	10	1	1
3	11	16	1
3	12	17	1
3	13	18	1
4	14	21	3
4	15	22	1
4	16	23	1
4	17	24	1
4	18	25	1
5	19	28	3
5	20	29	1
5	21	30	1
5	**22**	**31**	**1**

The implementation of the modelling of organic materials and products in contact with drinking water and the assessment of the estimated concentrations of migrants is explained using examples in the Annex (separate document).

3 Modelling assumptions

The mass transfer from organic materials to drinking water is limited by the mass transport of substances (diffusion) and the solubility in organic material and the solubility in drinking water. The mass transfer of a substance from one medium into another (different polymer layers or from organic material into drinking water) is determined by diffusion in the layers and by transfer at the boundary layers. In the following, the polymer layers are designated with the index P_k, whereby the value of k can range from 1 to the total number of polymer layers. The polymer layer touched with water shall always be designated as P1. The index W stands for the water phase. An exemplary structure of polymer layers is shown in Figure 1.

The equation that can be used to quantify the time- and location-dependent diffusion of a substance in a medium (P or W) in space (Fick's 2nd law) is as follows:

Equation 1 $$\frac{\partial\, c}{\partial\, t} = \mathrm{div}\ (\mathrm{Dgrad}c)$$

where: the differential operators div are the divergence and grad is the gradient, t is the migration time, c is the local concentration and D is the local diffusion coefficient of the substance in the water or in a polymer layer. The diffusion coefficient D characterises the mobility of the molecules of the substance in the water or in the polymer. Diffusion coefficients D are temperature-dependent and may be time- and location-dependent. A uniform diffusion coefficient in the respective medium (layer of a material) which differs only by the temperature to be considered (cold (23 °C), warm (60 °C) and hot water (85 °C) test) shall be assumed for modelling the mass transfer of a substance. The diffusion coefficient also differs for the substance under consideration. In Cartesian coordinates with the coordinates x, y and z, equation (1) thus reads:

Equation 2 $$\frac{\partial c_{P/W}}{\partial t} = D_{P/W}\left(\frac{\partial^2 c_{P/W}}{\partial x^2} + \frac{\partial^2 c_{P/W}}{\partial y^2} + \frac{\partial^2 c_{P/W}}{\partial z^2}\right)$$

or in cylindrical coordinates with the coordinates r, φ, z:

Equation 3 $$\frac{\partial c}{\partial t} = D\left(\frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial c}{\partial r}\right) + \frac{1}{r}\frac{\partial^2 c}{\varphi^2} + \frac{\partial^2 c}{\partial z^2}\right)$$

From a physical point of view, according to equation (1), the rate $\frac{\partial c}{\partial t}$, at which substance concentration c changes at a point (x,y,z) in the system is equal to the divergence (div) of the product of a local diffusion coefficient $D_{Pk/W}$ (D_P in the polymer layer k or D_W in water) and of the spatial change (grad) of the local concentration c.[3] The direction of diffusion is along the concentration gradient (polymer ⇢ water). In order to simplify the equation and make it easier to solve mathematically, a location-independent diffusion coefficient (excluding dependence on the material of the different layers) and a one-dimensional concentration gradient shall be assumed and the diffusion in the direction of this one-dimensional gradient shall be considered: $\left(\frac{\partial c}{\partial x}\right)$ or $\frac{\partial\, c}{\partial\, r}$. The direction is without restriction of generality in the x-direction if it is chosen orthogonal to the layer boundaries or in the r-direction with a cylindrical structure of the layers. The other spatial directions can be neglected. The equations to be solved are therefore in Cartesian coordinates.

Equation 4 $$\frac{\partial c}{\partial t} = D\frac{\partial^2 c}{\partial x^2}$$

or in cylindrical coordinates:

Equation 5 $$\frac{\partial c}{\partial t} = \frac{1}{r}D\frac{\partial}{\partial r}\left(r\frac{\partial c}{\partial r}\right) = \frac{1}{r}D\frac{\partial c}{\partial r} + D\frac{\partial^2 c}{\partial r^2}.$$

The transfer at the boundary layer is determined by the partition coefficient. The partition coefficient K is the equilibrium distribution of a substance between two different media, e.g. the

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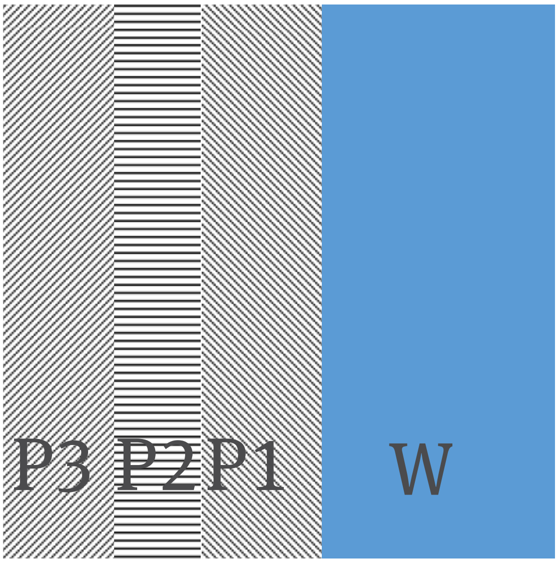
[3] For tubes with DN ≤ 80 mm, the equation should be solved with cylindrical coordinates.

partition coefficient $K_{P1/P2}$ for a substance between the 1st and 2nd polymer layer or the partition coefficient $K_{P1/W}$ between the polymer layer P1 and water W.

Abbildung 1 Beispielhafter Aufbau der Polymerschichten



The following assumptions are made for the model:

- No convection (flow) occurs during the water phase.
- Media (material layers or water phase) are parallel to each other (one-dimensional problem)
- The mass transfer is restricted by the mass transport (diffusion) in the organic material layers:
  - Nevertheless, the mass transport in the water phase is taken into account. A uniform diffusion coefficient of 10^{-4} cm²/s shall be used to simulate rapid mixing.
- The boundary resistance between the media is neglected: On the boundary surfaces of different layers or on the water/polymer
- boundary layer, the equilibrium state described by the partition coefficient is spontaneously set.
- The polymer and water system under consideration is a closed system.
  - The amount of substance in the overall system remains constant at all times (mass conservation).
  - There is no mass transfer to the outside at the edges of the two extreme media (water phase and extreme material layer).
  - A distribution of the migrant takes place on the polymer-water contact surface. The partition coefficient K_{PW} has the same value at all points of the surface at a constant temperature.
  - No chemical reactions take place (no hydrolysis of the migrant, no formation or reaction of the migrant in the solid).

- The diffusion and distribution coefficients are homogeneous within a medium and constant over time (for example, partial swelling of the polymer is not taken into account), but are temperature-dependent.
- If there is a change of temperature (hot/cold rinsing), a homogeneous temperature distribution in the media under consideration is always assumed. Possible temperature gradients should not be taken into account.
  - The density for water is temperature-dependent. The exact density can be found in corresponding tables. Alternatively, for practical reasons, a density of 1 g/cm^3 can be used.
  - The usual software for migration modelling outputs concentrations as mass-related concentrations [mg/kg] and requires the input of the density for water.

Necessary material constants and characteristic values for validated methods for assessing material constants are included in the bibliographical references in Annex 2 and 3.

The starting condition for single-layer materials and products shall be as follows:

Before the start of the first migration cycle, the migrating substance is homogeneously distributed in the polymer (initial concentration $c_{P,0}$).

Note: For substances migrating to the surface or blooming on their own, such as antistatic agents or lubricants, this condition is not met and migration would be underestimated. As a result, the starting condition is not met.

The following starting conditions are assumed for multi-layered materials and products (see 5.7 of the KTW evaluation criteria):

- Immediately after manufacture, the migrating substance is homogeneously distributed in the layers in which it was added (initial concentration $c_{P,0}$).
- Prior to the migration test, storage at room temperature (23 °C) of 30 days is modelled. The resulting concentrations for the migrating substance shall be calculated for all layers and used as the initial condition for contact with water.

Or

- A separate assessment of the individual layers is possible. It must be ensured that the addition of the migration results of the individual layers corresponds to the multilayered product. The same migrants of all layers to be assessed are to be added to assess MTC_{tap}.

The assumptions set out above, as well as the starting and boundary conditions applied, simplify the differential equation described above, thus making it easier to solve.

4 Solution of the differential equation

The differential equation describing the diffusion can be solved numerically in Cartesian or cylindrical coordinates, taking into account the starting and boundary conditions, whereby the solution describes the temporal change in the local concentration of the substance under consideration in the respective material layers and in the drinking water under the test conditions corresponding to the application depending on different variables (input parameters).

The solution of the differential equation of Fick's 2nd Law (see Chapter 3) for repeated contact in accordance with DIN EN 12783-1/2 is only possible using numerical algorithms. Different algorithms are necessary for the mathematical estimate of the migration from planar or cylindrical test specimen geometries. Algorithms should be applicable to mono- or multi-layered organic materials and products in contact with drinking water. Software solutions are necessary for the application of these algorithms.

Note: The inaccuracy of the numerical calculation itself should only make a negligible contribution to the overall inaccuracy of the assessment method, which is essentially determined by the inaccuracy of the input parameters (mass balance of the calculation < 1 % deviation, see 4.1). The relative and absolute inaccuracy of such an algorithm would then be at least one order of magnitude below the inaccuracy of analytical methods used for the experimental determination of migration (CEN TR 16364:2012).

4.1 Validation of the software used

Assuming that an organic material consists of a monolayer, drinking water has a limited volume and migration follows Fick's 2nd law, there are mathematical solutions for the differential equation to calculate the time-dependent migration from the organic material to drinking water.

For multiple contact in accordance with the migration standard DIN EN 12873-1/2, this simulation and its boundary conditions are not precise enough. As an initial condition, it can only be based on a homogeneous distribution in the material of the migrant to be considered. Contact with drinking water generates concentration gradients in the material, which must be used as the starting condition for the next migration cycle. This can only be done using numerical methods. The software must be able to map the test specification of the migration standard DIN EN 12873-1/-2.

The software solutions available on the market present themselves as a 'closed' algorithm in which the calculations cannot be traced by the user of the software.

In order to ensure that the simulations deliver correct results, the following criteria must be taken into account:

1. The accuracy of the simulation shall be tested using the examples given in the Annex. Software solutions that can only calculate planar test specimens shall be able to reproduce examples 1 to 3 and software solutions for cylindrical test specimens shall be able to reproduce examples 4 to 8. The deviations of the calculated concentrations from the solutions in the above-mentioned examples may not exceed 5 %.
2. For each calculation, the assumptions made must be plausible and comprehensible (source or justification).
3. The results obtained must be checked for plausibility (see 5.3).
4. The mass balance of the amount of the substance before and after the modelling calculation must be calculated and, after calculation using a numeric method, may not deviate from the amount of the starting material by less than 1 %. The mass balance compares the sum of the amount of substance of the migrating substance in all polymer layers at time t = 0 (i.e. before modelling) with the sum of the amount of substance in all polymer layers at the last migration contact plus the sum of the amounts of substance in the migration waters of all cycles including preliminary treatment.

5 Input parameters

The solution of the differential mass balance contains variables that are to be specified for the calculations of the migration of the substance under consideration into the water:

- **Geometric sizes** (layer thickness, contact surface, volume) as well as time and temperature are chosen according to the experimental migration test approach in accordance with the KTW evaluation criteria. This allows a direct comparison of the calculated and the tested migration values. The geometric sizes of the test specimens and the migration test conditions are known.
- In the case of **pipes**, cylindrical coordinates must be used for pipe diameters smaller than 80 mm, as the modelling can otherwise lead to an intolerable underestimation of the calculated concentrations in the migration water.
- **Complex geometries** may be disassembled into single geometries. The result of the different geometries is then added together, provided that no underestimation occurs as a result of the disassembly and individual simulations. Alternatively, an average thickness can be calculated from the ratio of the component volume to the surface in contact with drinking water and may be used for the simulation.
- **The initial concentration of the individual substance $C_{P.0}$** in the respective material layers must be known (e.g. in the case of polymers, residual monomer content, additive content, etc.) or analytically determined using validated (including in-house) test methods. In some cases, standards are also available (e.g. DIN EN 13130 series, official collection of analysis procedures according to § 64 LFBG, § 38 TabakerzG, § 28b GenTG). The real residual contents may change in the course of manufacturing and processing procedures (e.g. monomers in POM or polyamide, reaction and degradation products of crosslinkers or stabilisers). It is therefore important that the actual fluctuation range of $c_{P,0}$ is known or determined batch by batch. Provided that the concentration of the migrant does not change during the manufacturing and processing procedures, the quantity used in the formulation, e.g. in the case of an additive, can also be used.
- **The diffusion and distribution coefficients** are generally not known for the respective media and must be assessed using scientifically recognised methods (see bibliographical references in Annex 2 and Annex 3). If values measured with validated methods are available for the parameters, these can be used.
- During the pre-storage of a multi-layer material and during each individual migration or stagnation period for single and multi-layer materials, **concentration profiles** are formed in each layer. These must be used for the next test period. The use of the mean concentration per layer is not permitted instead.

5.1 Assessment of substance constants (assessment methods)

The relevant diffusion and partition coefficients are usually determined according to assessment methods. Annex 2 contains possible assessment methods for diffusion coefficients and Annex 3 contains possible assessment methods for partition coefficients. The bibliographical references of the assessment methods are listed. A detailed description of the assessment methods is not provided.

The parameters of the assessment methods of the diffusion and partition coefficients are calculated by interpolation of experimentally determined substance constants.

Validated parameters of the assessment methods for determining the diffusion and partition coefficients can be found in the bibliographical references.

5.2 Addition of further assessment methods for certain polymers

In order to supplement further assessment methods or the parameters for additional polymers, it must be shown that the assessment method is able to reproduce the real, experimentally determined diffusion or distribution coefficients with sufficient precision. The validation is material-specific. At least 15 experimental determinations of the diffusion/distribution coefficient for the polymer under consideration must be available. Results must be available for at least 5 migrants with different physico-chemical properties and 3 different temperatures in the 20 °C to 85 °C temperature range for the polymer under consideration.

For validation, the experimental diffusion or partition coefficients logarithmised to base 10 are plotted on the x-axis against the diffusion or partition coefficients logarithmised to base 10 that result from the respective assessment method. The plot is performed for each set of parameters as they are to be listed in the respective annex.

The respective assessment method should be published in a scientific journal, preferably open access.

5.3 Application of the numerical method (numerical algorithm)

The migration is calculated using a numerical algorithm to solve the differential equation of Fick's 2nd law (see Chapters 3 and 4). The references for solving the Fick's 2nd law are listed in Chapter 8.

5.3.1 Selection of the appropriate algorithm (planar or cylindrical)

Depending on the geometry of the test specimen, a numerical method (algorithm; see 4) can be used for the mathematical estimate of migration from planar or cylindrical monolayer or multilayer organic materials and products in contact with drinking water. Both algorithms can be integrated in one software. For the selection of the algorithm (planar or cylindrical) and the necessary input parameters, Chapters 5 and 5.1 shall be followed. The limits of the assessment methods for the necessary constants of substances must be observed.

5.3.2 Application of the above-mentioned assessment methods of Annex 2 and 3

If the assessment methods in Annex 2 or 3 are used to calculate the migration, the following conditions shall be taken into account when calculating the migration:

- The mathematical estimate of migration must be based on a recognised scientific method (bibliographical references in Annex 2 and 3 or newly published method/parameters in open access).
- The estimated concentrations of the migration period under assessment must be systematically overestimated.

Note: If the calculated concentrations are continuously significantly overestimated, the final result leads to an underestimation of migration.

Solution approach for strongly overestimated parameters: In the KTW evaluation criteria, the 3rd or 9th test period is used for the cold water test and the 7th or 22nd test period for the warm and hot water test for the purposes of the assessment. 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 examination, this underestimation can only occur if it is mathematically overestimated and more than 20 % at 23 °C or more than 10 % at 60 °C and 85 °C of the total substance present in the organic material is transferred to drinking water during the first 24-hour stagnation period (pretreatment of the test specimens in the migration test). These scenarios are easy to identify from the simulation. The first simulated test period should then be used as relevant for the assessment of the mass transfer.

The results of the migration calculation and their input parameters used shall be checked for plausibility, describing the following information in the modelling report:

- Documents used, in particular when using assessment methods in accordance with 5.3.3.
- For each calculation, the assumptions made must be plausible and comprehensible (source or justification).
- The mass balance (see 4.1), calculated using a numeric method, shall be less than 1 % of the initial amount of the substance (sum of the amount of the migrating substance in all polymer layers prior to modelling and in all layers including the water layers of all migration cycles after modelling).
- In case of doubt, an appropriate experimental measurement is recommended for plausibility checks to support the assessment carried out.

The plausibility check for the mathematical estimate of migration must be part of the modelling report.

5.3.3 Use of assessment methods other than those listed in Annex 2 and 3

If assessment methods are used which are not included in the bibliographical references of Annex 2 and Annex 3, in addition to the above criteria in 5.3.2, these must be checked and documented in particular for the plausibility of the input parameters. This also applies to assessment methods for matrices, conditions or substances for which there are no applicable parameters.

6 Modelling results

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

Instead of an analytical report containing the test results in accordance with DIN EN 12873-1/-2, an appropriate modelling report must be drawn up, containing the data input, the assessment parameters used, the software used and the simulated concentrations in the respective polymer layer (c_{Pk}) and the migration water for each migration period ($c_{calculated}$). In addition, information (see test report in accordance with DIN EN 12873-1/-2) is necessary as to which polymers and test specimens were covered by the modelling.

The plausibility check according to 5.3.2 or 5.3.3. shall be part of the modelling report.

The results of the calculated concentrations in the migration periods shall be reported as an average by integrating the concentration profile for each layer.

The migration results of the migration period relevant to the assessment must be normalised to the tap concentration c_{tap}, taking into account the migration conditions (surface/volume ratio and time) and the conversion factor for the product group F_c.

c_{tap} is compared with the MTC_{tap} of the positive list for the substance under consideration.

If the calculated c_{tap} is above the MTC_{tap} value, compliance with the migration restriction can be demonstrated by the experimental determination. The calculated migration water concentrations for all periods are used to assess the requirement of the KTW evaluation criteria 'no increasing trend'. The assessment of the non-increasing trend in calculated concentrations for individual migrants is carried out in accordance with the provisions of the KTW-BWGL in Chapter 5.5.2.

7 References for the solution of Fick's 2nd law

Roduit, B., Borgeat, C.H, Cavin, S., Fragniere, C. & Dudler, V. (2005). Application of Finite Element Analysis (FEA) for the simulation of release of additives from multilayer polymeric packaging structures. Food Additives and Contaminants 22(10): 945-955.

Tosa, V., Kovacs, K., Mercea, P & Piringer, O. (2008). A Finite Difference Method for Modelling Migration of Impurities in Multilayer systems. Numerical Analysis and Applied Mathematics 1048: 802 – 805.

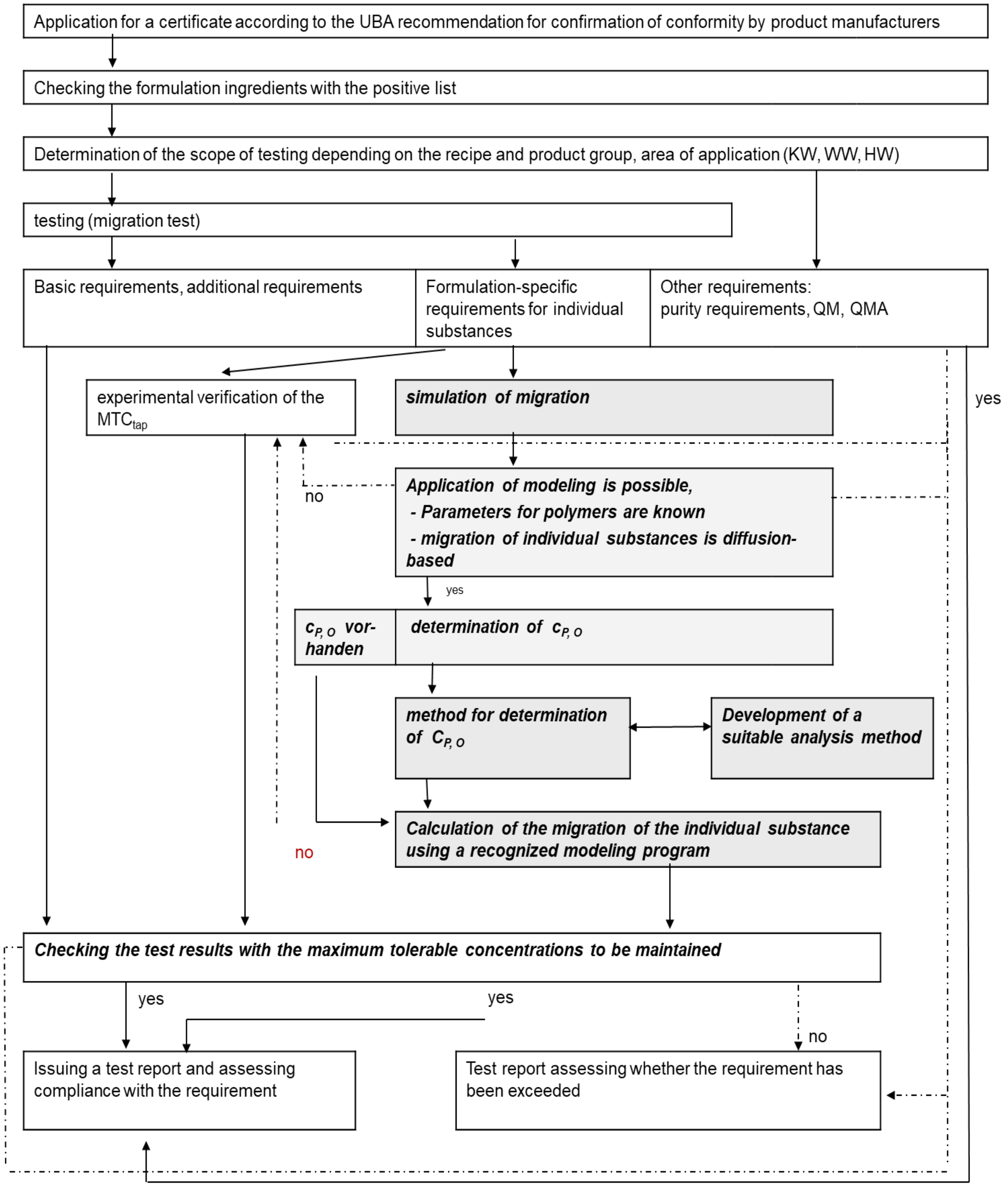
Reynier, A., Dole, P.& Feigenbaum, A. (2002). Integrated approach of migration prediction using numerical modelling associated to experimental determination of key parameters. Food Additives and Contaminants 19 (Supplement), 42–55.

Brandsch, R. & Schuster, D. (2020): Repeated use food contact materials: A categorisation approach in support of risk assessment. Food Additives & Contaminants: Part A. 37 (12): 2184-22-3. (DOI: 10.1080/19440049.2020.1798512).

Crank, I.: The Mathematics of Diffusion. (Clarendon Press 2nd edition 1979).

Tosa, V. & Kovács, K.: Numerical model to solve impurities migration in water pipes. (2009). Journal Physics: Conference Series 182. 012042. (for cylindrical geometry).

Annex 1 Flow chart for the integration of modelling for the verification of formulation-specific individual substance requirements of the KTW evaluation criteria



Annex 2 Assessment methods for diffusion coefficients

The diffusion coefficient of a substance in a plastic (D_P) is a size that reflects the mobility of the molecules of the substance in the organic material. The greater the diffusion coefficient, the faster the substance can be transported.

The diffusion coefficient D_P can be determined experimentally or calculated using a theoretical model and algorithm. For assessing the diffusion coefficient D_P different approaches are possible.

The details of the methods can be found in the literature.

No concrete quantitative quality criteria have yet been defined for the assessment methods. The list is therefore provisional.

Note: In the multiple migration calculation corresponding to the stagnation periods according to DIN EN 12873-1, -2, the use of conservative parameters may lead to an underestimation of the final result. Therefore, the most realistic parameters should be used.

Table 3: Bibliographical references for assessment methods of diffusion coefficients

Assessment method of the diffusion coefficients	Bibliographical references
DIN CEN/TR 16364, DIN SPEC 19811:2012-09	Influence of materials on water intended for human consumption – Influence due to migration – Prediction of migration from organic materials using mathematical modelling; German version of CEN/TR 16364:2012
Piringer assessment method	Mercea, P.V., Kalisch, A., Ulrich, M., Benz, H., Piringer, O.G., Tosa, V., Schuster, R. & Sejersen, P. (2018). Modelling migration of substances from polymers into drinking water. Part 1 – Diffusion coefficient estimations. Polymer testing 65: 176-188 Mercea, P., Losher, C., Benz, H., Petrasch, M., Costa, C., Stone, V. W. & Toşa, V. (2021). Migration of substances from unplasticised polyvinyl chloride into drinking water. Estimation of conservative diffusion coefficients. Polymer testing 104: 107385. Begley, T., Castle, L., Feigenbaum, A., Franz, R., Hinrichs, K., Lickly, T., Mercea, P., Milana, M., O'Brien, A., Rebre, S., Rijk, R. & Piringer, O. (2005). Evaluation of migration models that might be used in support of regulations for food-contact plastics. Food Additives and Contaminants 22(1): 73-90.

Assessment method of the diffusion coefficients	**Bibliographical references**
Brandsch assessment method	Brandsch, R. (2017). Probabilistic migration modelling focused on functional barrier efficiency and low migration concepts in support of risk assessment. Food Additives and Contaminants 34: 1743-1766.
Welle assessment method	Welle, F. (2013). A new method for the prediction of diffusion coefficients in Poly(ethylene terephthalate). Journal of Applied Polymer Science 129(4): 1845-1851. Ewender, J. & Welle, F. (2013). Determination of the Activation Energies of Diffusion of Organic Molecules in Poly(ethylene terephthalate). Journal of Applied Polymer Science 128 (6): 3885-3892 Welle, F. (2014). Activation energies of diffusion of organic migrants in cycloolefin polymer. International Journal of Pharmaceutics 473(1): 510-517. Ewender, J. & Welle, F. (2019). Diffusion Coefficients of n-Alkanes and 1-Alcohols in Polyethylene Naphthalate (PEN). International Journal of Polymer Science 2019: 9. Welle, F. (2021). Diffusion Coefficients and Activation Energies of Diffusion of Organic Molecules in Polystyrene below and above Glass Transition Temperature. Polymers 13(8): 1317. Kaiser, K.M.A., Ewender, J. & Welle, F. (2020). Recyclable Multilayer Packaging by Means of Thermoreversibly Crosslinking Adhesive in the Context of Food Law. Polymers (Basel) 12(12).
JRC	Brandsch, R., Dequatre, C., Mercea, P., Milana, M., Stoermer, A., Trier, X., Vitrac, O., Schaefer, A. & Simoneau, C. Practical guidelines on the application of migration modelling for the estimation of specific migration. EUR 27529. Luxembourg (Luxembourg): Publications Office of the European Union; 2015. JRC98028 https://publications.jrc.ec.europa.eu/repository/handle/JRC98028
Huang assessment method	Huang, L., Fantke, P., Ernstoff, A. & Jolliet, O. A quantitative property-property relationship for the internal diffusion coefficients of organic compounds in solid materials. Indoor Air 2017; 27: 1128-1140.

Annex 3 Assessment methods for partition coefficients

The partition coefficient of a substance between two immiscible media (K) is a size that expresses the ratio of the equilibrium concentrations c_{eq} of the substance in these two media.

The more K deviates from 1, the greater the difference in solubility in the two media is. During migration modelling for plastics in contact with drinking water, a basic distinction can be made between two types of K coefficients:

On the one hand, this is the partition coefficient $K_{P\text{-}W}$ of the migrating substance between the plastic and drinking water.

On the other hand, in the case of a plastic or other organic product consisting of several (different) layers, there are the partition coefficients $K_{P\text{-}P}$ between the layers of this product. Both types of partition coefficients can be determined experimentally or assessed using a theoretical model and algorithm.

In the following table, possible assessment methods are listed with the bibliographical references.

No concrete quantitative quality criteria have yet been defined for the assessment methods. The list is therefore provisional.

Note 1: In the multiple migration calculation corresponding to the stagnation periods according to DIN EN 12873-1, —2, the use of conservative parameters may lead to an underestimation of the final result. Therefore, the most realistic parameters should be used.

Note 2: If partition coefficients e.g. of two polymers compared to the same matrix (e.g. water or air) are known, the partition coefficient between the two polymers can be obtained by dividing the two partition coefficients to the same matrix.

Table 4: Bibliographical references for assessment methods of partition coefficients

Assessment methods for the partition coefficients	Bibliographical references
DIN CEN/TR 16364, DIN SPEC 19811:2012-09	Influence of materials on water intended for human consumption – Influence due to migration – Prediction of migration from organic materials using mathematical modelling; German version of CEN/TR 16364:2012
Fabes assessment method	Baner, A. & Piringer O., (2008). Partition coefficients", In "Plastic Packaging-Interactions with Food and Pharmaceuticals Eds. Piringer O.G., Baner, A.L.,Wiley-VCH, Weinheim. Mercea, P., Kalisch, A., Ulrich, M., Benz, H., Piringer, O., Tosa, V., Schuster, R. & Sejersen, P., (2019). "Modelling migration of substances from polymers into drinking water.

Assessment methods for the partition coefficients	Bibliographical references
	Part 2 – Partition coefficient estimations", Polymer Testing 76: 420-432.
Floy-Huggins method	Vitrac, O. & Gillet, G., (2008). Prediction of partition coefficients between food simulants and packaging materials using molecular simulation and a generalised Flory-Huggins approach, 18th European Symposium on Computer Aided Process-Engineering, Eds, Braunschweig, B., Xavier, J., Elsevier, Amsterdam.
Correlation between the partition coefficient and the logarithmic octanol/water coefficient	Asako Ozaki, A., Gruner, A., Störmer, A., Brandsch, R., & Franz, R. (2010). Correlation between Partition Coefficients Polymer/Food Simulant, $K_{P,F}$, and Octanol/Water, Log P_{OW} – a New Approach in support of Migration Modelling and Compliance Testing, DLR 106: 203-208 Pintado-Herrera, M.G., Lara-Martin, P.A., Gonzalez-Mazo, E. & Allan, I.J. (2016). Determination of silicone rubber and low-density polyethylene diffusion and polymer/water partition coefficients for emerging contaminants. Environmental Toxicology and Chemistry 35(9): 2162-2172.
Abraham-type linear solvation energy relation ships	Egert, T. & Langowski, H.-C. (2022). Linear Solvation Energy Relationships (LSERs) for Robust Prediction of Partition Coefficients between Low Density Polyethylene and Water Part I: Experimental Partition Coefficients and Model Calibration. European Journal of Pharmaceutical Sciences 172: 106137. Egert, T. & Langowski, H.-C. (2022). 'Linear solvation energy relationships (LSERs) for robust prediction of partition coefficients between low-density polyethylene and water. Part II: Model evaluation and benchmarking.' European Journal of Pharmaceutical Sciences **172**: 106138.
Quantitative property-property relationship (QPPR)	Huang, L & Jolliet, O. (2019). A combined quantitative property-property relationship (QPPR) for estimating packaging-food and solid material-water partition coefficients of organic compounds. Science of The Total Environment **658**: 493-500.