

SML5によるシミュレーション操作例の説明

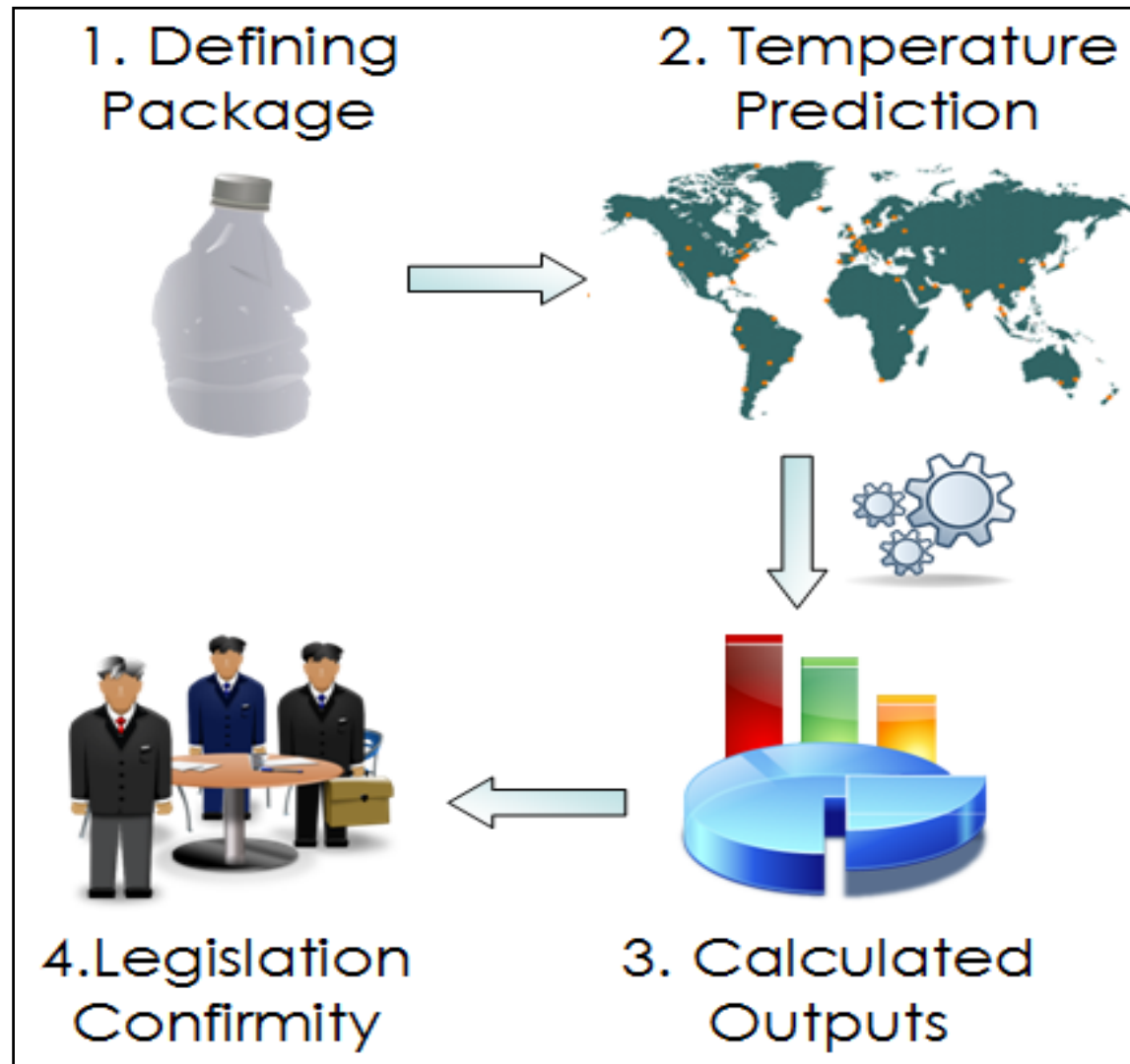


PETのAp-ValueはEU規制のガイドラインに沿って、Tg点温度前後の70°C以下と70°C以上の2種類から選択可能 Version 5.09より対応可能
ただしデータベースのAp-Valueは1種類につき、手動で操作する。

作成 2018-02-21 Ver. 5.231
AKTS日本総代理店 (株)パルメトリクス

1: 溶出試験条件の設定

2: 環境温度での溶出量予測



4: 規制に従っているか？

3: 予測(計算)結果の出力

SML5の9ステップ操作手順

- | | |
|---|--------------------------|
| ① Package (食品包装物) 形状を設定 | SML geometry |
| ② ポリマー (Layer) 数を定義 Max n=10 | |
| ③ ポリマーの種類を定義
ポリマーの厚さ (μm単位) | SML5 database |
| ④ 食品接触材料 (Contact medium) を定義 | SML5 database |
| ⑤ 移行物質 (Substance) を定義
Substanceの濃度 (ppm) n=10 | SML5 database |
| ⑥ 拡散定数の設定 (選択) | Ap-Value, Tg, Bransdsch, |
| ⑦ 分配係数の設定 | Solibility, Pow, Kp=1, |
| ⑧ 溶出試験条件の温度条件設定 | |
| ⑨ <u>SML5によるシミュレーション</u> | 計算実行 |

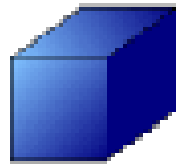
Version 5.231の画面 この操作説明にはVersion 5.09も混在していますが基本操作は同じです。
Wizard機能をOFFとした場合の表示例となっています。

The screenshot displays the SML v 5.231 software interface. The main window is titled "Article 1 (Package 0)". On the left, a tree view shows "Package 0" containing "Article 1". The central area has a "Surface (cm²)" input field set to 600 and an "Article" list. Below this are tabs for "Concentration", "Diffusion coefficient", "Partition coefficient", and "Solubility", along with "Add substance(s)" and "Run prediction..." buttons. The right sidebar shows "Package 0" settings: Geometry (Rectangular), Contact surface (cm²): 600, Volume of contact medium (cm³): 1000, and dimensions (Width, Height, Length) all set to 10. A table titled "Surface and mass of contact medium by article" is shown below, with one row for "Article 1" having a surface of 600 and a checked "Mass (g)" column. The total surface of all articles is 600 cm². A "Switch package in fitting mode" button is at the bottom of the sidebar. The Windows taskbar at the bottom shows the time as 16:50 on 2018/02/20.

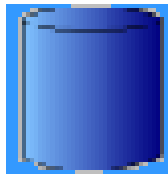
Articles	Surfaces (cm ²)	Mass (g)
Article 1	600	<input checked="" type="checkbox"/>

① Package (食品包装物) 形状を設定

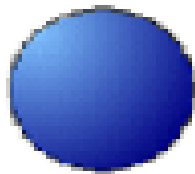
Packageの形状の種類を選択(前頁右端の画面のみ抽出)



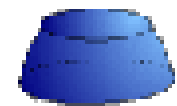
Rectangular



Cylindrical



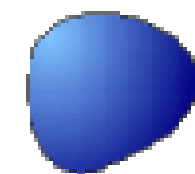
Spherical



Spherical segment




Truncated cone

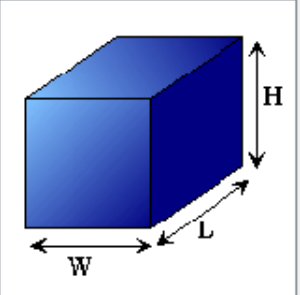


Surface / volume ratio


Package

Geometry:  Rectangular

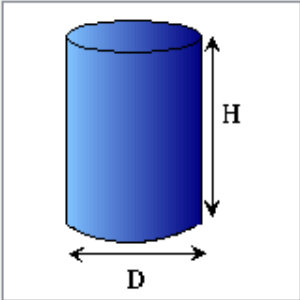
Contact surface (cm²): 600 Width (cm): 10
Volume of contact medium (cm³): 1000 Height (cm): 10
Length (cm): 10




Package

Geometry:  Cylindrical

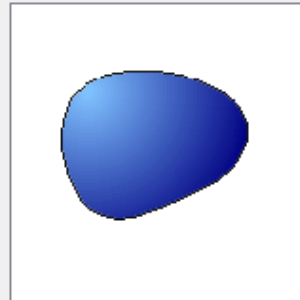
Contact surface (cm²): 213.6 Diameter (cm): 4
Volume of contact medium (cm³): 188.5 Height (cm): 15



Package

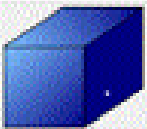
Geometry:  Surface / volume ratio

Surface/volume ratio (dm⁻¹): 0.4836 Contact surface (cm²): 483.598
Volume of contact medium (cm³): 1000 Volume of foodstuff (cm³): 1000



① Package (食品包装物) 形状を設定
直方体 W/L/H 寸法 & 表面積 cm^2

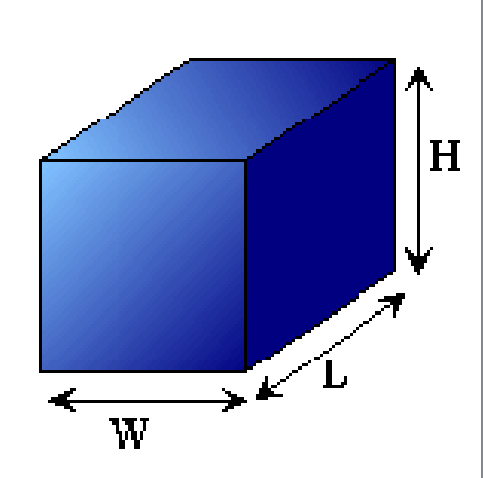
Package

Geometry:  Rectangular

Contact surface (cm^2): 600 Width (cm):

Volume of contact medium (cm^3): 1000 Height (cm):

Length (cm):



Articles

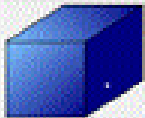
Articles	Surfaces (cm^2)	X

Total: 0 cm^2

New Article をクリックしてSurfaceを入力する。

① Package (食品包装物) 形状を設定

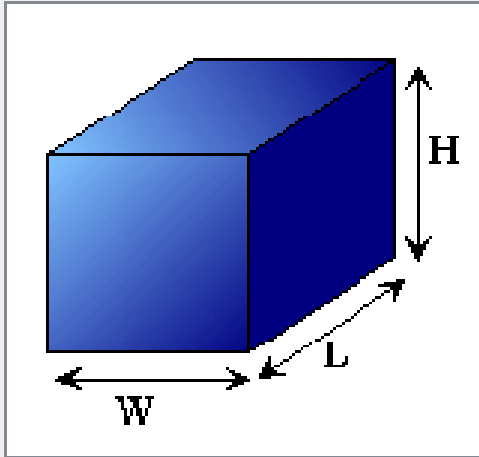
Package

Geometry:  Rectangular

Contact surface (cm²): 600 Width (cm): 10

Volume of contact medium (cm³): 1000 Height (cm): 10

Length (cm): 10




Articles

Articles	Surfaces (cm ²)	Total: 600 cm ²
Article 1	600	

New article

Use wizard for articles

Continue 

Cancel

EU方式⇒6面体: 600cm²
JP方式⇒5面体: 500cm²

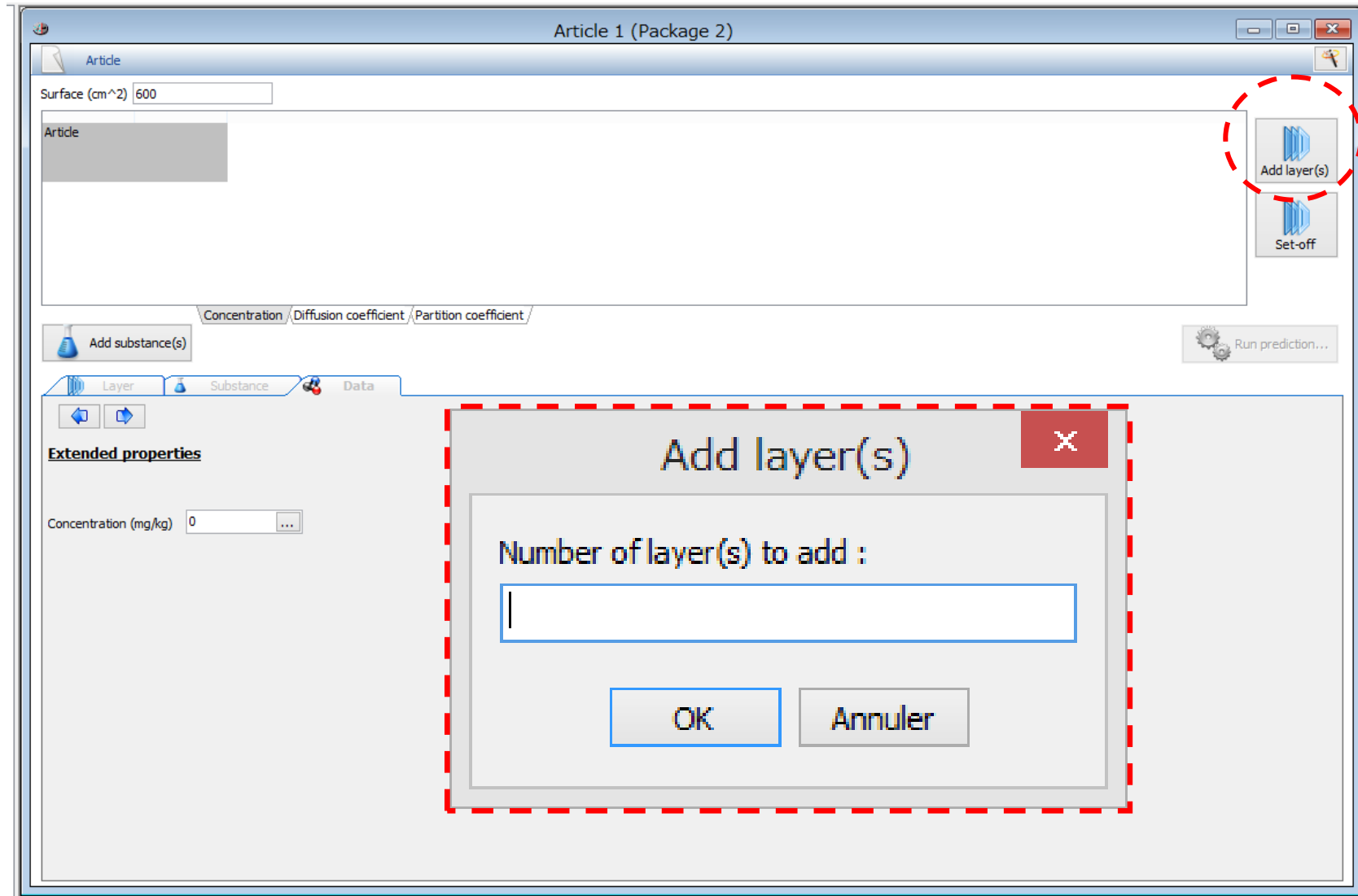
② ポリマー(Layer)数を定義 最大 n=10

The screenshot displays the SML v 5.231 software interface. The main window shows the configuration for 'Article 1 (Package 0)'. The 'Surface (cm²)' is set to 600. The 'Article' section is currently empty. A red dashed circle highlights the 'Add layer(s)' button in the top right corner of the article configuration area. A dialog box titled 'Add layer(s)' is open in the center, with a text input field for 'Number of layer(s) to add :'. The right-hand panel shows the 'Package 0' configuration, including 'Geometry: Rectangular' and dimensions: Width (cm): 10, Height (cm): 10, Length (cm): 10. Below this, a table titled 'Surface and mass of contact medium by article' shows the following data:

Articles	Surfaces (cm ²)	Mass (g)
Article 1	600	<input checked="" type="checkbox"/>

Below the table, the 'Total surface of all articles (cm²):' is shown as 600. The bottom status bar indicates the version '5.231' and the date '2018/02/20'.

② ポリマー(Layer)数を定義 最小n=2 最大 n=10
Add layerのコマンドをクリックすると赤破線枠が表示されます。



② ポリマー(Layer)数を定義

最大 $n=10$

Setoffの計算 $n=\infty$

Article 1 (Package 3)

Article

Surface (cm²)

Article	Layer 1	Layer 2
	Not defined	Not defined
Thickness (μm)	100	100

単層フィルムの場合

Layer1はポリマー

Layer2は食品溶媒

Version5.231ではLayer 0(ポリマー),
Layer1(食品溶媒)になっています。

Package 0
Article 1

Article 1 (Package 0)

Surface (cm²) 600

Article	Layer 0	Layer 1
	Not defined	Not defined
Thickness (µm)	100	100

Concentration / Diffusion coefficient / Partition coefficient / Solubility

Add substance(s)

Run prediction...

Add layer(s) Set-off

Layer (Layer 0) Substance Data

Copy from...
 Reset layer
 Database
 Set to user defined

Type: Polymer Contact medium

Thickness (µm): 100

Density (g/cm³): 1

Layer abbreviation: Layer 0

Material: Not defined

Layer details


Molecular weight (g/mol): 160 Glass transition temperature (°C): -100

Electronegativity (kJ/mol): 10

Material specific constants for estimation of diffusion coefficients according to Piringer

Upper limit: A^{*p}: 13.1 Tau: 1577 A^{*p}: 7.721
 Realistic case: A^p: 13.1 Tau: 1577 A^p: 7.721

Package 0

Geometry: Rectangular 

Contact surface (cm²): 600

Volume of contact medium (cm³): 1000

Width (cm): 10

Height (cm): 10

Length (cm): 10

Add Article

Surface and mass of contact medium by article

Articles	Surfaces (cm ²)	Mass (g)
Article 1	600	<input checked="" type="checkbox"/>

Total surface of all articles (cm²): 600

Switch package in fitting mode

Article	Layer 1	Layer 2
	Not defined	Not defined
Thickness (μm)	100	100

③ Layer1:ポリマーの種類を選択(定義)します。

ポリマーの厚さ (μm 単位)を入力します。

④ Polymeの選択を確認してDatabaseをクリックします。

Concentration / Diffusion coefficient / Partition coefficient

Add substance(s)

Layer (Layer 1) Substance Data

Type: Polymer Contact medium

Thickness (μm): 100 ...

Density (g/cm^3): 1 ...

Copy from...

Reset layer

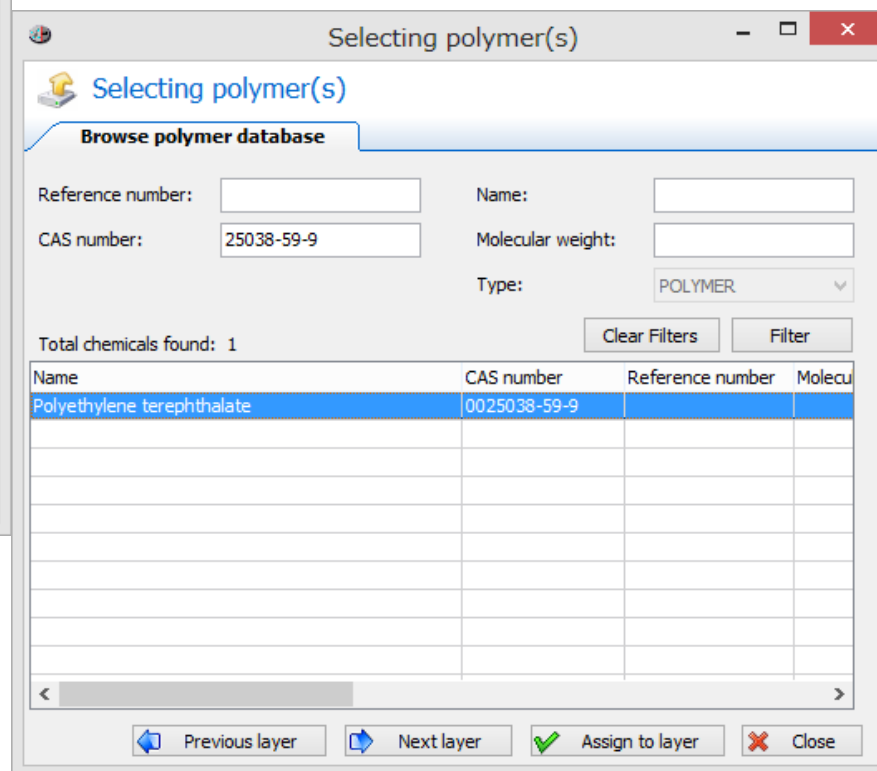
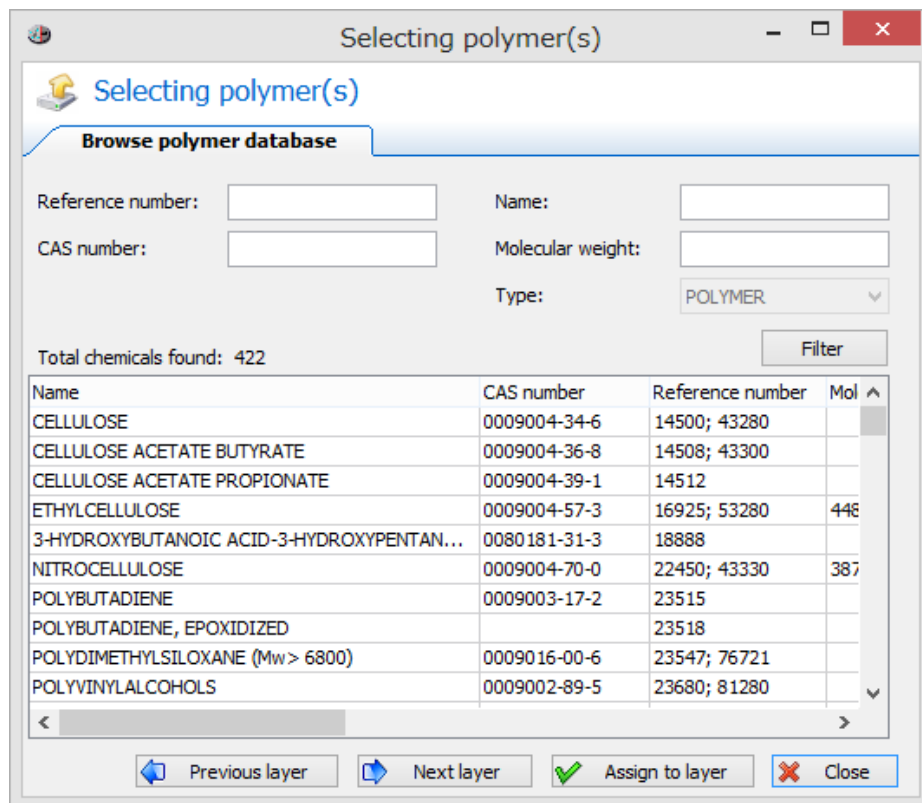
Material : Not defined

Layer abbreviation : Layer 1

④ Database をクリックします。

polymer としてPET (Cas.No25038-59-9)を入力

下図はVersion5.082の場合です。
Version5.231は次ページに示します。



④ Layer1: ポリマーの種類を選択(定義)します。

polymer としてPET (Cas.No25038-59-9)を入力すると

Polyethylene terephthalate (modelling T < 70-C) 0025038-59-9

Selecting polymer(s)

Selecting polymer(s)

Browse polymer database

Reference number:

CAS number:

Name:

Molecular weight:

Type: POLYMER

Total chemicals found: 1

Clear Filters Filter

Name	CAS number	Reference number	Molecu
Polyethylene terephthalate (modelling T < 70-C)	0025038-59-9		

PETについては溶出条件がT_g温度の70°C前後で移行モデルの拡散係数の選択を行う必要があります。

溶出条件が70°C以下の場合、databaseにあるPET T_g<70°Cを選択します。

溶出条件が70°C以上の場合、Table6に示すようにAp-Valueは6.4となります。

そのため、次ページに示すようにSet to user defineでAp-Valueを手動入力にて再登録します。

Polymer	A _p ^{1*}	τ
PET >T _g (70 °C)	6.4	1577
PET <T _g (70 °C)	3.1	1577
PEN	5.0	1577

PETの場合、注意！

Table 6: Parameters for PET and PEN

Version.5.231の画面

Reference number:

Name:

CAS number:

Molecular weight:

Type:

Total chemicals found: 3

Name	CAS number	Reference number	Molecu
Polyethylene terephthalate (PET) (modeling all T)	0025038-59-9		
Polyethylene terephthalate (PET) (modeling T > 7...	0025038-59-9		
Polyethylene terephthalate (PET) (modeling T < 7...	0025038-59-9		50000

Clear Filters Filter

Previous layer Next layer Assign to layer

Reference number:

Name:

CAS number:

Molecular weight:

Type:

Total chemicals found: 3

Name	CAS number	Reference number	Molecu
Polyethylene terephthalate (PET) (modeling all T)	0025038-59-9		
Polyethylene terephthalate (PET) (modeling T > 7...	0025038-59-9		
Polyethylene terephthalate (PET) (modeling T < 7...	0025038-59-9		50000

Clear Filters Filter

Previous layer Next layer Assign to layer Finish

Missing parameters

Molecular weight not available in the database.

Input of molecular weight is required for estimation of diffusion coefficients and partition coefficients.

Please enter molecular weight (g/mol)

Glass transition temperature not available in the database.

Input of polymer Tg (glass transition temperature) is required for estimation of diffusion coefficients with 'Interpolation based on Tg'.

Please enter glass transition temperature (°C)

Electronegativity not available in the database.

Input of electronegativity is required for estimation of partition coefficients based on solubility and temperature.

Please enter electronegativity (kJ/mol)

Don't show this window again

If you have no information, keep the default value displayed.
If you keep the default value, please be aware that the calculation results will be a rough estimate only.

PETの場合、Tg点温度を入力すること

数値を入力して

かつ

確認ボタンをクリックすることが必要

Missing parameters

Molecular weight not available in the database.

Input of molecular weight is required for estimation of diffusion coefficients and partition coefficients.

Please enter molecular weight (g/mol)

Glass transition temperature not available in the database.

Input of polymer Tg (glass transition temperature) is required for estimation of diffusion coefficients with 'Interpolation based on Tg'.

Please enter glass transition temperature (°C)

Electronegativity not available in the database.

Input of electronegativity is required for estimation of partition coefficients based on solubility and temperature.

Please enter electronegativity (kJ/mol)

Don't show this window again

If you have no information, keep the default value displayed.
If you keep the default value, please be aware that the calculation results will be a rough estimate only.

OK

SML v 5.231

File Administration Window ?

Physical memory used: 30%

Package

Package 0

Article 1

Article 1 (Package 0)

Surface (cm²) 600

Article	Layer 0	Layer 1
	Polyethylene...	Not defined
Thickness (μm)	100	100

Concentration / Diffusion coefficient / Partition coefficient / Solubility

Add substance(s)

Run prediction...

Add layer(s)

Set-off

Layer (Layer 0)

Substance

Data

Copy from... Reset layer Database Set to user defined

Type: Polymer Contact medium

Thickness (μm): 100

Density (g/cm³): 1.4

Layer abbreviation: Layer 0

Material: Polyethylene terephthalate (PET) (modeling T > 70-C)

Layer details

Molecular weight (g/mol): 1000000 Glass transition temperature (°C): 70

Electronegativity (kJ/mol): 10

Material specific constants for estimation of diffusion coefficients according to Piringer

Upper limit: A¹p: 6.4 Tau: 1577 A²p: 1.021

Realistic case: A¹p: 3.2 Tau: 1577 A²p: -2.179

Package 0

Geometry: Rectangular

Contact surface (cm²): 600

Volume of contact medium (cm³): 1000

Width (cm): 10

Height (cm): 10

Length (cm): 10

Add Article

Surface and mass of contact medium by article

Articles	Surfaces (cm ²)	Mass (g)
Article 1	600	<input checked="" type="checkbox"/>

Total surface of all articles (cm²): 600

Switch package in fitting mode

5.231

Version_5.09の場合 Version5.231では改善されています。
いったんはTgが70°C以下のPETを選択してからSet to user definedをクリックしてupper limit
のAp-Valueを3.1から6.4に手動入力する。Materialの欄も書き換えておくこと。 不要

Layer (Layer 1) Substance Data

Type: Polymer Contact medium Thickness (µm): 100 ...

Density (g/cm3): 1.4 ...

Copy from... Layer abbreviation: Layer 1

Reset layer

Database Material: Polyethylene terephthalate (modelling T >70 degee C (手動入力する))

Set to user defined

Material specific constants for estimation of diffusion coefficients according to Piringer

Upper limit: A*p: 6.4 ... Tau: 1577 ... A*p: 1.021

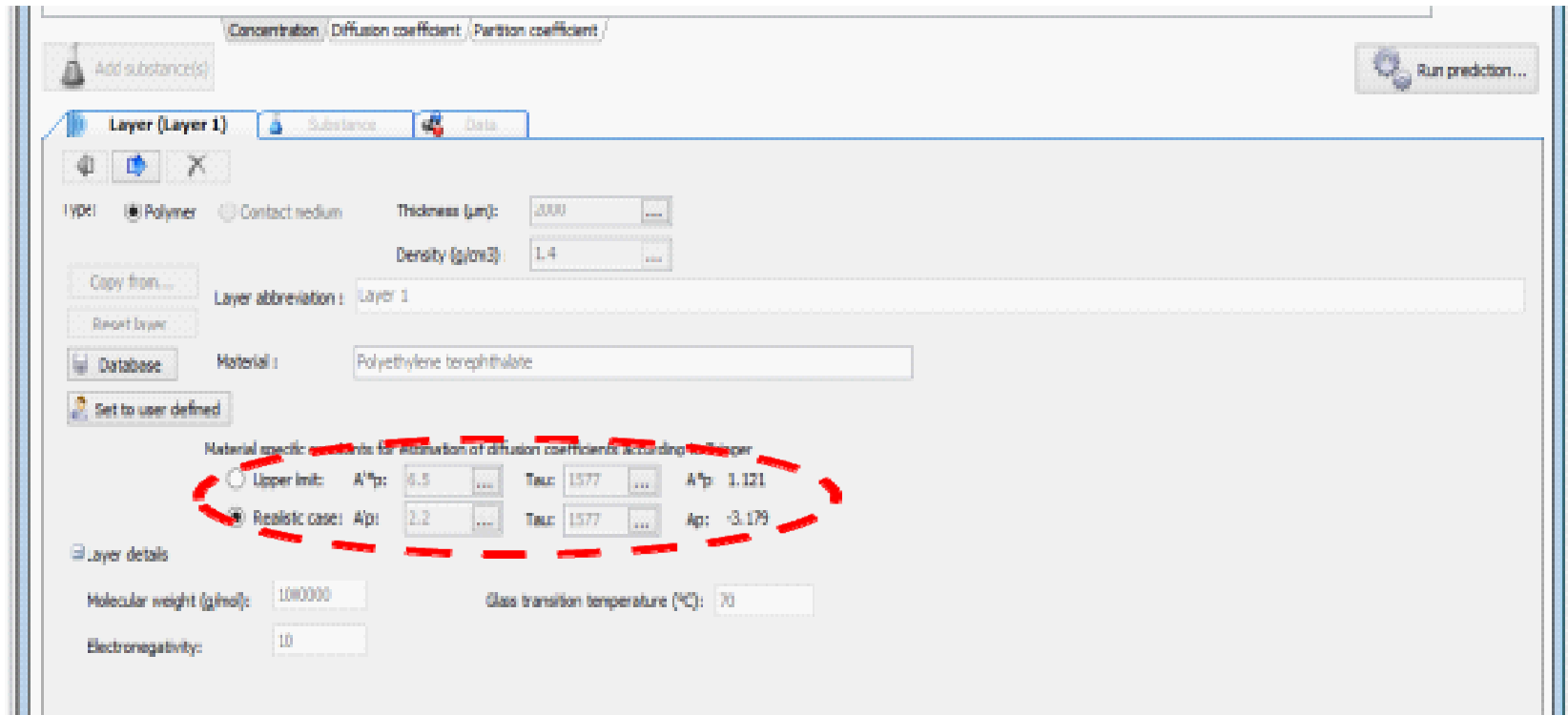
Realistic case: A*p: -1.5 ... Tau: 1577 ... Ap: -6.879

Layer details

Molecular weight (g/mol): 1000000 Glass transition temperature (°C): 70

Electronegativity (kJ/mol): 10

より現実的な溶解曲線を求めるときは
拡散定数 (Ap-Value) はrealisticを選択



Upper と Realisticでは濃度が1桁違うことがあります。

PETの70°C以上の温度におけるRealistic値は別途手動入力すること

④Contact Medium(食品疑似物)リストは
Annex V of Regulation(EU)10/2011 and some more

注:日本で使用される食品疑似物が追加されています。

Layer (Contact Medium) Substance Data

← → ✕

Type: Polymer Contact medium

Thickness (µm): 16667 ...

Density (g/cm³): 1 ...

Copy from...

Reset layer

Layer abbreviation : Contact Medium

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

- User defined
- User defined
- lipophilic foods (fats and oils, free fat on surface) / lipophile Lebensmittel (Fette und Öle, freie Fette an
- Vegetable oil - food simulant (olive oil, sunflower oil, margarine, etc.) / Pflanzen- - Lebensmittelsimulan
- lipophilic foods - oil in water emulsion (milk and milk products, sour cream, etc.) / lipophile Lebensmittel -
- Ethanol 50% - food simulant (lipophilic foods - oil in water emulsions) / Lebensmittelsimulanz (lipophile L
- Ethanol 20% - food simulant (alcoholic foods < 20%) / Ethanol 20% - Lebensmittelsimulanz (alkoholisch
- Acetic acid 3% - food simulant (acidic foods, pH < 4.5) / Essigsäure 3% - Lebensmittelsimulanz (saure L
- Chocolate and chocolate products / Schokolade und Schokoladenprodukte

Article	Layer 1	Contact Medi...
	Polyethylene...	Ethanol 50...
Thickness (μm)	100	1.667E04

エタノール50%が選択された。

ポリマーに含まれる化学物質の選択

Concentration / Diffusion coefficient / Partition coefficient

Add substance(s)

Add substance(s) ✕

Number of substance(s) to add :

OK Annuler

Layer (Contact Medium) Substance Data

Navigation icons: back, forward, delete

Type: Polymer Contact medium

Thickness (μm): 16667

Density (g/cm3): 1

Copy from...

Reset layer

Layer abbreviation : Contact Medium

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

Ethanol 50% - food simulant (lipophilic foods - oil in water emulsions) / Lebensmittelsimulanz (lipophile I

Parameters for estimation of partition coefficients based on Pow

Worst Case A: 0.4 B: -2

Realistic A: 0.4 B: -1

⑤ 移行物質 (Substance) の選択

添加剤A

CAS NO.0002082-79-3

Selecting substance(s)

Selecting substance(s)

Browse substance database

Reference number:

Name:

CAS number:

Molecular weight:

Type:

Total chemicals found: 1

Name	CAS number	Reference number	Molecular weight	Density	Melting point
OCTADECYL 3-(3,5-DI-tert-BUTYL-4-HYDROXYPHE...	0002082-79-3	68320	530.88		241.01

化学データベースには分子量やPowの値が登録されています。
ただし登録されていないこともありますので要注意

Clear Filters

Filter

Electronegati...	Aip mean	Tau mean	Aip wc	Tau wc	Glass Trans 7...	pow
						13.41

⑤ 移行物質 (Substance) を定義

Substanceの濃度 (ppm) 添加剤Aの濃度を記入 (5000ppm)

Article

Surface (cm²) 600

Article	Layer 1	Contact Medi...
	Polyethylene...	Ethanol 50...
Thickness (µm)	100	1.667E04
Substance 1	OCTADECYL ...	0

Contact medium 初期濃度は0 ppm

Concentration / Diffusion coefficient / Partition coefficient

Add substance(s)

Layer (Layer 1) Substance (Substance 1) Data (concentration)

Extended properties

Concentration (mg/kg) 0

⑥ 拡散定数の設定 (主な選択枝) Piringer, Tg, Brandsch

Article 1 (Package 2)

Article

Surface (cm²) 600

Article	Layer 1	Contact Medi...	
	Polyethylene...	Ethanol 50...	
Thickness (μm)	100	1.667E04	
Substance 1	OCTADECYL ...	P(7.03E-15)	0.0001

Concentration / Diffusion coefficient / Partition coefficient

Add substance(s)

Layer (Layer 1) Substance (Substance 1) Data (diffusion coef) (2)

Diffusion coefficient

Known

Interpolation based on Tg (2)

Piringer (2)

Arrhenius

Customized equation

Brandsch equation

Diffusion coefficient (cm²/s): 1E-11 (1) Set to de

Set all to default value

Apply same mode to this layer (3)

Apply same mode to all layers

Diffusion coefficient

Known

Interpolation based on Tg (2)

Piringer (2)

Arrhenius

Customized equation

Brandsch equation (2)

Package 0
Article 1

Article 1 (Package 0)

Surface (cm²) 600

Article	Layer 1	Contact Medi...
	Polyethylene...	Ethanol 50%
	Thickness (µm) 100	1.667E04
Substance 1	OCTADECYL ... P(6.361E-15)	P(1.99E-06)

Concentration / Diffusion coefficient / Partition coefficient / Solubility

Add substance(s) Run prediction... Add layer(s) Set-off

Layer (Contact Medium 1) Substance (Substance 1) **Data (Diffusion coefficient)**

Diffusion coefficient Example temperature (°C): 20

Known
 Interpolation based on Tg
 Pringer Example for 20°C (cm²/s): P(1.99E-06)
 Arrhenius
 Customized equation
 Bransch equation
 Welle equation

Set all to default value
Apply same mode to this layer

Package 0

Geometry: Rectangular

Contact surface (cm²): 600
Volume of contact medium (cm³): 1000

Width (cm): 10
Height (cm): 10
Length (cm): 10

Add Article

Surface and mass of contact medium by article

Articles	Surfaces (cm ²)	Mass (g)	
Article 1	600	1000	<input checked="" type="checkbox"/>

Total surface of all articles (cm²): 600

Switch package in fitting mode

塩化ビニリデン樹脂の場合などでは
Ap-Valueがなく、Piringer法が選択できません。

SML5では代わって



2) ポリマーのTg温度によりAp-Valueを推定

3) ポリマーのTg温度と分子量によりAP-Valueを推定

Article	Layer 1	Contact Medi...
	Polyethylene...	Ethanol 50...
Thickness (µm)	100	1.667E04

重要！ : Ap-Value (Piringer法) を使用しない場合の操作
Reset LayerをクリックしてDatabaseから選択されたポリマーを削除します。

Concentration / Diffusion coefficient / Partition coefficient

Add substance(s)

Layer (Contact Medium) | Substance | Data

← | → | ✕

Type: Polymer Contact medium Thickness (µm): 16667 ...

Density (g/cm³): 1 ...

Copy from... Layer abbreviation: Contact Medium

Reset layer

Food group (according to Annex V of Regulation (EU) 10/2011 and some more)
Ethanol 50% - food simulant (lipophilic foods - oil in water emulsions) / Lebensmittelsimulanz (lipophile I ▼

Parameters for estimation of partition coefficients based on Pow

Worst Case A: 0.4 B: -2

Realistic A: 0.4 B: -1

Article 1 (20130524-01)

Article

Surface (cm²) 600

Layer	Contact Medi...
Not defined	Ethanol 50...
Thickness (μm) 100	1.667E04
Substance 1 OCTADECYL...	5000 0

Reset layerによりLayerはNot definedと表示が変化します。

Concentration / Diffusion coefficient / Partition coefficient

Add substance(s)

Run prediction...

Layer (Layer)

Type: Polymer Contact medium

Thickness (μm): 100

Density (g/cm³): 1

Copy from...

Layer abbreviation: Layer

Reset layer

Database

Material: Not defined

Set to user defined

Material specific constants for estimation of diffusion coefficients according to Piringer

Upper limit: A^{*p}: 13.1 Tau: 1577 A^{*p}: 7.721

Realistic case: A_p: 13.1 Tau: 1577 A_p: 7.721

Layer details

Molecular weight (g/mol): 1000000

Glass transition temperature (°C): -100

Electronegativity: 1

ここで初めて分子量 (g/mol) と Tg 温度 Glass transition temp が設定可能となります。

ポリマーがデータベースに登録されていなくても2つのパラメータを設定すれば Interpolation based on Tg と Brandsch 法が設定できます。

ポリマー中の移行物質の拡散定数は 優先1:Piringer式 $p(7.03E-15)$ を選択

Article	Layer 1	Contact Medi...
	Polyethylene...	Ethanol 50...
Thickness (μm)	100	1.667E04
Substance 1	OCTADECYL ...	P(7.03E-15) 0.0001

Concentration Diffusion coefficient Partition coefficient

Add substance(s)

Layer (Layer 1) Substance (Substance 1) Data (diffusion coefficient)

Diffusion coefficient

Known

Interpolation based on Tg

Piringer Example for 20°C (cm^2/s): P(7.03E-15)

Arrhenius

Customized equation

Brandsch equation

添加剤B,C,D すべてPiringer選択可能

補足説明

Article		Layer 1	Contact Medi...
		Polyethylene...	Ethanol 50...
	Thickness (μm)	100	1.667E04
Substance 1	OCTADECYL ...	P(7.03E-15)	0.0001

- Thickness(μm) 1.667E04とは
食品溶媒1000mL (cm³)が600cm² に接触したときの
平均厚み

$$1000/600 = 1.66\text{cm} = 1.66\text{E}04\text{mm}$$

⑦ 分配係数の設定

Solubility, Pow, Kp=1,

Article	Layer	Contact Medi...
	Polyethylene...	Ethanol 50...
Thickness (μm)	100	1.667E04
Substance 1	OCTADECYL ...	0

Concentration / Diffusion coefficient / Partition coefficient

Add substance(s)

Layer (Contact Medium) / Substance (Substance 1) / Data (partition coefficient)

Partition coefficient (Kp)

Known 1 ...

Solubility

Pow

通常はPowを選択します。

添加剤A CAS NO.0002082-79-3


Clear Filters Filter

Glass Trans T...	pow
	13.41

⑦ 分配係数の設定 Solubility, Pow

Article	Layer	Contact Medi...
	Polyethylene...	Ethanol 50...
	Thickness (μm)	100
		1.667E04
Substance 1	OCTADECYL ...	P(28.9)

P(28.9)

 Add substance(s)

Concentration / Diffusion coefficient / Partition coefficient

Layer (Contact Medium) / Substance (Substance 1) / Data (partition coefficient)

← →

Partition coefficient (Kp)

Known $K_{pf} = \exp(B + A * \log(\text{Pow}))$

Solubility
A [food]: 0.4
B [food]: -2

Pow
Log(Pow) [chemical]: 13.41
Kpf: 28.9

Partition coefficient (Kp)

Known $K_{pf} = \exp(B + A * \log(\text{Pow}))$

Solubility
A [food]: 0.4
B [food]: -2

Pow
Log(Pow) [chemical]: 13.41
Kpf: 28.9

P(28.9) ⇒ P(2112)となる。

SML v 5.231

File Administration Window ?

Physical memory used: 31%

Package

Package 0

Article 1

Article 1 (Package 0)

Surface (cm²) 600

Article	Layer 1	Contact Medi...
	Polyethylene...	Ethanol 50%
	Thickness (μm)	1.667E04
Substance 1	OCTADECYL ...	P(2312)

Concentration / Diffusion coefficient / Partition coefficient / Solubility /

Add substance(s)

Run prediction...

Add layer(s)

Set-off

Layer (Contact Medium 1) Substance (Substance 1) **Data (Partition coefficient)**

Partition coefficient (Kp)

$Kpf = 10^{(B + A * \log(Pow))}$

Known
 Solubility
 Arrhenius
 Pow

A [food]: 0.4
 B [food]: -2
 Log(Pow) [chemical]: 13.41
 Kpf: 2312

Note : The estimation of Kpf based on Pow is limited to temperature below 60°C

Set all to default value

Apply same mode to all layers and substances

Package 0

Geometry: Rectangular

Contact surface (cm²): 600

Volume of contact medium (cm³): 1000

Width (cm): 10

Height (cm): 10

Length (cm): 10

Add Article

Surface and mass of contact medium by article

Articles	Surfaces (cm ²)	Mass (g)	
Article 1	600	1000	<input checked="" type="checkbox"/>

Total surface of all articles (cm²): 600

Switch package in fitting mode

5.231



Run prediction...

⑧ 溶出温度条件の設定 121°C30min

Predictions

Time max 30 min

Without statistics

Predictions

Temperature profiles

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

Isothermal conditions

Temperature = 121 °C

$\Delta T = 20$ °C

Number of isotherms = 1

Final Temperature = 121 °C

Isothermal conditions

Temperature = 121 °C

$\Delta T = 20$ °C

Number of isotherms = 1

Final Temperature = 121 °C

Time max 30 min

Without statistics

Monte Carlo runs

Number of Runs 10

Include Sobol Runs

Fast distribution

Save... Load...

OK Cancel



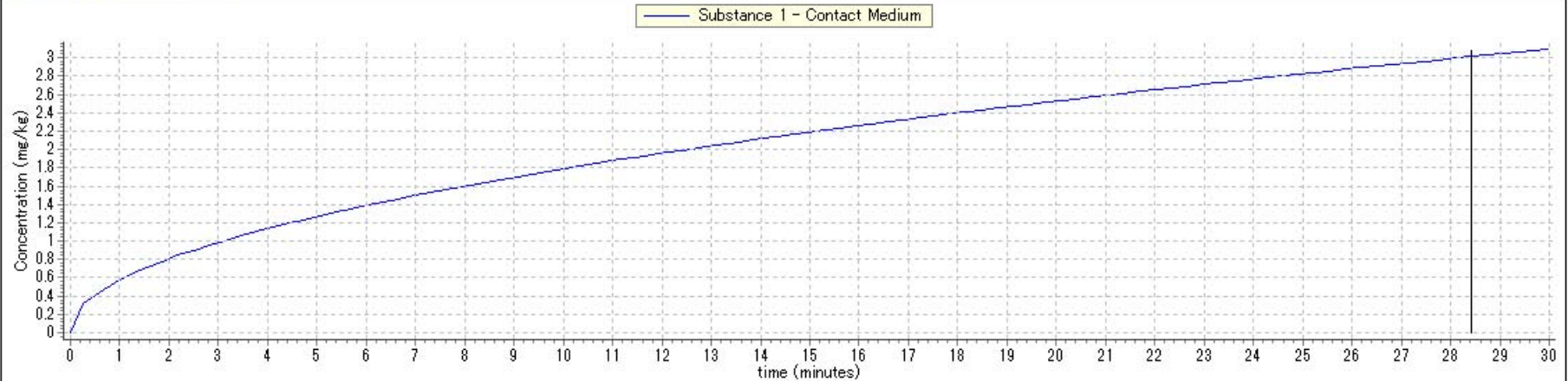
Output Calculation

121°C30minの溶出試験シミュレーション

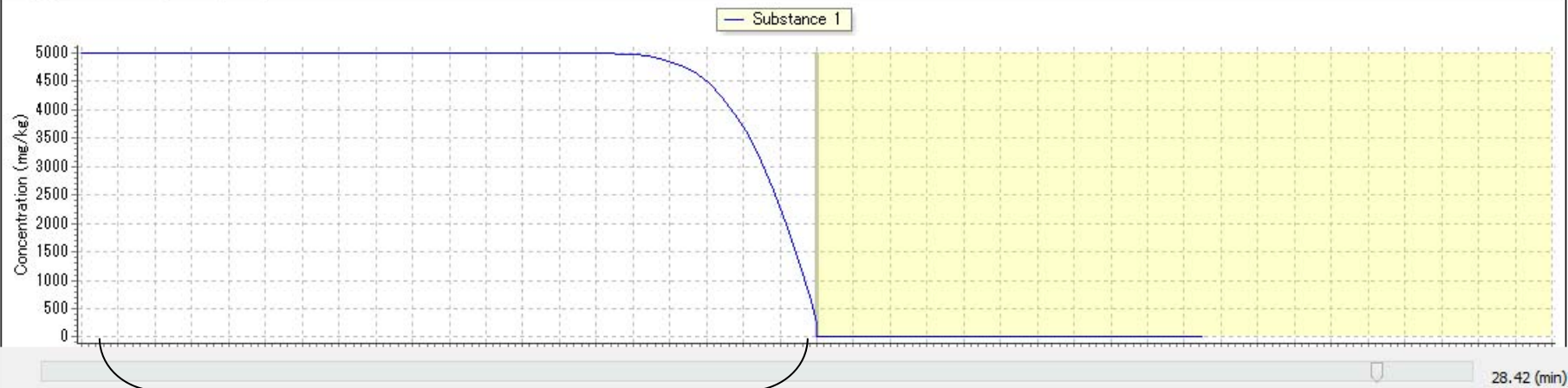


Grid

c(t) - Article 1 - Iso(121°C ,30min)



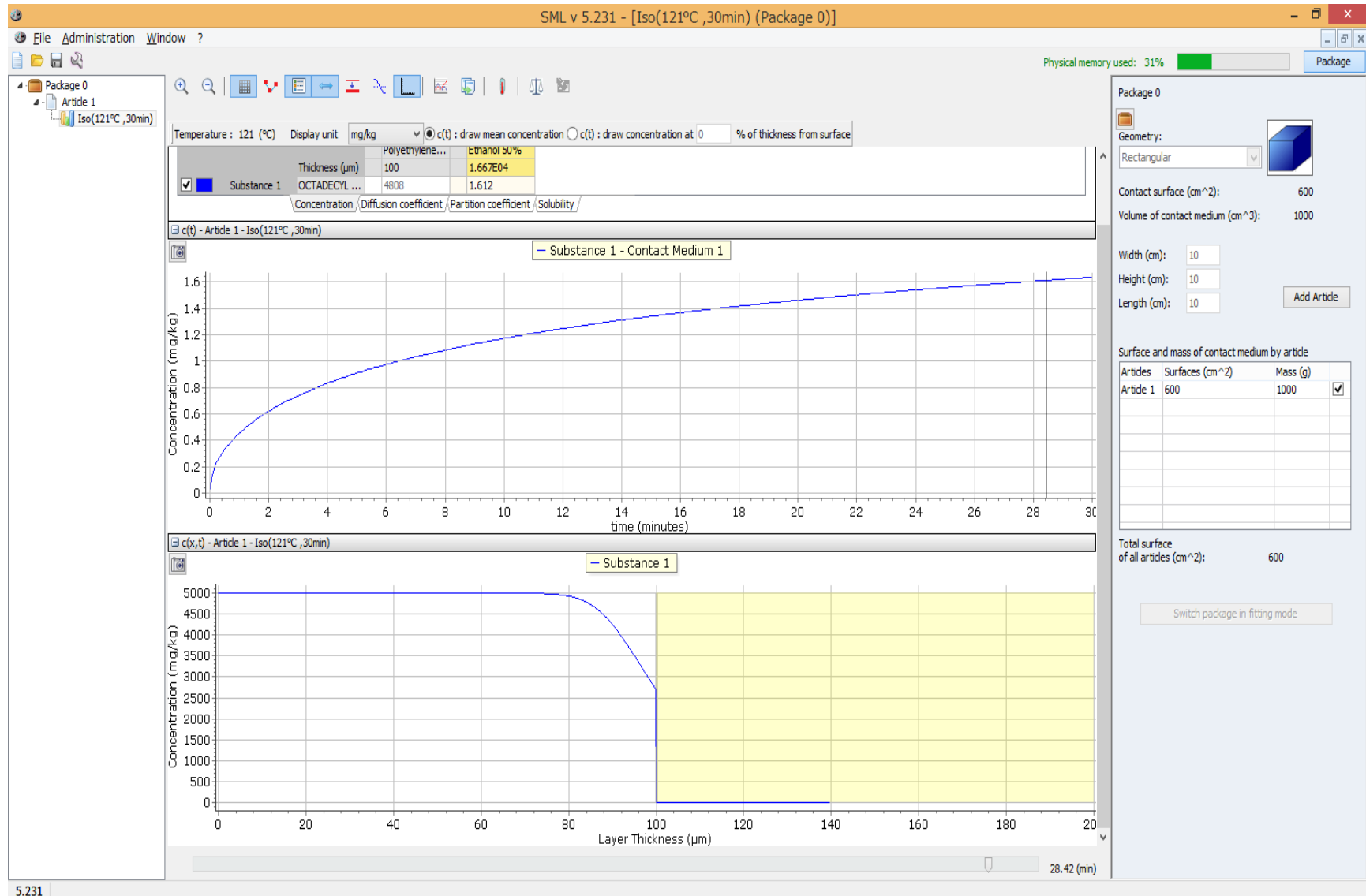
c(x,t) - Article 1 - Iso(121°C ,30min)



厚み方向の化学物質濃度分布

注PET :Tg>70°CのAp-Valueを使っています。

121°C 30minの溶出量 3ppm ⇒ 1.6ppm



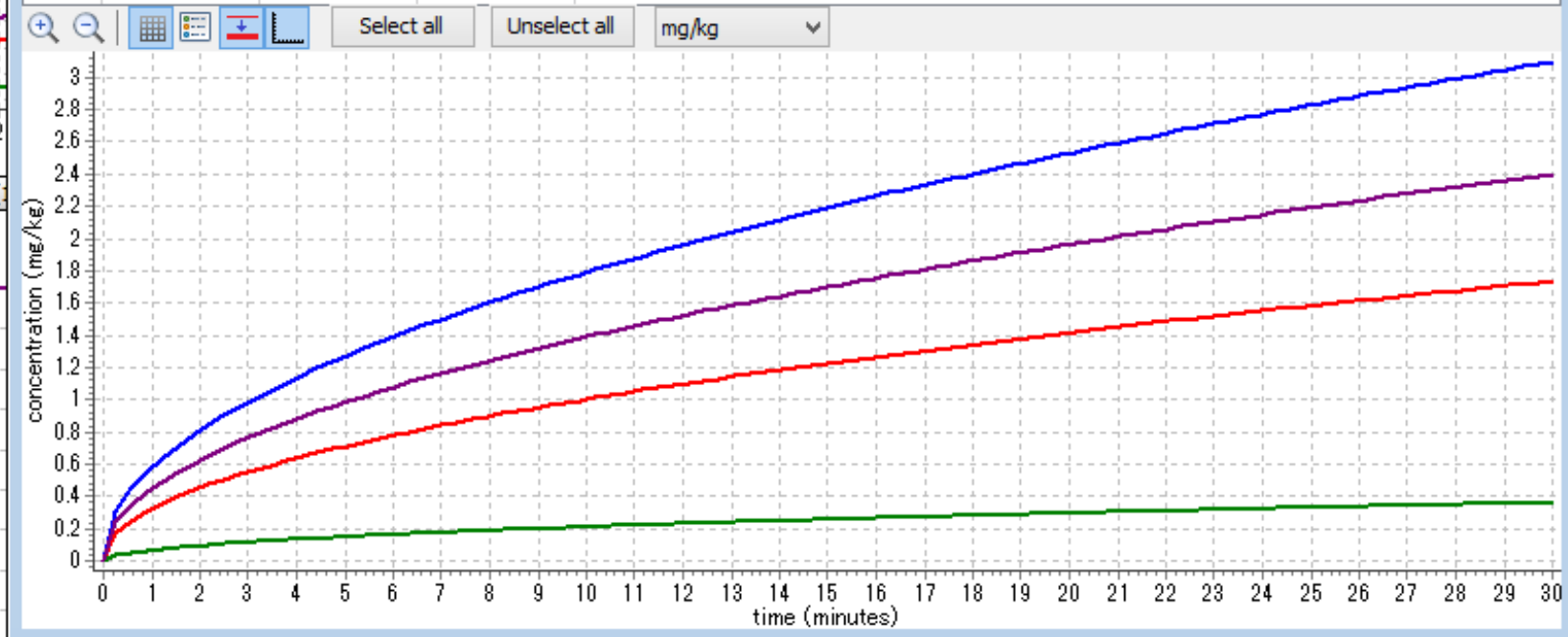
Article	Layer 1	Contact Medi...
	Polyethylene...	Ethanol 50...
	Thickness (μm)	100
Substance 1	OCTADECYL ...	P(28.9)
Substance 2	PHOSPHORO...	P(187.2)
Substance 3	PENTAERYT...	P(343.8)
Substance 4	Calcium stea...	P(0.1353)

PET1 100μm
 エタノール50%
 121°C・30min

Article 1 - Iso(121°C,30min)

	Layer 1	Contact Medium
■ Substance 1	<input type="checkbox"/>	<input checked="" type="checkbox"/>
■ Substance 2	<input type="checkbox"/>	<input checked="" type="checkbox"/>
■ Substance 3	<input type="checkbox"/>	<input checked="" type="checkbox"/>
■ Substance 4	<input type="checkbox"/>	<input checked="" type="checkbox"/>

Substance1	添加剤A	3.095ppm
Substance2	添加剤B	1.733ppm
Substance3	添加剤C	0.361ppm
Substance4	添加剤D	2.401ppm



Substance 1 - OCTADECYL 3-(3,5-DI-tert-BUTYL-4-HYDROXYPHENYL) PROPIONATE

Properties

Density (g/cm³) : 1

Molecular weight (g/mol) : 530.88

POW : 13.41

Initial concentration

Layer 1 : 5000mg/kg

Partition coefficient

Layer 1 / Contact Medium : 28.9 (POW based)

Diffusion coefficient

Layer 1 : 7.030E-15 cm²/s (Piringer based)

Contact Medium : 1.000E-04 cm²/s (Known)

Time/Temperature conditions :

Iso 121°C

30 min.

Migration :

SML (mg/kg of contact medium): Specific Migration Limit

QM (mg/kg of packaging) : Quantity Maximum

QMA (mg/dm² of packaging): Quantity Maximum per Area

DL (mg/kg of contact medium): Detection Limit

Green : Compliant

Red : Not compliant

Legislation (EU) No.10/2011
に 準拠するか否か？ の出力例

緑色表示は準拠する場合

赤色表示は準拠しない場合

☐ Substance 1 - 3.095E+00 mg/kg - OCTADECYL 3-(3,5-DI-tert-BUTYL-4-HYDROXYPHENYL) PROPIONATE

No ☐ European Union : Regulatory : (EU) No 10/2011

SML	QM	QMA	DL
6	-	-	-

☐ European Union : Regulatory : 2002/72/EC

SML	QM	QMA	DL
6	-	-	-

Japan/Tokyoの気候条件 40年間暴露試験 = 121°C・30min

