

Application note

AKTS-SML6 Software 操作トレーニング

MR-PETの移行モデル“Cmod”による汚染度算定

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Palmetrics

Application note

– Calculation of modelled C_{mod} contamination in recycled PET
再生PETの移行モデル“ C_{mod} ”による汚染度算定

Summary

In the European Union, the safety evaluation of a PET recycling process is performed by comparing the *residual concentration* of each contaminant in recycled PET (C_{res}) to a *modelled concentration* (C_{mod}) in PET [1]. This C_{mod} is calculated using generally recognized conservative migration models and it corresponds to a migration which cannot give rise to an unsafe dietary exposure

欧州連合では、PETリサイクルプロセスの安全性評価は、リサイクルPET(C_{res})中の各汚染物質の残留濃度はPETの移行モデルによる推定濃度(C_{mod})と比較することによって行われます[1]。

この C_{mod} は、一般的に認識されている保守的な移行モデルを使用して計算され、危険な飲食による曝露を引き起こさない移行量に対応しています。

This application note describes how to apply the AKTS-SML software to calculate C_{mod} for a contaminant used in a challenge test performed for the determination of the cleaning efficiency.

このアプリケーションノートでは、AKTS-SMLソフトウェアを適用して、洗浄効率を決定するために実行されるチャレンジテストであり、使用される汚染物質の C_{mod} を計算する方法について説明します。

[1] EFSA Panel on food contact materials, enzymes, flavourings and processing aids (CEF); **Scientific Opinion on the criteria to be used for safety evaluation of a mechanical recycling process to produce recycled PET intended to be used for manufacture of materials and articles in contact with food**. EFSA Journal 2011;9(7):2184. [25 pp.] doi:10.2903/j.efsa.2011.2184.

1] 食品接触材料、酵素、香料、加工助剤(CEF)に関するEFSAパネル。食品と接触する材料や物品の製造に使用されることを目的としたリサイクルPETを製造するためのメカニカル・リサイクルプロセスの安全性評価に使用される基準に関する科学的意見。EFSAジャーナル2011;9(7):2184. [25ページ] DOI: 10.2903/j.efsa.2011.2184.



Evaluation principles

Migration criterion

In the safety evaluation, EFSA considers that a contaminant present in recycled PET should not give rise to a migration in food which could result in a dietary exposure higher than $0.025 \mu\text{g}/\text{kg bw}/\text{day}$.

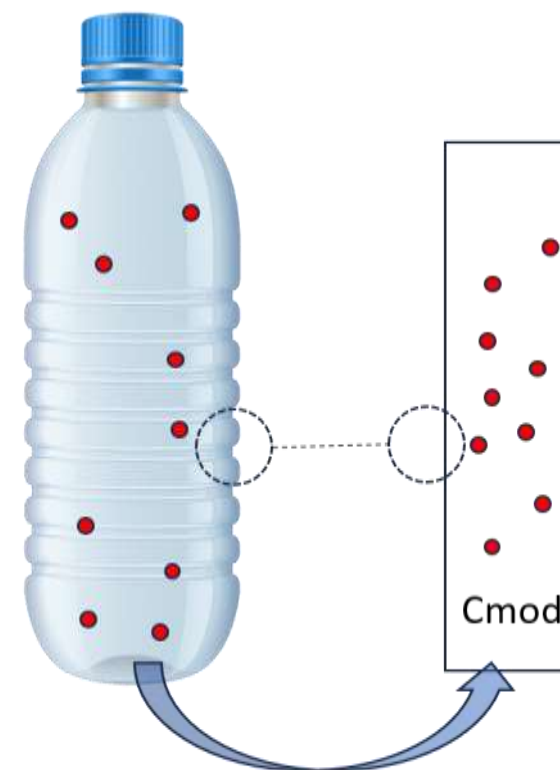
安全性評価において、EFSAは、リサイクルPETに存在する汚染物質が、 $0.025\mu\text{g}/\text{kg}$ 体重/日を超える食事曝露をもたらす可能性のある食品の移行を引き起こすべきではないと考えています。

Three exposure scenarios are considered. For the infants, the population group the most at risk, the exposure limit is respected if the concentration in water is lower or equal at $0.1 \mu\text{g}/\text{kg}$ (modelling over-estimation factor of 5 included).

3つの曝露シナリオが考慮されます。最もリスクの高い集団である乳児の場合、水中の濃度が $0.1 \mu\text{g}/\text{kg}$ 以下であれば曝露限界が尊重されます。(5の移行モデル_過大評価係数を含みます)

C_{mod} is the concentration in recycled PET that leads to a migration equal to $0.1 \mu\text{g}/\text{kg}$ food, using migration modelling.

C_{mod} は、移行モデルを使用して、食品中 $0.1 \mu\text{g}/\text{kg}$ に等しい移行をもたらすリサイクル PET 中の濃度です。



Backwards calculation

Evaluation principles

Modelling parameters

For the Cmod calculation (infant scenario), EFSA requires the following parameters to be applied in the modelling:

Cmod計算(乳幼児シナリオ)の場合、EFSAでは、モデリングとして次のパラメータを適用する必要があります。

Contact time:	12 months
Contact temperature:	25°C
Thickness of PET package:	300 µm
Density of PET material:	1.375 g/cm ³
Packaging geometry:	EU-cube (V=1l, S=6dm ²)
Diffusion coefficient, D:	estimated with Piringer model (Ap' = 3.1, Tau = 1577, worst case for T ≤ 70°C)
Partition coefficient, K_{p/F}	1.0 (good solubility)

Solving problem step by step

1) Create the traditional “EU cube” package (volume of 1 l, surface of 600 cm²), one layer PET of 300 μm

従来の「EUキューブ」パッケージ(容量1リットル、表面600cm²)、300μmの1層のPETを作成します。

The screenshot shows the SML v 6.62 software interface. The main window is titled "Article Creation Wizard" and is currently on step 2, "Layers".

- Step 1:** "Surface" (Number of layers: 2)
- Step 2:** "Layers" (Define all layers)
- Step 3:** "Migrants" (Add Migrant(s))
- Step 4:** "Data" (Concentration, Diffusion Coefficient, Partition Coefficient, Solubility)
- Step 5:** "Run prediction" (Run Prediction...)

The "Layers" table shows the following data:

Article	Thickness (μm)	Contact Me...
Not Defined	300	User Defined

The "Layer Details" for Layer 1 show:

- Type: Material (selected)
- Thickness (μm): 300
- Density (g/cm³): N/A
- Layer Abbreviation: Layer 1
- Material: Not Defined

The "Package 1" properties on the right show:

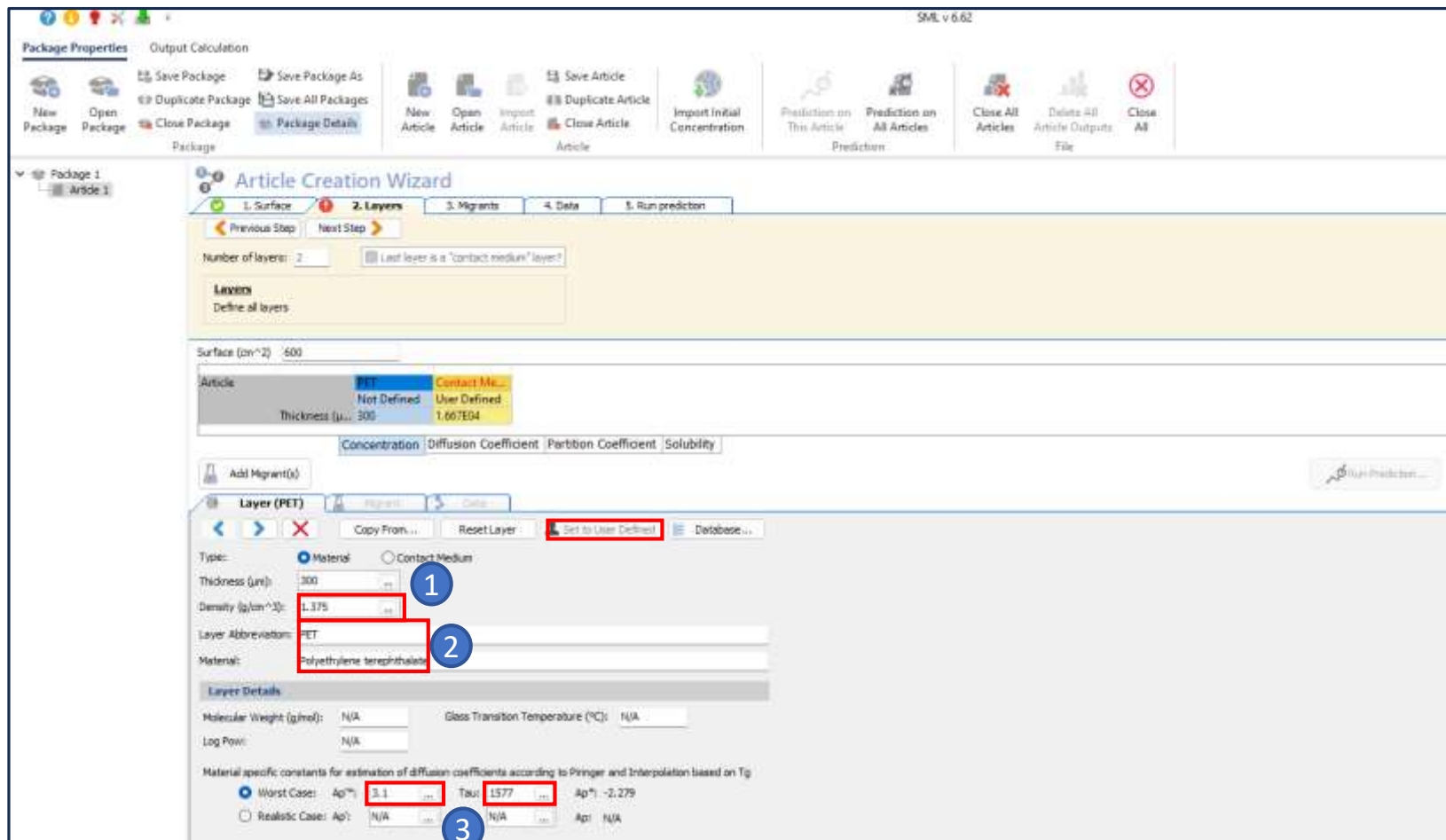
- Geometry: Rectangular
- Contact Surface (cm²): 600
- Volume of Contact Medium (cm³): 1000
- Width (cm): 10
- Height (cm): 10
- Length (cm): 10

The "Surface and mass of contact medium by article" table shows:

Articles	Surfaces (cm ²)	Mass (g)
Article 1	600	

The "Total surface of all articles (cm²):" is 600.

- 2) Define the characteristics of the PET layer in the tab “set to User Defined” (alternatively, material type can be selected and assigned using the database)
“set to User Defined” タブでPETレイヤーの特性を定義します (データベースを使用して材料タイプを選択して割り当てることもできます)



3) Select one migrant using the database (note: benzophenone is a common surrogate in challenge test of PET recycling process)



データベースを使用して移行物質を選択します(注:ベンゾフェノン、PETリサイクルプロセスのチャレンジテストで一般的な代理物質です)

The screenshot displays the SML software interface during the 'Article Creation Wizard' process. The wizard is at step 3, 'Migrants', where the number of migrants is set to 1. A table shows the properties for 'Migrant 1' (BENZOPHE...), including a thickness of 0 and a partition coefficient of 0. A 'Database...' button is highlighted with a red box and a blue circle labeled '2'. An 'Assign' button is also highlighted with a red box and a blue circle labeled '6'. A secondary window titled 'Selecting material for migrants' is open, showing a search for 'benzophenone' in the 'MasterDB (35)'. The search results table lists various compounds, with 'BENZOPHENONE' highlighted in blue and a red box around its row. A blue circle labeled '3' is next to the search input, a blue circle labeled '4' is next to the 'Filter' button, and a blue circle labeled '5' is next to the 'Assign' button in the wizard.

Article 1 (Package 1) - SML v 6.62

Package Properties Output Calculation

Package 1

Article 1

Article Creation Wizard

1. Surface 2. Layers 3. Migrants 4. Data 5. Run prediction

Number of migrants: 1

Migrants

Define all migrants

Surface (cm²): 600

Article	PET	Contact Me...
	Not Defined	User Defined
Thickness (μm)	300	1.667E04
Migrant 1	BENZOPHE...	0

Concentration Diffusion Coefficient Partition Coefficient Solubility

Add Migrant(s)

Migrant (Migrant 1)

Copy From... Reset Migrant Set to User Defined Database...

Migrant Abbreviation: Migrant 1

Migrant: BENZOPHENONE

Migrant Details

Molecular Weight (g/mol):	182.22	Melting Point (°C):	47.8
Density (g/cm ³):	1.1108		
Molecular Volume (Å ³):	174.44	Log Pow:	3.18

Selecting material for migrants

Browse Database

Reference Number: Name: benzophenone

CAS Number: Molecular Weight:

FCM number: Type: ALL

Clear Filters Filter

MasterDB (35) UserDB (1)

Copy To User Database

Name	CAS Number	Reference Number	FCM Number	Molecular Weight (g...	Density (g/cm...
4,4'-DIFLUOROBENZOPHENONE	0000345-92-6	15820	337	218.20	1.3399
4,4'-DIHYDROXYBENZOPHENONE	0000611-99-4	15970; 48720	359	214.22	1.302
4-HYDROXYBENZOPHENONE	0001137-42-4	18885		198.22	
BENZOPHENONE	0000119-61-9	38240	286	182.22	1.1108
4,4'-DIFLUOROBENZOPHENONE-HYDROQUINONE...	0029658-26-2	48470			
2,4-DIHYDROXYBENZOPHENONE	0000131-56-6	48640	318	214.22	0.694993278

Previous Migrant Next Migrant

Assign Close

- 4) Assign an initial concentration of benzophenone in the PET material
 PET材料中のベンゾフェノンの初期濃度 **0.3mg/kg** を割り当てます。

Package Properties Output Calculation

Package: New Package, Open Package, Save Package, Duplicate Package, Close Package, Save Package As, Save All Packages, Package Details

Article: New Article, Open Article, Import Article, Save Article, Duplicate Article, Close Article, Import Initial Concentration

Article Creation Wizard

1. Surface 2. Layers 3. Migrants 4. Data 5. Run prediction

Previous Step Next Step

Specify for each migrant:

- Concentration
- Diffusion coefficient
- Partition coefficient

Surface (cm²) 600

Article	PET	Contact Me...
	Not Defined	User Defined
Thickness (μm)	300	1.667E04
BzP	BENZOPHE...	0.3

Concentration Diffusion Coefficient Partition Coefficient Solubility

Add Migrant(s)

Layer (PET) Migrant (BzP) Data (Concentration)

Extended Properties

Concentration (mg/kg) 0.3

Note: the initial concentration of the contaminant is not important as it will be fitted backwards.

注:汚染物質の最終目標の初期濃度は後半で計算されます。

ここでは実際に含有されるmigrantの初期濃度を入力しています。

- 4) Select the Piringer model for the estimation of the diffusion coefficient, then define the partition coefficient $K_{p/f}$ equal to 1.0
 拡散係数の推定に“ピリンジャーモデル”を選択し、分配係数 $K_{p/f}$ として1.0に定義します。

Article Creation Wizard

1. Surface 2. Layers 3. Migrants 4. Data 5. Run prediction

Previous Step **Next Step** 2

Specify for each migrant:
 - Concentration
 - **Diffusion coefficient**
 - Partition coefficient

Surface (cm²) 600

Article	PET	Contact Me...
	Not Defined	User Defined
Thickness (μ...)	300	1.667E04
BzP	BENZOPHE...	P(7.51E-15) 0.0001

Concentration Diffusion Coefficient Partition Coefficient Solubility

Add Migrant(s)

Layer (PET) Migrant (BzP) **Data (Diffusion Coefficient)**

Diffusion Coefficient Example Temperature (°C): 20

Known
 Interpolation based on Tg
 Piringer 1
 Arrhenius
 Customized Equation
 Bransch Equation
 Welle Equation
 In-Silico

Piringer Calculation Parameters

Layer	Ap'*	3.1
	Tau:	1577
Migrant	Molecular Weight (g/mol):	182.2

Apply Same Mode to This Layer Set All to Default Value Apply Same Mode to All Layers



Article Creation Wizard

1. Surface 2. Layers 3. Migrants 4. Data 5. Run prediction

Previous Step **Next Step** 4

Specify for each migrant:
 - Concentration
 - Diffusion coefficient
 - **Partition coefficient**

Surface (cm²) 600

Article	PET	Contact Me...
	Not Defined	User Defined
Thickness (μ...)	300	1.667E04
BzP	BENZOPHE...	1

Concentration Diffusion Coefficient Partition Coefficient Solubility

Add Migrant(s)

Layer (Contact Medium) Migrant (BzP) **Data (Partition Coefficient)**

Partition coefficient (Kp)

Known 3
 Solubility
 Van't Hoff
 Pow
 Polarity Scale

Known Value

1

Set All to Default Value Apply Same Mode to All Layers and Migrants

- 6) Enter the density of the contact medium (water)
食品接触溶媒として(水)の密度を入力します。

Article Creation Wizard

1. Surface 2. Layers 3. Migrants 4. Data 5. Run prediction

Previous Step Next Step

Input of article parameters is finished.

You can now run a prediction on it.

Surface (cm²) 600

Article	PET	Intact Medium	1
	Not Defined	User Defined	
Thickness (μm)	300	1.667E04	
BzP	BENZOPHE...	1	

Concentration Diffusion Coefficient Partition Coefficient Solubility

Add Migrant(s)

Layer (Contact Medium) Migrant Data

Copy From... Reset Layer

Type: Material Contact Medium

Thickness (μm): 16667

Density (g/cm³): 1

Layer Abbreviation: Contact Medium

Contact Medium Details

Food group (according to Annex III of Regulation (EU) 10/2011 and some more)

Not Defined

Simulant

User Defined

- 7) Run a prediction of the diffusion for the benzophenone
ベンゾフェノンの拡散の予測を実行します。 25℃等温条件 1年間

Article Creation Wizard

1. Surface 2. Layers 3. Migrants 4. Data 5. Run prediction

Input of article parameters is finished.

You can now run a prediction on it.

Surface (cm²) 600

Article Thickness (μm) Contact Medium

PET No. 300

BzP BENZOPHE...

Add Migrant(s)

Layer (Contact Medium)

Type: Material

Thickness (μm): 16667

Density (g/cm³): 1

Layer Abbreviation: Contact Medium

Contact Medium Details

Food group (according to Annex III): Not Defined

Simulant: User Defined

Log Pow: N/A

Parameters required for estimation of partition coefficient based on Pow:

Predictions

Temperature Profiles

Iso Non-Iso Step Modulated Shock Worldwide STANAG Customized Repeated Use

Isothermal Conditions

Temperature = 25 °C

ΔT = 20 °C

Number of Isotherms = 1

Final Temperature = 25 °C

Time Max 1 year

Without Statistics

Monte Carlo Runs

Number of Runs 10

Include Sobol Runs

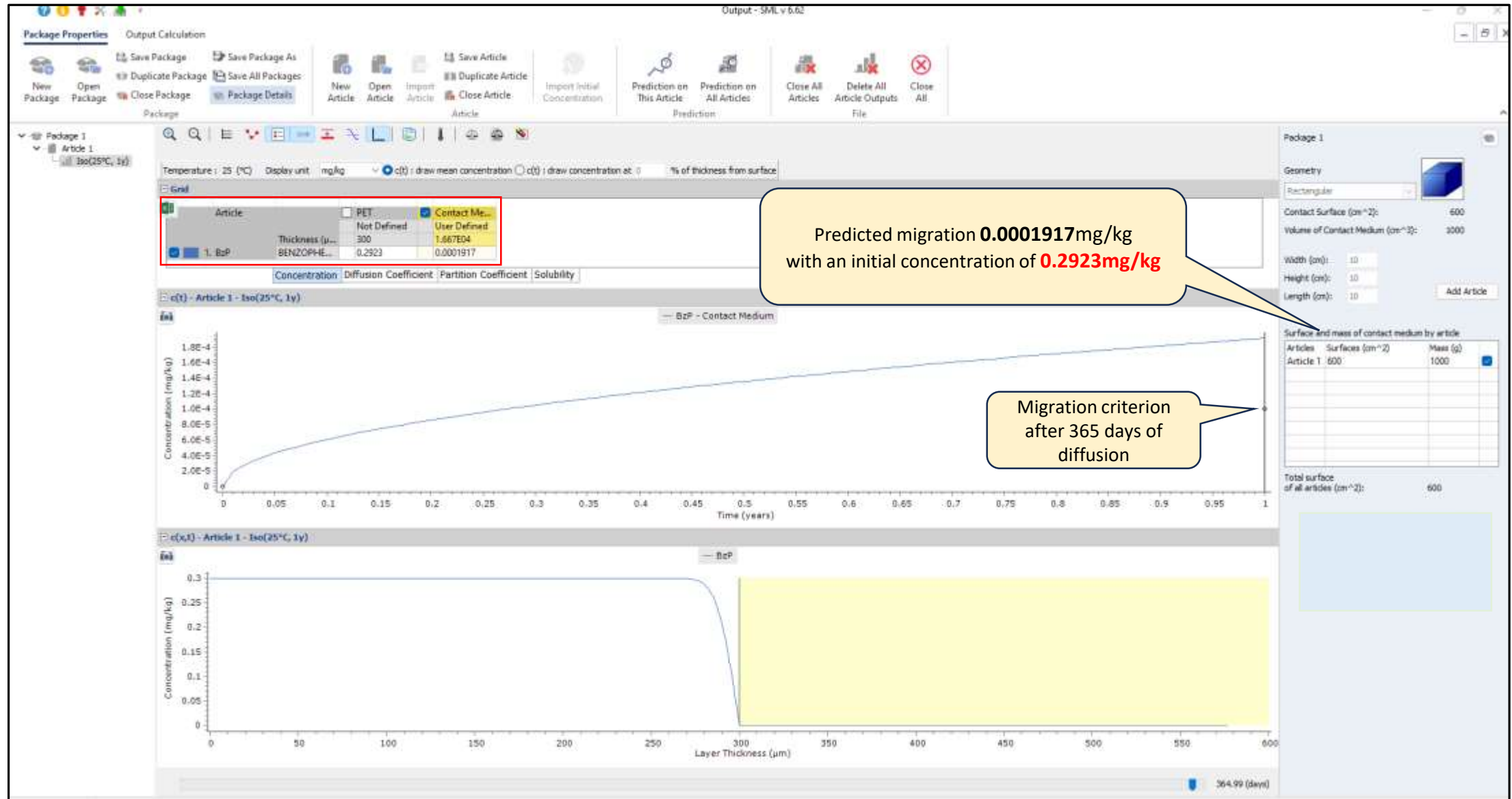
Fast Distribution

Save... Load...

Number of steps for this output: 100

OK Cancel

9) 赤線枠から25°C365日後の疑似溶媒中の移行量（溶出濃度）が0.2923mg/kgであることを示しています。



Predicted migration **0.0001917mg/kg**
with an initial concentration of **0.2923mg/kg**

Migration criterion
after 365 days of
diffusion

Cmod valueが 0.156と予測されました。

このようにSML6のOption機能Fitting_moduleを使用して最大許容濃度を越えない初期濃度の計算が可能です。

The screenshot shows the SML6 software interface. The main window is titled 'Article 1 (Package 1) - SML v 6.62'. The 'Article Creation Wizard' is active, showing the '5. Run prediction' step. The 'Input of article parameters is finished' message is displayed. The 'Surface (cm²)' is set to 600. The 'Article' table shows 'PET' with 'Not Defined' and 'Benzophenone' with 'Defined'. The 'Concentration (mg/kg)' field is set to 0.156, and the 'Optimize' button is highlighted. The 'Fitting Mode' window is open, showing a graph of Cmod vs Loops. The graph shows Cmod starting at a high value and dropping to a constant value of 0.156 after approximately 2 loops. The 'Fitting Mode' window also shows the 'Optimize' button highlighted. The 'Extended Properties' section shows the 'Concentration (mg/kg)' field set to 0.156, and the 'Optimize' button is highlighted. The 'Parameter Name' table shows 'PET-Concentration(mg/kg)' with a 'Value' of 0.156.

ただしこのFitting_moduleを使用しなくてもSML6の基本機能により、初期濃度計算が可能です。最終ページの15ページを参照してください。

Final remarks

This calculation can be adapted to fit different scenarios (i.e. EFSA scenarios for toddler or adult) or to calculate Cmod of other surrogates used in challenge test of PET recycling process: use the prepared package “Cmod_calculation” and enter the parameters of the desired migrant.

この計算は、さまざまなシナリオ(幼児または成人向けのEFSAシナリオなど)に適合させるか、PETリサイクルプロセスのチャレンジテストで使用される他のサロゲートのCmodを計算するように調整できます:

準備されたパッケージ「Cmod_calculation」を使用して、目的とする移行物質のパラメータを入力します。移行物質の入力は10種類をセットすることができます。(最大18種類まで確認済み)

other than bottles.

また、物品の接触時間や温度を変更して、ボトル以外の包装容器について拡散係数を評価することができます

Fitting_moduleの機能は実測値から拡散係数を求めることができることが基本機能です。

Data files for SML 6.7



Cmod_calculation.sml



migration_infant_scenario.txt



migration_toddler_scenario.txt



migration_adult_scenario.txt

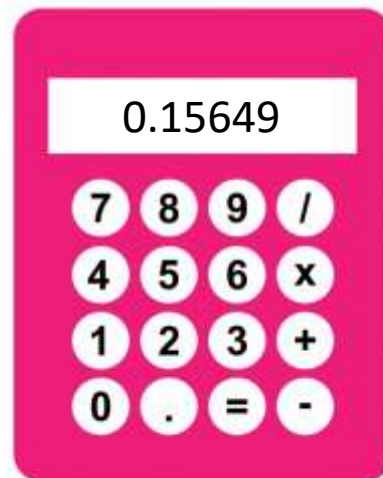
初期濃度**0.3mg/kg**,25℃365日後の疑似溶媒中の移行量_溶出濃度が**0.0001917mg/kg**であることを示しています。

25℃365日後の疑似溶媒中の移行量（溶出濃度）が**0.0001mg/kg**となるときの初期濃度 X は？

$$0.3\text{mg/kg} : 0.0001917\text{mg/kg} = X \text{ mg/kg} : 0.0001 \text{ mg/kg}$$

移行モデルのガイドラインによれば、FCM中の初期濃度が1%以内であれば、初期濃度と食品疑似溶媒への移行量は比例関係が成立するとされています。

比例関係があることから簡単な移行量が1点求まればこの値からポリマーに含まれる移行物質の初期濃度が算出できます。



$$\begin{aligned} X &= (0.3 \times 0.0001) / 0.0001917 \\ &= 0.156\text{mg/kg} \end{aligned}$$

筆算または電卓で計算できます！