SLOVENSKI STANDARD
SIST-TP CEN/TR 16364:2012

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Vpliv materiala na pitno vodo - Vpliv migracije - Ocenjevanje migracije iz organskih snovi z uporabo matematičnega modeliranja

Influence of materials on water intended for human consumption - Influence due to migration - Prediction of migration from organic materials using mathematical modelling

Einfluss von Materialien auf Wasser für den menschlichen Gebrauch - Einfluss infolge der Migration - Abschätzung der Migration aus organischen Materialien mittels mathematischer Modellierung

Influence des matériaux sur l'eau destinée à la consommation humaine - Influence de la migration - Utilisation de modèles mathématiques pour prévoir la migration depuis des matériaux organiques

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Foreword

This document (CEN/TR 16364:2012) has been prepared by Technical Committee CEN/TC 164 “Water supply”, the secretariat of which is held by AFNOR.

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Introduction

During the last two decades, several scientific investigations have demonstrated that migration from organic materials into liquid simulants is a physical process that can be modelled successfully. Mass transfer from an organic material into a liquid simulant is predictable because in many cases it follows Fick´s law of diffusion, i.e. the diffusion process is the rate determining step. To predict migration from organic materials into contacting media a corresponding diffusion model was established.

This Technical Report describes the application of predictive diffusion modelling to the estimation of the migration of a substance from a product intended for contact with water intended for human consumption – for convenience, and where appropriate, referred to as drinking water in this report. The application applies to organic materials, such as polymers, used to make such products.

The purpose of the report is to stimulate the use of such techniques in member states such that sufficient experience is generated to enable the value of such modelling to be assessed in relation to complementing or substituting the conventional approach.

Normally in member states the estimation of such migration is performed by standardised procedures based on laboratory testing and analysis, i.e. an experimental approach. Migration modelling is an alternative to this type of experimental testing. The experimental determination of the specific migration of substances into test water (simulated drinking water) often requires a considerable amount of time and it can be costly. This conventional approach has worked well and, of course, it generates data on the actual concentration of a substance in test water. However, in some cases the analysis is difficult or even impossible due to problems caused, for example, by chemical degradation, volatilisation of the substance. In addition, the substance may not be amenable to, or the target concentration of interest may be too low for, available analytical techniques Therefore, the application of a mathematical model could have considerable benefits for industry and regulators, as experience has shown in the control of migration from plastic materials in contact with foodstuffs.

Thus, the modelling approach is attractive because, in principle, it is quicker and more flexible than the conventional testing approach, in that different exposure conditions can be readily investigated - and it should be cheaper.

Modelling of migration has been used for several years in the United States as an additional tool in support of regulatory decisions. Also, the European Union has introduced such diffusion modelling by means of EU Directive 2001/62/EC (the 6th amendment of Directive 90/128/EEC), consolidated in Directive 2002/72/EC as a compliance and quality assurance tool for plastic materials intended to come in contact with foodstuff [3].

The European project SMT-CT98-7513, *Evaluation of Migration Models in Support of Directive 90/128/EEC*, successfully demonstrated the practical value of such diffusion models. The main objectives of this project were to demonstrate:

— the validity of migration models for compliance purposes;

— that a relationship between the specific migration limit (SML) and the concentration of a substance in the finished product can be established.

A report of this project has been finalised and the project results were published in a scientific journal [4]. As indicated above, a major advantage of migration modelling is that it enables calculation of migration values independent of the limitations that affect the experimental/analytical approach. For example, at low cost one can quickly investigate, for compliance or research purposes, a wide range of conditions of contact between material with test water.

The diffusion modelling approach described was originally developed for, and accepted by, the European Commission in the area of plastic materials in contact with foodstuffs. It has been successfully used to simulate the conventional experimental/analytical approach to compliance testing of plastics in contact with foodstuffs. In this latter approach different liquid food simulants, including aqueous simulants, are used.

In principle, the approach is applicable to many organic materials. However, today it has been applied mainly to different types of polyethene, polypropene, polystyrene and polyvinyl chloride.

Like the experimental approach, the mathematical approach has its limitations. An accurate prediction of the migration of a substance from an organic material to water requires detailed knowledge of the diffusion behaviour of the materials and substances under investigation. The level of information may well require extensive experimental studies – more than the experimental, analytical approach would require. An important feature of the mathematical approach is the possibility of generalisation. Based on known average diffusion behaviour of polymers and substances, a maximum or 'upper-limit' migration can be calculated. This so-called 'worst-case' result may then be used for compliance purposes.

1 Scope

This Technical Report describes a procedure, based on a diffusion model, to be applied to the estimation of specific migration of substances into drinking water from organic materials intended to come into contact with drinking water.

The modelling approach is readily applicable to certain organic materials, as explained in this report. In principle, the diffusion modelling approach is applicable to other organic materials but practical difficulties, in relation to obtaining data to feed into the diffusion model, may restrict or prevent its application. Accordingly, in addition to the diffusion model, scientific estimation procedures for the required data inputs need to be considered.

The approach is normally applicable to organic substances that are soluble in the material matrix. Substances applied externally to a product made of an organic material, e.g. antistatic agents, lubricants, etc. are excluded from the diffusion modelling approach, as are electrolytes, salts, oxides and metals. Only organic substances with well-defined molecular weight or mixtures with well-defined ranges of molecular weights are amenable to the diffusion modelling approach.

The diffusion modelling approach is readily applicable to amenable organic materials in the form of a pipe or a sheet, where data such as material thickness is readily calculable. More complicated product shapes, such as fittings, require assumptions to be made.

It may not be possible to model the effects of test waters that are chemically active, for example test waters to which chlorine has been added to simulate chlorinated drinking water. This is because substances that migrate from a material into water containing chlorine can be converted by chemical reaction into substances with different properties.

2 Normative references

Not applicable.

3 Terms and definitions

For the purpose of this document, the following terms and definitions apply.

3.1
diffusion model
Fick's Second Law of diffusion that simulates the diffusion of substances from a material into drinking water

3.2
experimental test
technical operation that consists of the determination of one or more characteristics of a given product

3.3
experimental testing procedure
set of instructions for determining by experiment the migration of a substance from a material into water

3.4
software tool
set of instructions for a computer (e.g. a computer program)

Note1 to entry: In this document it refers to instructions designed to model migration of substances from a material into water.

3.5
product
manufactured item intended for contact with drinking water

3.6
monolayer
product this is or contains a material that consists of one layer

3.7
multilayer
product this is or contains a material that consists of more than one layer

3.8
migration
movement of a substance or substances from one compartment (a material) into a second compartment (water)

3.9
migration period
period of time in which the migration is carried out under specified conditions

3.10
migration rate
mass of a measured substance or substances migrating from the surface of a test piece into the test water in one day

3.11
substance
chemical that is a constituent of a material used in contact with drinking water with the potential to migrate into drinking water

3.12
contact area
surface area of a material in contact with a specific volume of water

3.13
volume to area ratio
ratio of the volume of water in contact with a specific area of material

3.14
test water
water used for migration testing

3.15
diffusion equation
partial differential equation known as Fick's Second Law that describes the variation of the concentration of a substance in a system (e.g. a polymer in contact with water) depending on time and location

3.16
diffusion coefficient
factor of proportionality representing the amount of substance diffusing across a unit area through a unit concentration gradient in unit time (e.g. from polymer to water)

3.17
molecular weight
mass of one mole of molecules calculated using standard atomic weights, expressed as g/mol

3.18
partition coefficient
ratio of the concentrations, at equilibrium, of a substance in the two phases of a mixture of two immiscible solvents

Note1 to entry: Examples are polymer and water or in the case of the Octanol-Water Partition Coefficient, 1-octanol and water.

4 Principle

Current predictive mathematical models for the estimation of migration of a substance from an organic material into another medium, such as a food simulant or drinking water, are based on diffusion theory and partitioning effects. Various parameters and information are needed to make the diffusion model work, in terms of calculating the concentration of a substance in test water or a migration rate.

Various assumptions need to be valid for the model to work satisfactorily.

If the described data inputs are available, or can be estimated, and the various assumptions valid, then the model can be used to estimate reliably the concentration of a substance in water after a specific time of contact between an organic material and water - and at a specific temperature. If required this concentration can be used to calculate a migration rate.

Depending on how the various data inputs are obtained, or used, the diffusion model can be used to estimate a worst-case value of migration, i.e. to produce a value that is likely to be higher than a value estimated by means of the conventional experimental/analytical approach.

The diffusion model can be used in a manner that simulates the conditions applied in the conventional analytical approach used in member states.

Annex A provides detail on the principles on which the diffusion modelling approach is based.

5 Apparatus

In order to predict migration a personal computer set-up capable of running an appropriate validated software tool is required. See Annex C for information on validation of the numerical algorithm and the software. Currently suitable software to run the diffusion model is available.

6 Assumptions that need to be valid

The diffusion model is based on the following assumptions being valid:

1) the migration process of the substance within organic materials shall obey the law of diffusion (Fick's Second Law);

2) the migrant is an uncharged, organic substance;

3) the mass of the substance in the system is conserved, i.e. no substance is consumed or built up;

4) the initial concentration of the substance in the material shall be homogeneous, i.e. it does not vary significantly and is constant, i.e. is non-degradable by chemical reaction; this applies to each layer in the case of multilayer products;

5) the material thickness shall be uniform (i.e. it does not vary significantly);

6) the volume of the organic material and the water is finite;

7) there shall be no boundary resistance for the transfer of the substance between the organic material and water;

8) the uptake of the substance by the water shall be fast, i.e. the water is a high diffusivity medium or well-mixed liquid;

9) the interaction between the organic material and water shall be negligible such that no swelling of organic material by uptake of water occurs during the migration process.

7 Required data inputs

7.1 General

The data inputs required to use the diffusion model are described in 7.2 to 7.10.

7.2 Diffusion coefficient of the substance (D_P)

The diffusion coefficient is a parameter dependant on the properties of the substance and of the organic material. It relates to the mobility of the substance in the organic material. It may be obtained in several ways:

a) from tables;

b) determined by experiment [5];

c) estimated by a validated scientific estimation procedure:

1) Arrhenius equation [6];

2) estimation procedure developed by Piringer validated in the EU Project SMT-CT98-7513 [4]; the diffusion coefficients for various organic materials can be estimated from their polymer-specific parameter, A_P [7];

d) assumed to be a worst-case value.

A detailed explanation on how to obtain and use diffusion coefficients, see A.4.

7.3 Partition coefficient of the substance ($K_{P,W}$).

The partition coefficient $K_{P,W}$ is a parameter dependant on the relative solubility of the substance in relation to the organic material and the water. It relates to what extent the substance moves from the organic material into water at thermodynamic equilibrium. It may be obtained in several ways:

a) from tables;

b) determined by experiment;

c) estimated by a validated scientific estimation procedure;

1) estimation from the solubility of the substance in water, i.e. the concentration in the water will not exceed its water solubility (worst-case assumption) [8];

2) estimated from the octanol/water partition coefficient of the substance [9,10];

d) assumed to be a worst-case value.

A detailed explanation on how to obtain and use partition coefficients, see A.5.