

Introduction to Migration Modelling

オプション機能 Fitting_module **Part2**

等温温度条件・2水準、溶出量実測データ 各1点から
アレニウス式の**拡散式のみ**を算出します。
分配係数 K_{pf} は既知、またはPowアプローチとし、Fitting計算は**拡散式のみ**に限定しています。
(40°Cと70°Cの溶出量実測データ 各1点から 40°C~70°Cの溶出試験を予測します。)



2023_07_02 Version1.0

この操作マニュアルを独習する前に、必ずお読みください。

この資料はSML6のOption:Fitting_Moduleの独習するためにAKTS社が作成した [操作トレーニング・マニュアル](#) です。下記の40, 70°Cの実測データ 2ファイルと解析SMLファイル_4ファイルがあれば独習することが可能です。これらのファイルは最終ページに記載されています。このファイルが必要な方は パルメトリクスまでご連絡ください。メールに添付してお送りします。

“溶出温度条件が2水準で各温度条件で2点の実測データがあれば、アレニウス式で拡散係数を求めることが可能”としています。この事例ではさらにシンプルな条件で初期濃度(0 min後の溶出量)をゼロとし、1点の実測値から拡散係数を求めています。このような場合、MigrantとSimulant間の分配係数 K_{pf} はPowアプローチ、あるいは K_{pf} =既知とし、拡散係数のみを算出しています。この事例では酢酸3, 4%水溶液を疑似溶媒としており、Powアプローチが使うことができないので、分配係数は既知とし、 $K_{pf}=1$ を使用しています。なお拡散係数と分配係数の2つを実測データから算出するには、各温度水準ごとに実測データは3個以上、必要です。3個以上の実測データから拡散係数と分配係数を求める操作マニュアルも作成されています。

この操作マニュアルは150ページありますが、すべてSML6.6の操作画面で説明しています。150ページすべてについて解説・説明はしていませんが、説明のない部分の画面はなにをしているのか？ご自分で考えながら最後まで読破してください。説明文があるページは部分は画面を次々に送ると、パラパラ動画のような画面の動きを見ることができます。Fitting_ModuleはSML6のOption機能の中で、操作の難易度が高いソフトウェアです。当社でFitting_moduleの操作方法がどうしてもわからず、AKTSから操作マニュアルを支給されて初めて操作手順を理解することができました。Fitting_Moduleの機能を理解するにはこのマニュアルを読破することが必要です。

SML6.6のオプション機能 Fitting moduleの操作トレーニング・マニュアル
Fitting_Moduleを独習するためのトレーニング・キットです。

溶出温度が40°Cと70°Cの2水準の実測データ2点から アレニウス式で拡散式を解析します。

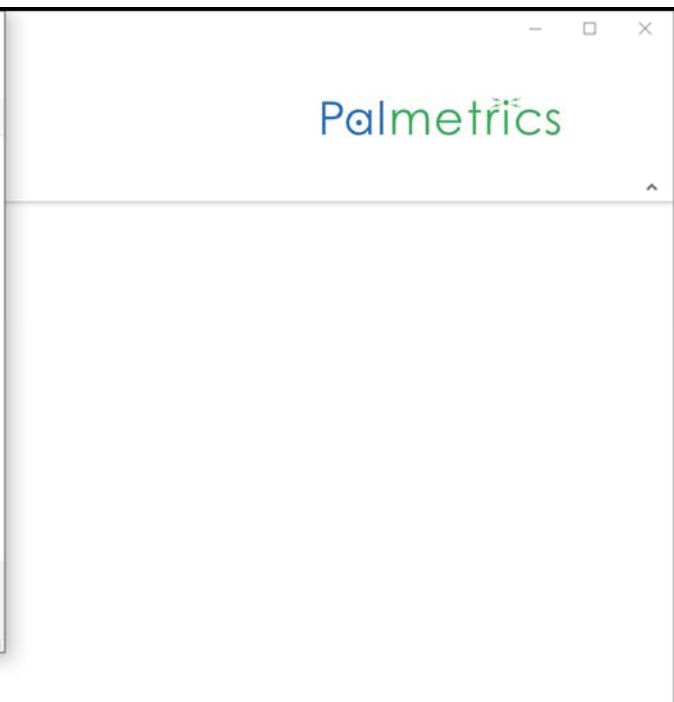
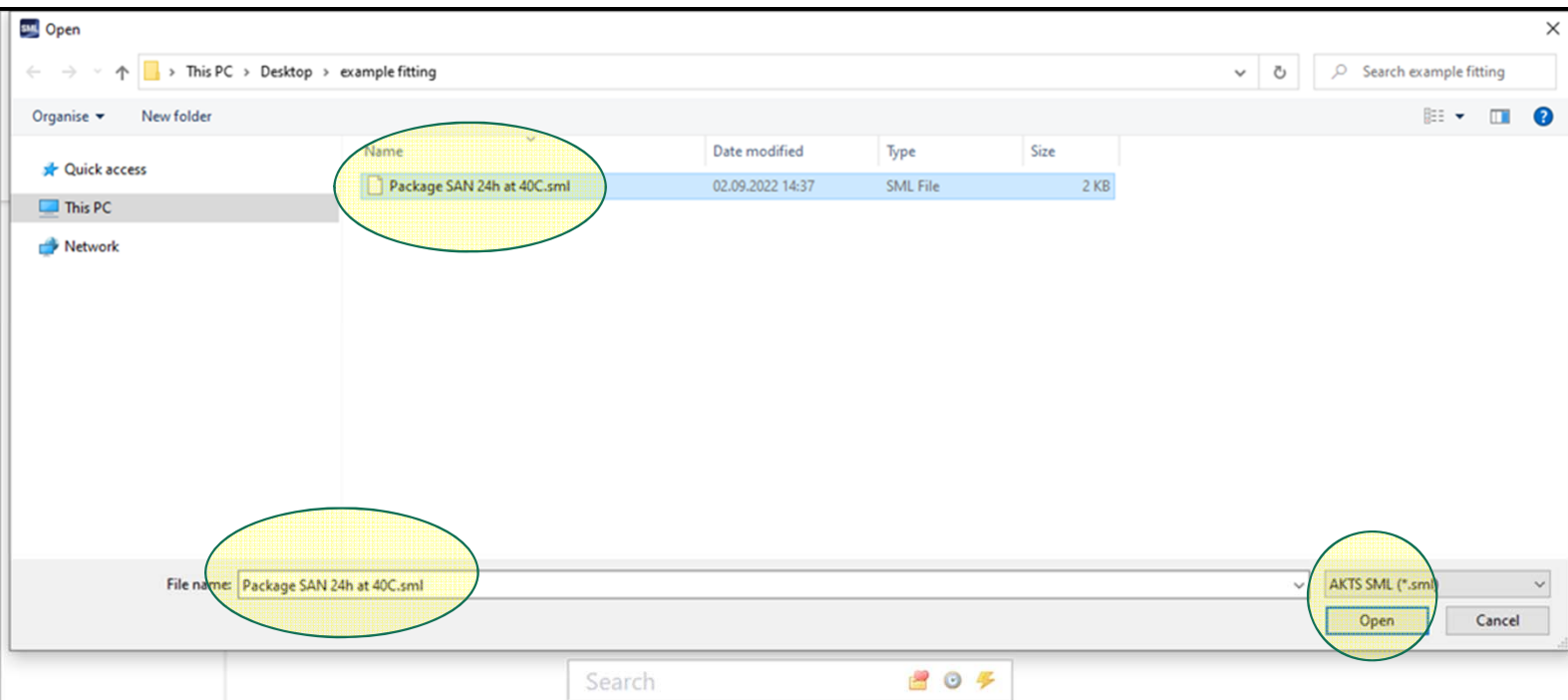
03: 下段のような40,70°C溶出試験データが得られたとします。このデータから拡散式と分配係数を求めます。
初期値は0と仮定しているので、実際には各温度で溶出量データは1点ということになります。

File 名		
220902_To_0_24h at ...		
ファイル(E) 編集(E) 書式(O) 表示(V) ヘルプ(H)		
t (h)	T (° C)	S (mg/kg)
0	40	0
24	40	0.0058

File 名		
220902_To_0_2h at 70C -...		
ファイル(E) 編集(E) 書式(O) 表示(V) ヘルプ(H)		
t (h)	T (° C)	S (mg/kg)
0	70	0
2	70	0.0054



04: クリックして Package を Open します。



05: Package SAN 24h at 40C.sml ファイルをクリックして Open をクリックします。

Surface (cm²) 600

Article	Layer 1	Contact Me...
	ACRYLONIT...	Acetic acid ...
Thickness (μ...	300	1.667E04
Migrant 1	ACRYLONIT...	P(N/A)

Concentration Diffusion Coefficient Partition Coefficient Sol

Partition coefficient (Kp) Example Temperature (°C): 0

Known
 Solubility
 Van't Hoff
 Pow
 Polarity Scale

Pow Calculation Parameters

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

Food A: Missing
Food B: Missing
Migrant Log Pow: 0.25

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

この事例では拡散係数Dpのみを解析します。分配係数を実測データから予測することはしません。Powアプローチが選択できないので、分配係数は既知としてKpf = 1を定義します。

Surface (cm²) 600

Article	Layer 1	Contact Me...
	ACRYLONIT...	Acetic acid ...
Thickness (μ...	300	1.667E04
Migrant 1	ACRYLONIT...	1

Concentration Diffusion Coefficient Partition Coefficient Sol

Partition coefficient (Kp)

Known
 Solubility
 Van't Hoff
 Pow
 Polarity Scale

Known Value

1

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

この事例では拡散係数Dpのみを解析します。分配係数を実測データから予測することはしません。今回のように初期値の0データ以外の実測データが1点の場合は、分配係数はPowアプローチ または分配係数は既知とします。この事例では疑似溶媒が酢酸3%, or 4%のためPowアプローチは選択できません。

Package Properties Output Calculation

- Package SAN 24h at 40C
- Article 1

Surface (cm²) 500

Article	Layer 1	Contact Medi...
	ACRYLONIT...	Acetic acid 3%
Thickness (μm)	300	1.667E04
Migrant 1	ACRYLONIT...	0

Layer (Layer 1) Migrant Data

Type: Polymer Contact Medium

Thickness (μm): 300

Density (g/cm³): 1.09

Layer Abbreviation: Layer 1

Material: ACRYLONITRILE-STYRENE, COPOLYMER (AS)

Layer Details

Molecular Weight (g/mol): 471.64 Glass Transition Temperature (°C): 97

Log Pow: N/A

Material specific constants for estimation of diffusion coefficients according to Pringer

Upper Limit: A^{*}p: N/A τ: N/A A^{*}p: N/A
 Realistic Case: A^{*}p: N/A τ: N/A A^{*}p: N/A

Coefficients for estimation of diffusion coefficients according to Welle

a (K⁻¹): N/A c (A³): N/A
 b (cm²*s⁻¹): N/A d (K⁻¹): N/A

07:Layer1はアクリルニトロル_コポリマー 厚み300μm
Migrantはアクリルニトリル 濃度 15ppm

Package SAN 24h at 40C

Geometry: Rectangular

Contact Surface (cm²): 600

Volume of Contact Medium (cm³): 1000

Width (cm): 10

Height (cm): 10

Length (cm): 10

Surface and mass of contact medium by article

Articles	Surfaces (cm ²)	Mass (g)
Article 1	600	1000

Total surface of all articles (cm²): 600

Package SAN 24h at 40C
Article 1

Surface (cm²) 500

Article	Layer 1	Contact Medi...
	ACRYLONIT...	Acetic acid 3%
	Thickness (μm)	300
		1.567E04
Migrant 1	ACRYLONIT...	1E-11
		0.0001

Concentration Diffusion Coefficient Partition Coefficient Solubility

Add Migrant(s)

Run Prediction...

Layer (Layer 1) Migrant Data

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

Type: Polymer Contact Medium

Thickness (μm): 300

Density (g/cm³): 1.09

Layer Abbreviation: Layer 1

Material: ACRYLONITRILE-STYRENE, COPOLYMER (AS)

Layer Details

Molecular Weight (g/mol): 471.64 Glass Transition Temperature (°C): 97

Log Pow: N/A

Material specific constants for estimation of diffusion coefficients according to Pringler

Upper Limit: A^{*p}: N/A Tau: N/A A^{*p}: N/A

Realistic Case: A^p: N/A Tau: N/A A^p: N/A

Coefficients for estimation of diffusion coefficients according to Welle

a (K⁻¹): N/A c (A³): N/A

b (cm²*s⁻¹): N/A d (K⁻¹): N/A

08:Layer1の拡散係数は 1E-11
ContactMediumの拡散係数は 0.0001に設定する。

Package SAN 24h at 40C

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

Total surface of all articles (cm²): 600

Switch Package in Fitting Mode

Package SAN 24h at 40C

Article 1

Surface (cm²) 600

Article	Layer 1	Contact Medi...
	ACRYLONIT...	Acebic acid 3%
	Thickness (μm)	300
		1.667E04
Migrant 1	ACRYLONIT...	1E-11
		0.0001

Layer (Layer 1) Migrant (Migrant 1) Data (Diffusion Coefficient)

Diffusion Coefficient

Known

Interpolation based on Tg

Pringer

Arrhenius

Customized Equation

Bransch Equation

Welle Equation

In-Silico

Diffusion Coefficient (cm²/s): 1E-11

09:Layer1の拡散係数は knownを選択して 1E-11
ContactMediumの拡散係数は 0.0001に設定する。

Package SAN 24h at 40C

Geometry: Rectangular

Contact Surface (cm²): 600

Volume of Contact Medium (cm³): 1000

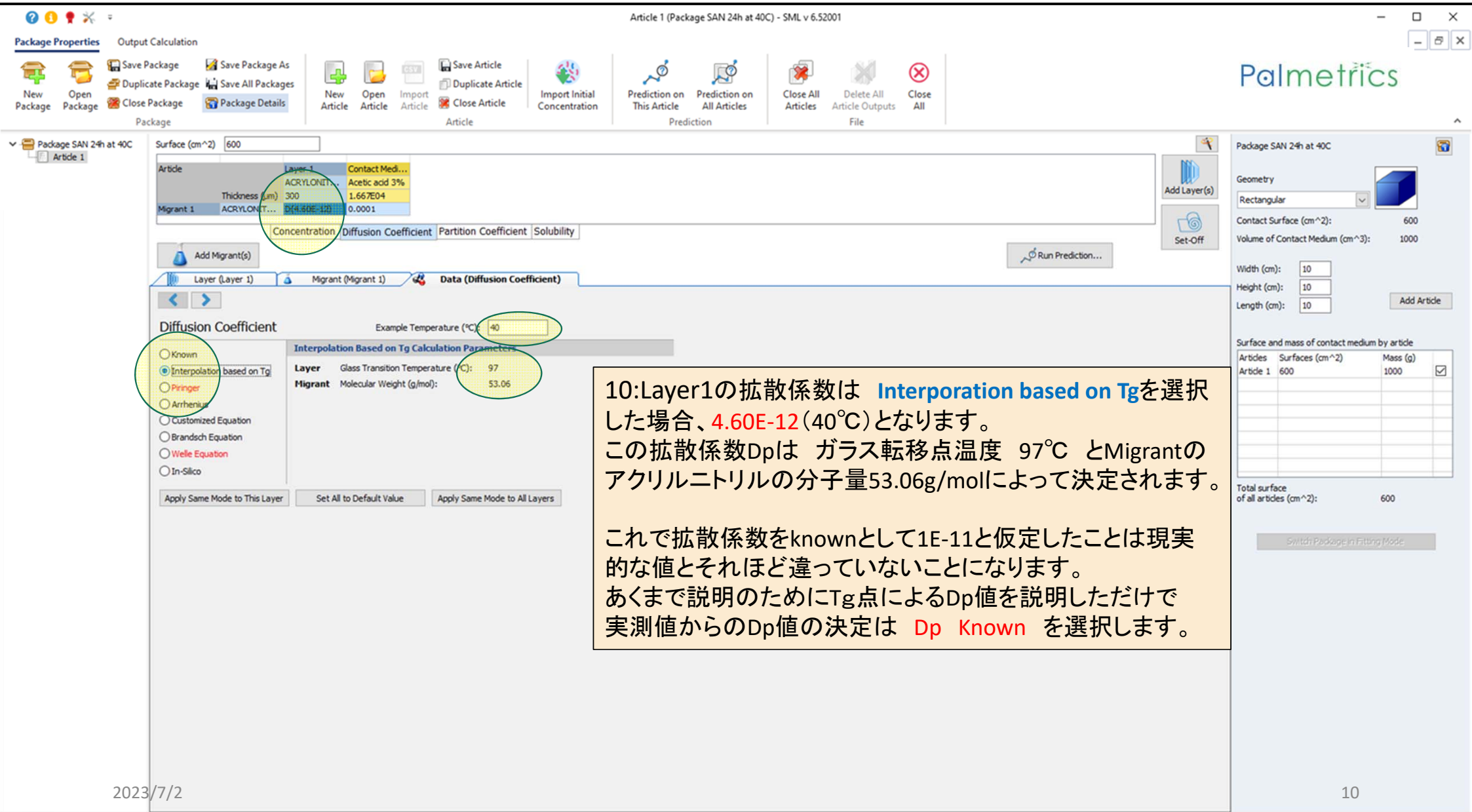
Width (cm): 10

Height (cm): 10

Length (cm): 10

Articles	Surfaces (cm ²)	Mass (g)
Article 1	600	1000

Total surface of all articles (cm²): 600



10:Layer1の拡散係数は **Interporation based on Tg**を選択した場合、**4.60E-12** (40°C)となります。
この拡散係数Dpは ガラス転移点温度 97°C とMigrantの アクリルニトリルの分子量53.06g/molによって決定されます。

これで拡散係数をknownとして1E-11と仮定したことは現実的な値とそれほど違っていないことになります。
あくまで説明のためにTg点によるDp値を説明しただけで 実測値からのDp値の決定は **Dp Known** を選択します。

Package SAN 24h at 40C

Surface (cm²) 600

Article	Layer 1	Contact Medi...
	ACRYLONIT...	Acetic acid 3%
	Thickness (μm)	300
		1.667E04
Migrant 1	ACRYLONIT...	IE-11
		0.0001

Concentration Diffusion Coefficient Partition Coefficient Solubility

Add Migrant(s)

Run Prediction...

Layer (Layer 1) Migrant (Migrant 1) Data (Diffusion Coefficient)

Diffusion Coefficient

Known

Interpolation based on Tg

Pringer

Arrhenius

Customized Equation

Bransch Equation

Welle Equation

In-Silico

Known Value

Diffusion Coefficient (cm²/s): 1E-11

Set to Default Values

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

Package SAN 24h at 40C

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

Total surface of all articles (cm²): 600

Switch Package in Fitting Mode

11: 実測値からのDp値の決定は Dp Known を選択します。設定する暫定値は 拡散係数が既知の値と仮定しています。

Article 1 (Package SAN 24h at 40C) - SML v 6.52001

Palmetrics

Package SAN 24h at 40C

Surface (cm²) 600

Article	Layer 1	Contact Medi...
	ACRYLONIT...	Acebic acid 3%
	Thickness (μm)	300
		1.667E04
Migrant 1	ACRYLONIT...	4.6E-12
		0.0001

Concentration Diffusion Coefficient Partition Coefficient Solubility

Add Migrant(s)

Layer (Layer 1) Migrant (Migrant 1) Data (Diffusion Coefficient)

Diffusion Coefficient

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

Known Value

Diffusion Coefficient (cm²/s): 4.6E-12

Set to Default Values

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

Run Prediction...

Package SAN 24h at 40C

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

Total surface of all articles (cm²): 600

Switch Package in Fitting Mode

2023/7/2

6.52001

12 : Diffusion Coefficient値は 4.6E-12と入力します。
 ただし1E-11の値でも構いません。

Tg温度から予測した 4.6E-12 の値でも 1E-11 の値でも
 実測値にFitting計算すれば、Fitting後に到達する溶解濃度
 は同じなので、推定されるDp値は同じ値になります。

Package Properties Output Calculation

Save Package Save Package As
 Duplicate Package Save All Packages
 Close Package Package Details

New Package Open Package

New Article Open Article Import Article Save Article Duplicate Article Close Article

Import Initial Concentration

Prediction on This Article Prediction on All Articles

Close All Articles Delete All Article Outputs Close All

Package SAN 24h at 40C

Surface (cm²) 600

Article	Layer 1	Contact Medi...
	ACRYLONIT...	Acetic acid 3%
	Thickness (μm) 300	1.667E04
Migrant 1	ACRYLONIT...	4.6E-12 0.0001

13:40°C_1日間の溶出予測データを表示する設定です。

Concentration Diffusion Coefficient Partition Coefficient Solubility

Add Migrant(s)

Layer (Layer 1) Migrant (Migrant)

Diffusion Coefficient

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

Apply Same Mode to This Layer Set All to Default

Predictions

Temperature Profiles

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

Isothermal Conditions

Temperature = 40 °C

ΔT = 20 °C

Number of Isotherms = 1

Final Temperature = 40 °C

Time Max 10 day

Without Statistics
 Monte Carlo Runs
 Include Sobol Runs
 Fast Distribution

Number of Runs 10

Save... Load...

Number of steps for this output: 100 OK Cancel

Package SAN 24h at 40C

Geometry Rectangular

Contact Surface (cm²): 600
 Volume of Contact Medium (cm³): 1000

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

Surface and mass of contact medium by article

Articles	Surfaces (cm ²)	Mass (g)
Article 1	600	1000

Total surface of all articles (cm²): 600

Switch Package in Fitting Mode

Package Properties Output Calculation

Package SAN 24h at 40C

Article 1

Surface (cm²) 600

Article	Layer 1	Contact Medi...
	ACRYLONIT...	Acebic acid 3%
	Thickness (μm)	300
		1.667E04
Migrant 1	ACRYLONIT...	4.6E-12
		0.0001

14:40°C_1dayを設定して OKをクリックします。

Concentration Diffusion Coefficient Partition Coefficient Solubility

Add Migrant(s)

Layer (Layer 1) Migrant (Migrant)

Diffusion Coefficient

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

Apply Same Mode to This Layer Set All to Default

Predictions

Temperature Profiles

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

Time Max: 1 day

Without Statistics
 Monte Carlo Runs
 Include Sobol Runs
 Fast Distribution

Number of Runs: 10

Save... Load... OK Cancel

Number of steps for this output: 100

Isothermal Conditions

Temperature = 40 °C

ΔT = 20 °C

Number of Isotherms = 1

Final Temperature = 40 °C

Package SAN 24h at 40C

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

Total surface of all articles (cm²): 600

Switch Package in Fitting Mode

Package Properties Output Calculation

Package SAN 24h at 40C

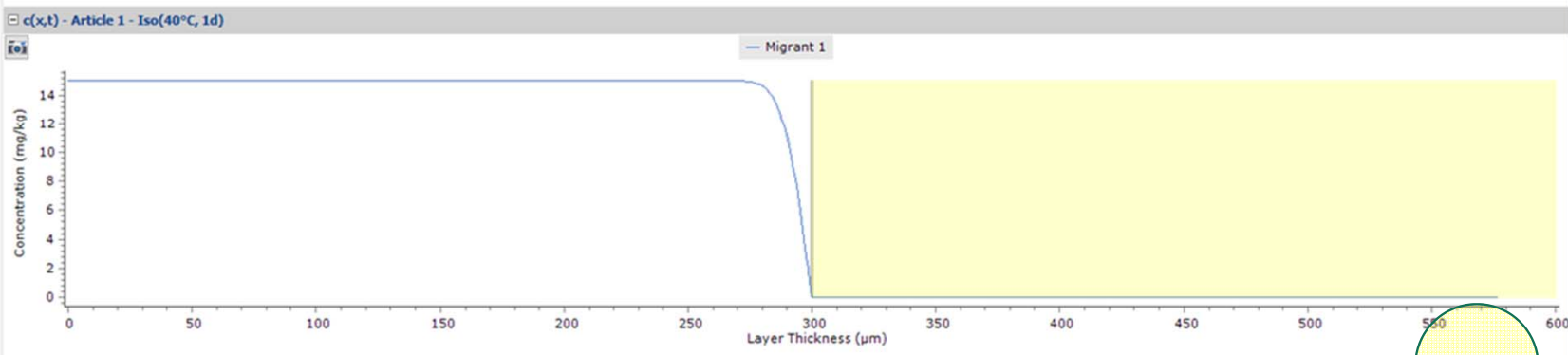
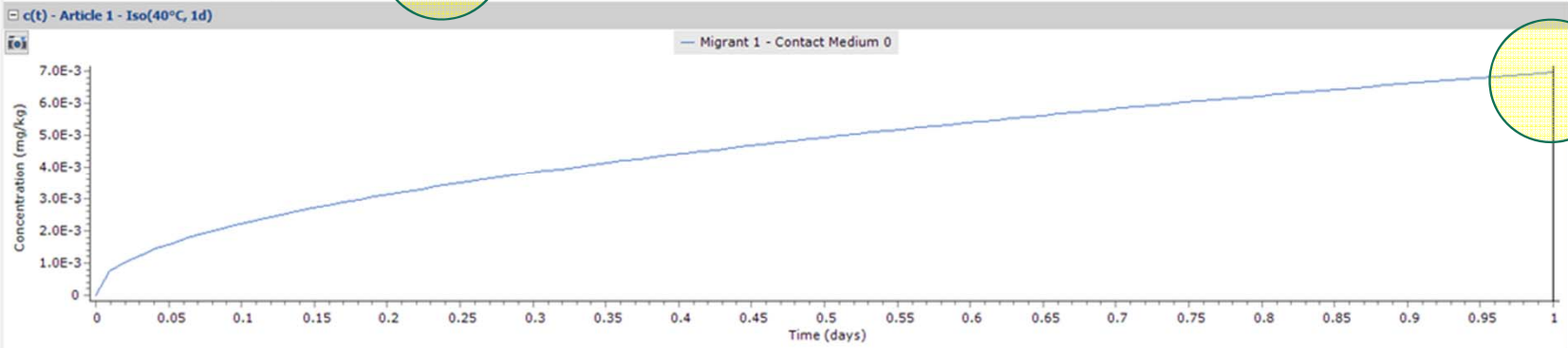
- Article 1
 - Iso(40°C, 1d)

Temperature : 40 (°C) Display unit mg/kg c(t) : draw mean concentration c(t) : draw concentration at 0 % of thickness from surface

Grid

Article	Layer 1	Contact Med...
	ACRYLONIT...	Acetic acid 3%
	Thickness (µm)	1.667E04
	300	
<input checked="" type="checkbox"/> Migrant 1	ACRYLONIT...	14.64
		0.006981

15: 40°C_1day後の溶出量は0.006981mg/kgになりました。



Package SAN 24h at 40C

Geometry

Rectangular

Contact Surface (cm²): 600

Volume of Contact Medium (cm³): 1000

Width (cm): 10

Height (cm): 10

Length (cm): 10

Surface and mass of contact medium by article

Articles	Surfaces (cm ²)	Mass (g)
Article 1	600	1000

Total surface of all articles (cm²): 600

23.98 (hours)

Package Properties

- New Package
- Open Package
- Save Package
- Duplicate Package
- Close Package
- Save Package As
- Save All Packages
- Package Details

- New Article
- Open Article
- Import Article
- Save Article
- Duplicate Article
- Close Article
- Import Initial Concentration

- Prediction on This Article
- Prediction on All Articles

- Close All Articles
- Delete All Article Outputs
- Close All

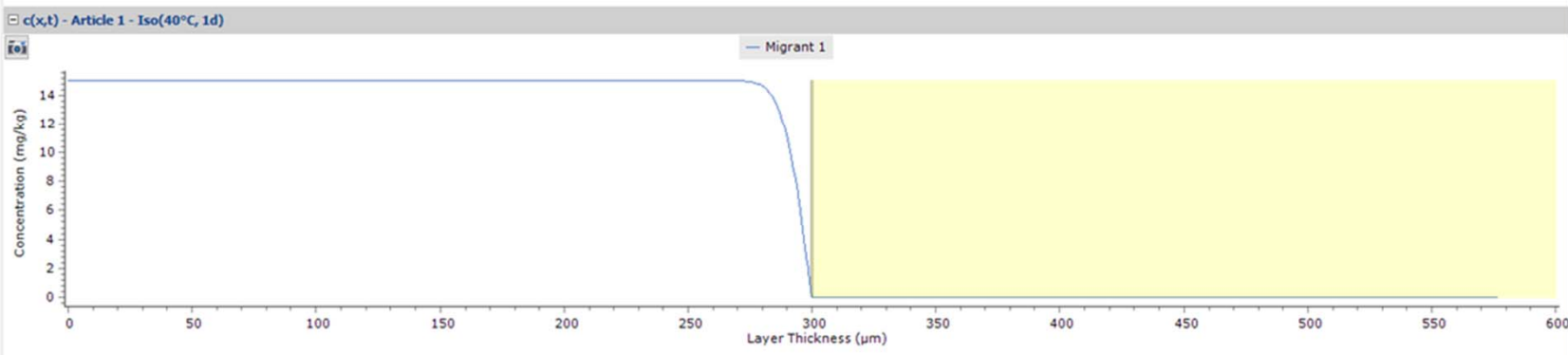
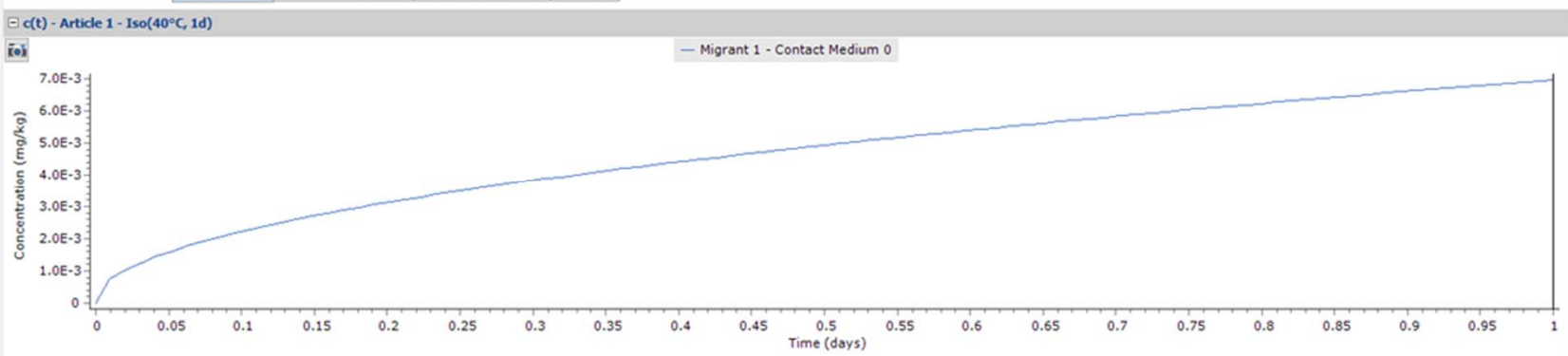
Package SAN 24h at 40C

- Save Output
- Export Migration c(t)
- Export Concentration c(x,t)
- Import Migration c(t)
- Import Concentration c(x,t)
- Delete Output

Unit mg/kg c(t) : draw mean concentration c(t) : draw concentration at 0 % of thickness from surface

Layer	Material	Acetic acid 3%
Layer 1	ACRYLONIT...	1.667E04
	Thickness (µm)	300
	ACRYLONIT...	14.64
	Contact Med...	0.006981

16: 40°C_1dayの溶出曲線を表示したまま、Iso_40°C,1d をクリックして赤枠の設定選択内容を表示させます。



Package SAN 24h at 40C

Geometry: Rectangular

Contact Surface (cm²): 600

Volume of Contact Medium (cm³): 1000

Width (cm): 10

Height (cm): 10

Length (cm): 10

Surface and mass of contact medium by article

Articles	Surfaces (cm ²)	Mass (g)
Article 1	600	1000

Package Properties Output Calculation

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

New Article
 Open Article
 Import Article
 Duplicate Article
 Close Article
 Import Initial Concentration

Prediction on This Article
 Prediction on All Articles
 Close All Articles
 Delete All Article Outputs
 Close All

Package SAN 24h at 40C

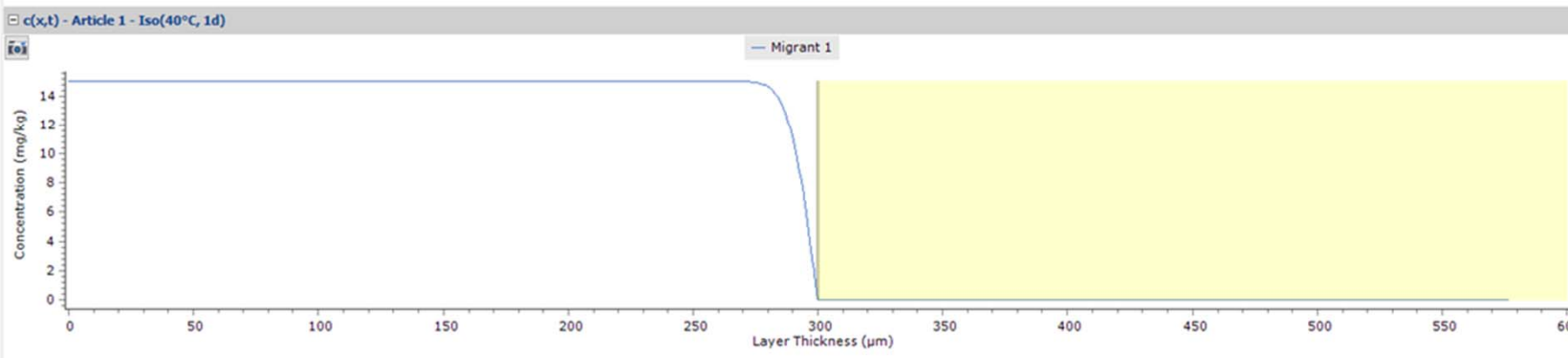
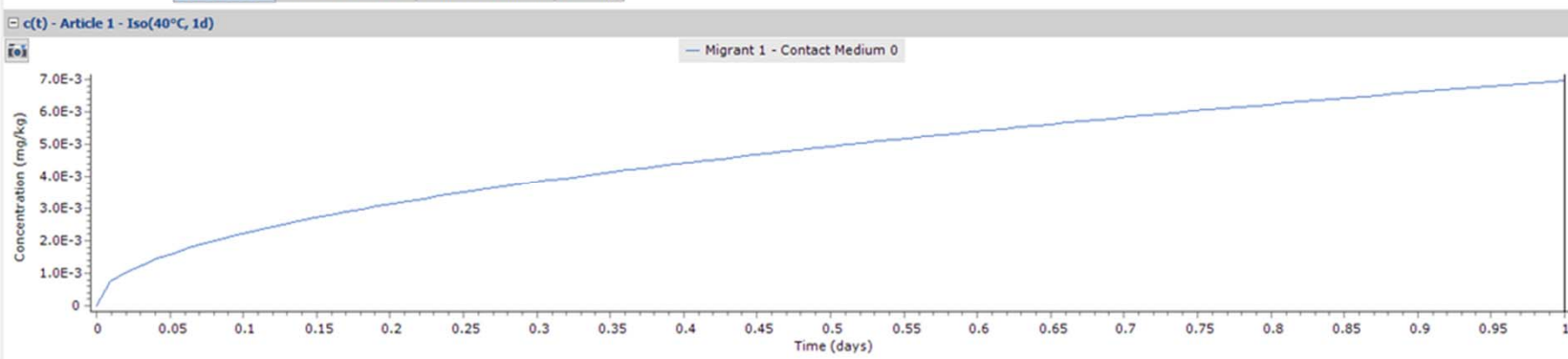
Article 1

- Save Output
- Export Migration c(t)
- Export Concentration c(x,t)
- Import Migration c(t)**
- Import Concentration c(x,t)
- Delete Output

Layer unit mg/kg c(t) : draw mean concentration c(t) : draw concentration at 0 % of thickness from surface

Layer	Material	Acetic acid 3%
Layer 1	ACRYLONIT...	1.667E04
	Thickness (µm)	300
	ACRYLONIT...	14.64
	Contact Med...	0.006981

17: 設定選択の **Import Migration** を選択します。
 目的は40°C, 1dayの実測溶出曲線(データ点数2個)をimportするためです。



Package SAN 24h at 40C

Geometry: Rectangular

Surface (cm²): 600
 Contact Medium (cm³): 1000

Length (cm): 10

Surface and mass of contact medium by article

Articles	Surfaces (cm ²)	Mass (g)
Article 1	600	1000

Total surface of all articles (cm²): 600

18: **Import Migration** をクリックすると溶出実測データファイルから **220902_To_0_24h at 40C** を選択してImportします。
 Importすると下記の赤線枠が表示されます。
 Columnの番号をセットし、Timeの0.1secなどを適切な単位に変更します。

Import Experimental Migration Profile

Import

t(h) T(°C) S(mg/kg)

	column 1	column 2	column 3
1	0	40	0
2	24	40	0.0058

Time is in: [Select Column] 0.1 sec
 Concentration is in: [Select Column] mg/kg

Buttons: Open Customized Profile..., OK, Cancel

Package Properties Output Calculation

Save Package Save Package As Duplicate Package Save All Packages Close Package Package Details

New Package Open Package

New Article Open Article Import Article

Package SAN 24h at 40C

Article 1

Iso(40°C, 1d)

Temperature: 40 (°C) Display unit mg/kg c(t): draw

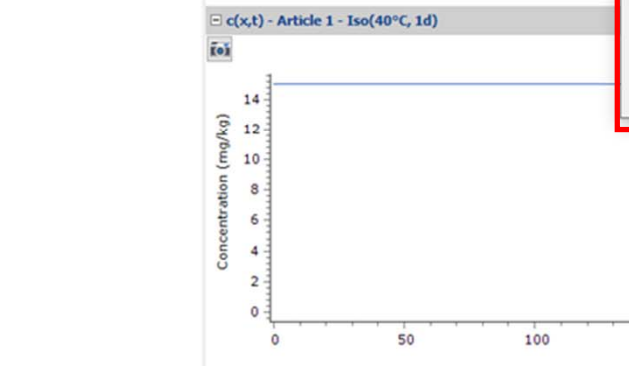
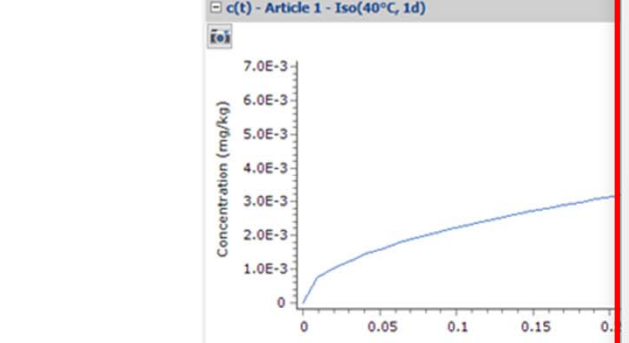
Grid

Article Layer 1

Thickness (µm) 300

Migrant 1 ACRYLONIT... 14.64

Concentration Diffusion Coefficient



Package SAN 24h at 40C

Geometry Rectangular

Contact Surface (cm²): 600

Volume of Contact Medium (cm³): 1000

Width (cm): 10

Height (cm): 10

Length (cm): 10

Surface and mass of contact medium by article

Articles	Surfaces (cm ²)	Mass (g)
Article 1	600	1000

Total surface of all articles (cm²): 600

19: Column 1は Time(時間)ですが、時間単位はhoursです。
18ページ~20ページで適切な単位を選択します。

Package Properties Output Calculation

Save Package Save Package As
Duplicate Package Save All Packages
Close Package Package Details

New Package Open Package

New Article Open Article Import Article

Package SAN 24h at 40C

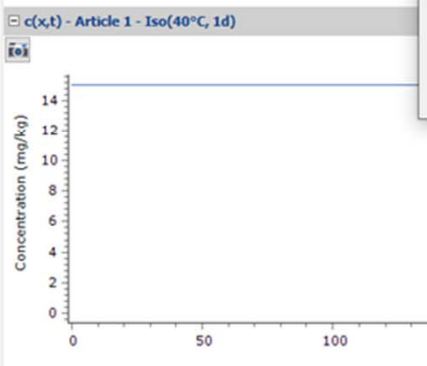
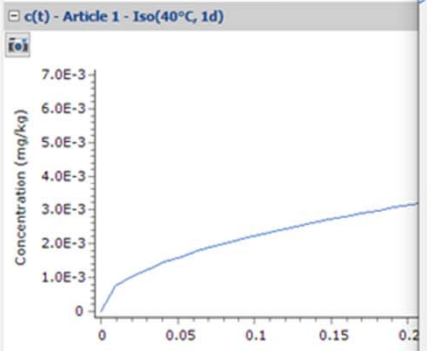
Article 1

Iso(40°C, 1d)

Temperature : 40 (°C) Display unit mg/kg c(t) : draw mean concentration c(t) : draw concentration at 0 % of thickness from surface

Grid

Article	Layer 1	Thickness (µm)	Migrant 1	ACRYLONIT...	14.64
		300			



Import Experimental Migration Profile

Import

t(h) T(°C) S(mg/kg)

	column 1	column 2	column 3
1	0	40	0
2	24	40	0.0058

Time is in [Select Column] 0.1 sec Concentration is in [Select Column] mg/kg

column 1
column 2
column 3

Open Customized Profile... OK Cancel

Package SAN 24h at 40C

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

Total surface of all articles (cm²): 600

Switch Package in Fitting Mode

Package Properties Output Calculation

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

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

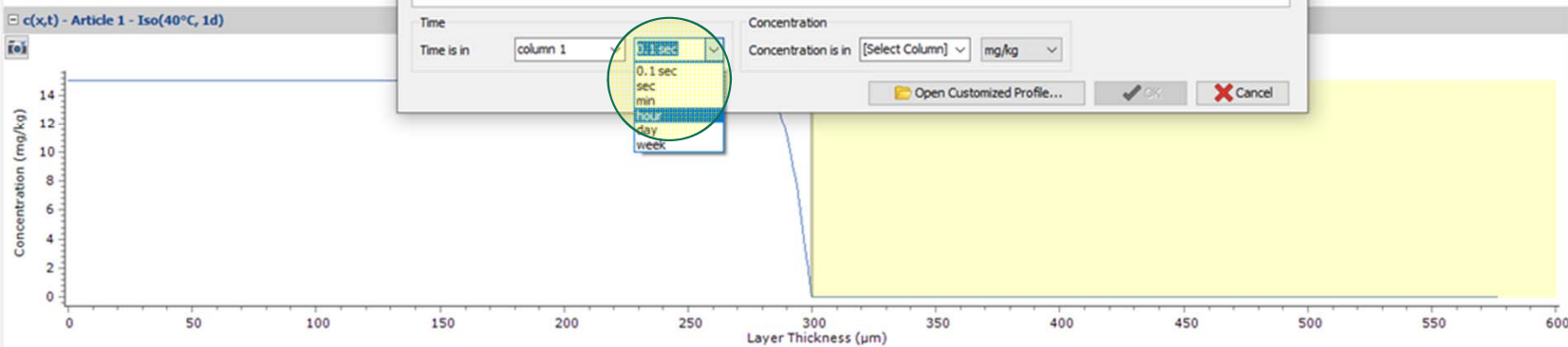
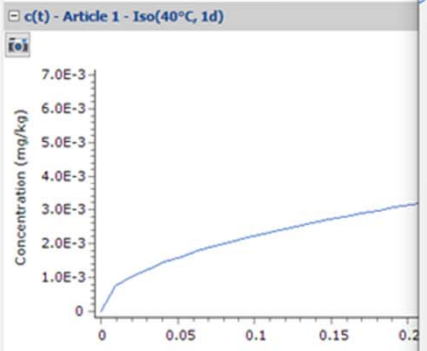
Prediction on This Article
 Prediction on All Articles
 Close All Articles
 Delete All Article Outputs
 Close All

Package SAN 24h at 40C
 Article 1
 Iso(40°C, 1d)

Temperature : 40 (°C) Display unit mg/kg c(t) : draw mean concentration c(t) : draw concentration at 0 % of thickness from surface

Grid

Article	Layer 1	ACRYLONIT...
Thickness (µm)		300
Migrant 1	ACRYLONIT...	14.64



Import Experimental Migration Profile

Import

t(h) T(°C) S(mg/kg)

	column 1	column 2	column 3
1	0	40	0
2	24	40	0.0058

Time is in: sec min hour day week

Concentration is in: mg/kg

Package SAN 24h at 40C

Geometry

Rectangular

Contact Surface (cm²): 600

Volume of Contact Medium (cm³): 1000

Width (cm):

Height (cm):

Length (cm):

Surface and mass of contact medium by article

Articles	Surfaces (cm ²)	Mass (g)
Article 1	600	1000

Total surface of all articles (cm²): 600

Package Properties Output Calculation

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

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

Prediction on This Article
 Prediction on All Articles
 Close All Articles
 Delete All Article Outputs
 Close All

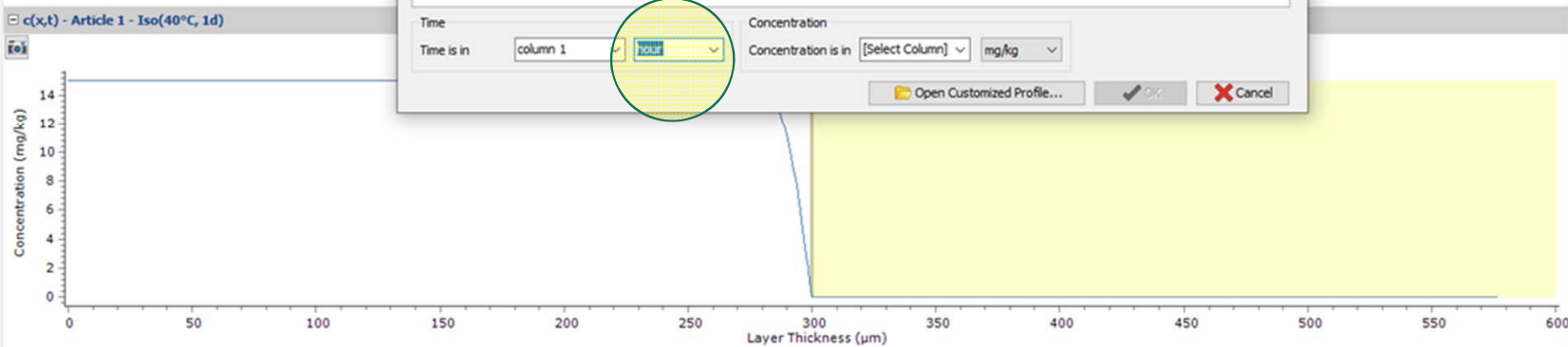
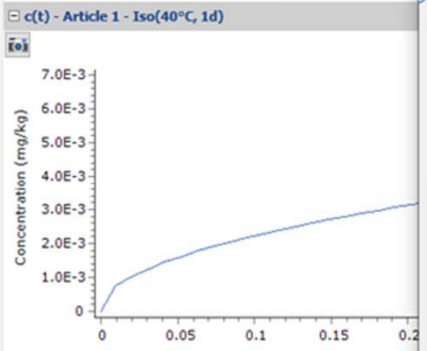
Package SAN 24h at 40C

- Article 1
 - Iso(40°C, 1d)

Temperature : 40 (°C) Display unit mg/kg c(t) : draw mean concentration c(t) : draw concentration at 0 % of thickness from surface

Grid

Article	Layer 1	Thickness (µm)	Migrant 1	ACRYLONIT...	14.64
	ACRYLONIT...	300			



Import Experimental Migration Profile

Import

t(h) T(°C) S(mg/kg)

	column 1	column 2	column 3
1	0	40	0
2	24	40	0.0058

Time is in: Concentration is in: mg/kg

Package SAN 24h at 40C

Geometry

Rectangular

Contact Surface (cm²): 600

Volume of Contact Medium (cm³): 1000

Width (cm): 10

Height (cm): 10

Length (cm): 10

Surface and mass of contact medium by article

Articles	Surfaces (cm ²)	Mass (g)
Article 1	600	1000

Total surface of all articles (cm²): 600

21: column3 は濃度です。濃度の単位はmg/kg です。

Package Properties Output Calculation

Save Package Save Package As
Duplicate Package Save All Packages
Close Package Package Details

New Package Open Package

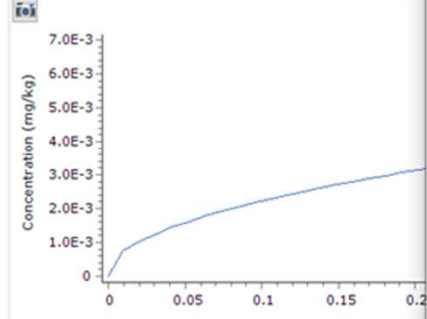
Package SAN 24h at 40C
Article 1
Iso(40°C, 1d)

Temperature: 40 (°C) Display unit: mg/kg c(t) : draw mean concentration c(t) : draw concentration at 0 % of thickness from surface

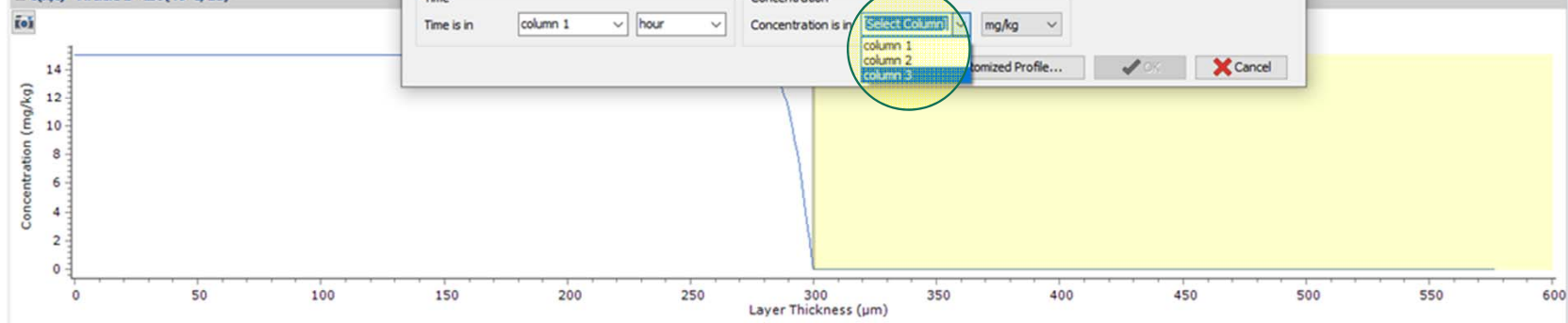
Grid

Article	Layer 1	ACRYLONIT...
Thickness (µm)		300
Migrant 1	ACRYLONIT...	14.64

Concentration Diffusion Coefficient



c(x,t) - Article 1 - Iso(40°C, 1d)



Import Experimental Migration Profile

Import

t(h) T(°C) S(mg/kg)

	column 1	column 2	column 3
1	0	40	0
2	24	40	0.0058

Time is in: column 1 hour Concentration is in: **Select Column** mg/kg

column 1
column 2
column 3

OK Cancel

Package SAN 24h at 40C

Geometry: Rectangular

Contact Surface (cm²): 600
Volume of Contact Medium (cm³): 1000

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

Surface and mass of contact medium by article

Articles	Surfaces (cm ²)	Mass (g)
Article 1	600	1000

Total surface of all articles (cm²): 600

Switch Package in Fitting Mode

22: 設定が完了したら OKをクリックします。

Package Properties Output Calculation

Save Package Save Package As
 Duplicate Package Save All Packages
 Close Package Package Details

New Package Open Package

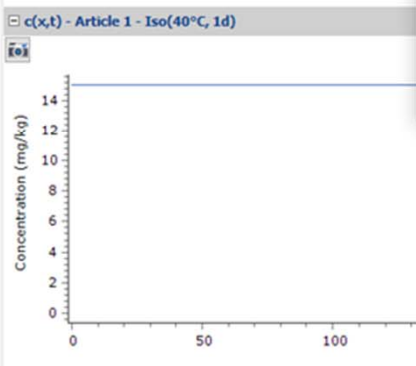
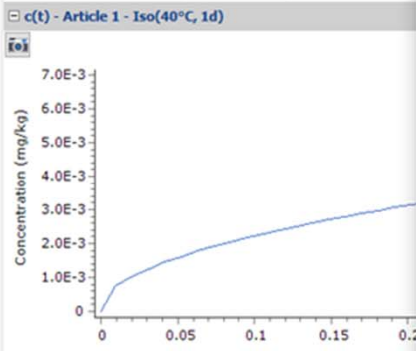
New Article Open Article Import Article Save Article

Package SAN 24h at 40C
 Article 1
 Iso(40°C, 1d)

Temperature : 40 (°C) Display unit mg/kg c(t) : draw mean concentration c(t) : draw concentration at 0 % of thickness from surface

Grid

Article	Layer 1	Thickness (µm)	Migrant 1	ACRYLONIT...	14.64
		300			



Import Experimental Migration Profile

Import

t(h) T(°C) S(mg/kg)

	column 1	column 2	column 3
1	0	40	0
2	24	40	0.0058

Time is in: column 1 hour Concentration is in: column 3 mg/kg

Open Customized Profile... OK Cancel

Package SAN 24h at 40C

Geometry: Rectangular

Contact Surface (cm²): 600
 Volume of Contact Medium (cm³): 1000

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

Surface and mass of contact medium by article

Articles	Surfaces (cm ²)	Mass (g)
Article 1	600	1000

Total surface of all articles (cm²): 600

Package Properties Output Calculation

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

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

Prediction on This Article
 Prediction on All Articles
 Close All Articles
 Delete All Article Outputs
 Close All

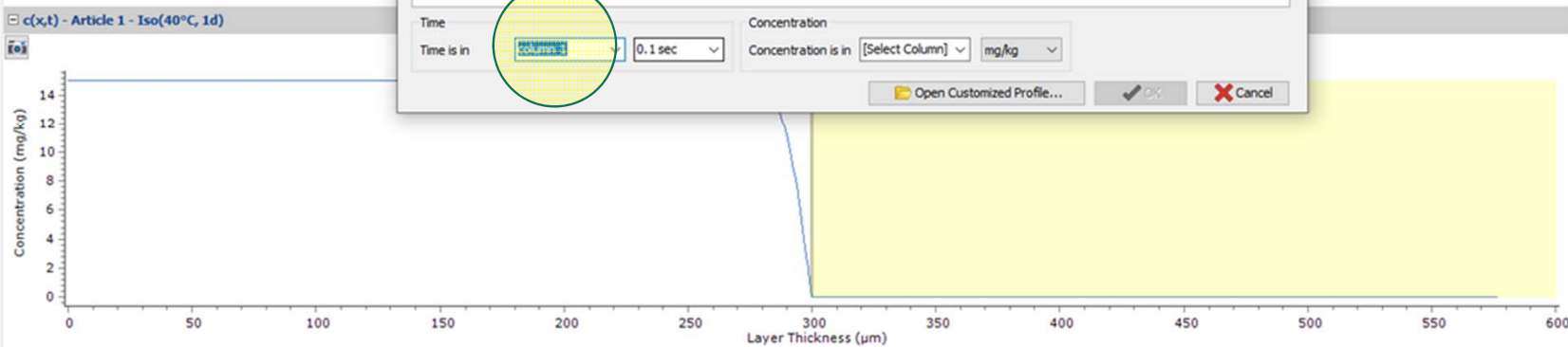
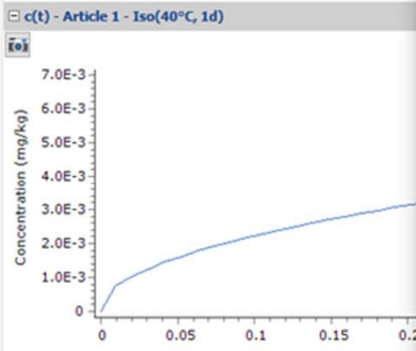
Package SAN 24h at 40C

- Article 1
 - Iso(40°C, 1d)

Temperature : 40 (°C) Display unit mg/kg c(t) : draw mean concentration c(t) : draw concentration at 0 % of thickness from surface

Grid

Article	Layer 1	Thickness (µm)	Migrant 1	ACRYLONIT...	14.64
	ACRYLONIT...	300			



Import Experimental Migration Profile

Import

t(h) T(°C) S(mg/kg)

	column 1	column 2	column 3
1	0	40	0
2	24	40	0.0058

Time is in **column 3** 0.1 sec Concentration is in [Select Column] mg/kg

Package SAN 24h at 40C

Geometry

Rectangular

Contact Surface (cm²): 600

Volume of Contact Medium (cm³): 1000

Width (cm): 10

Height (cm): 10

Length (cm): 10

Surface and mass of contact medium by article

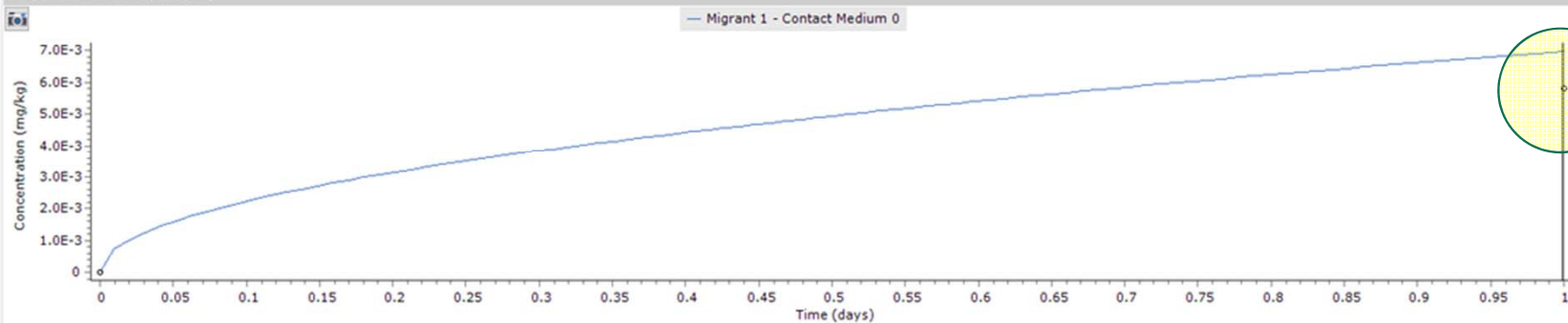
Articles	Surfaces (cm ²)	Mass (g)
Article 1	600	1000

Total surface of all articles (cm²): 600

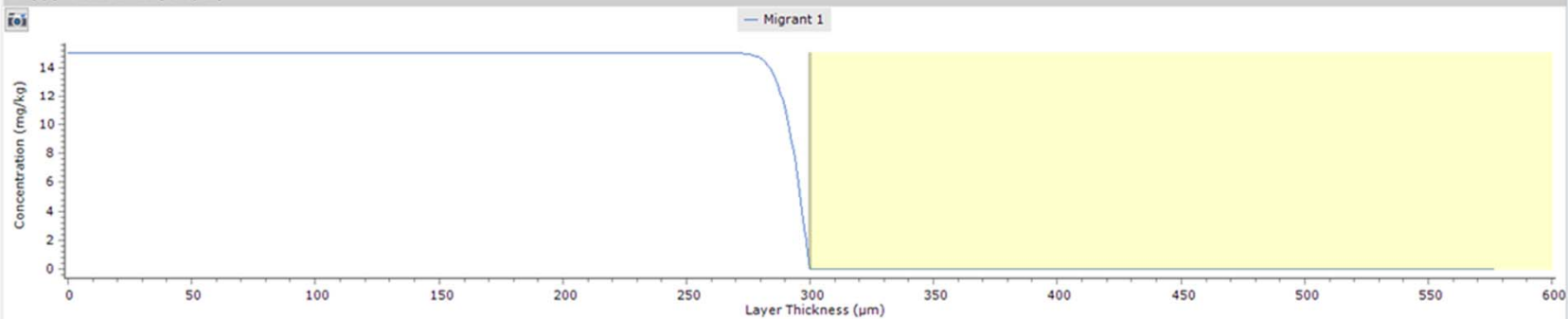
25: 拡散係数を既知とした溶出曲線から実測溶出量はずれています。実測値と溶出曲線が一致するようにFitting計算をします。実測値と溶出曲線が一致した時の拡散係数が目的とする拡散係数です。

Article	Layer 1	Contact Med...
	ACRYLONIT...	Acetic acid 3%
	Thickness (μm)	300
		1.667E04
<input checked="" type="checkbox"/> Migrant 1	ACRYLONIT...	14.64
		0.006981

c(t) - Article 1 - Iso(40°C, 1d)



c(x,t) - Article 1 - Iso(40°C, 1d)



Articles	Surfaces (cm ²)	Mass (g)
Article 1	600	1000

Total surface of all articles (cm²): 600

Switch Package in Fitting Mode

Package Properties Output Calculation

Package

Article

Prediction File

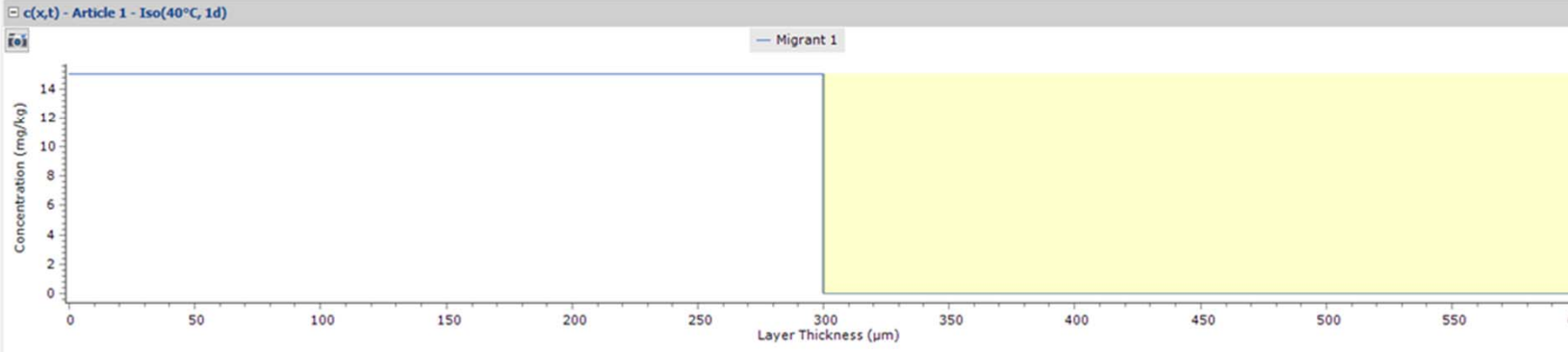
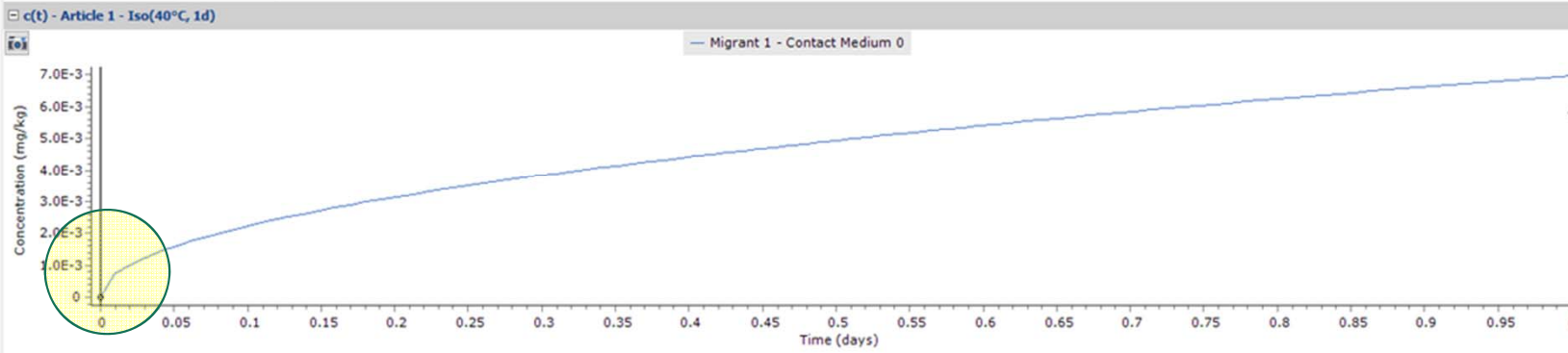
Package SAN 24h at 40C

- Article 1
 - Iso(40°C, 1d)

Temperature : 40 (°C) Display unit mg/kg c(t) : draw mean concentration c(t) : draw concentration at 0 % of thickness from surface

Grid

Article	Layer 1	Contact Med...
	ACRYLONIT...	Acetic acid 3%
	Thickness (µm)	1.667E04
<input checked="" type="checkbox"/> Migrant 1	ACRYLONIT...	0



Package SAN 24h at 40C

Geometry

Rectangular

Contact Surface (cm²): 600

Volume of Contact Medium (cm³): 1000

Width (cm): 10

Height (cm): 10

Length (cm): 10

Surface and mass of contact medium by article

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

Total surface of all articles (cm²): 600

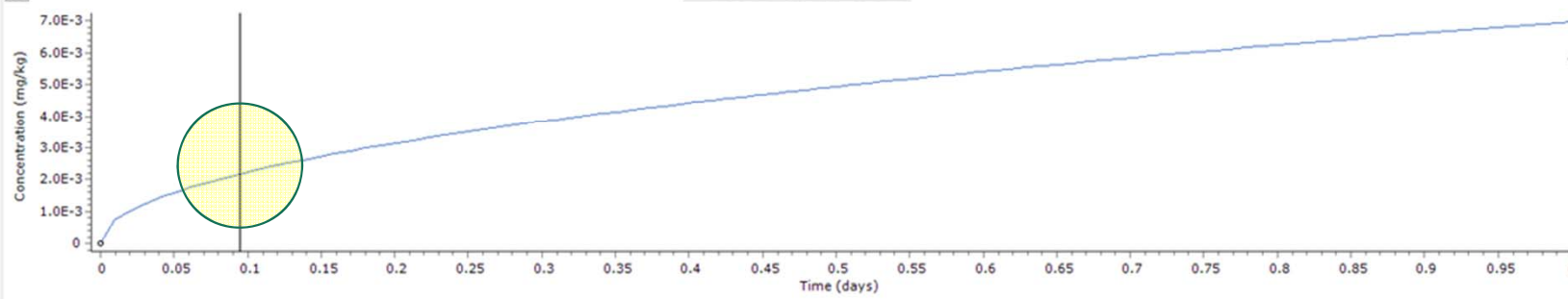
Package Properties Output Calculation

- Package SAN 24h at 40C
 - Article 1
 - Iso(40°C, 1d)

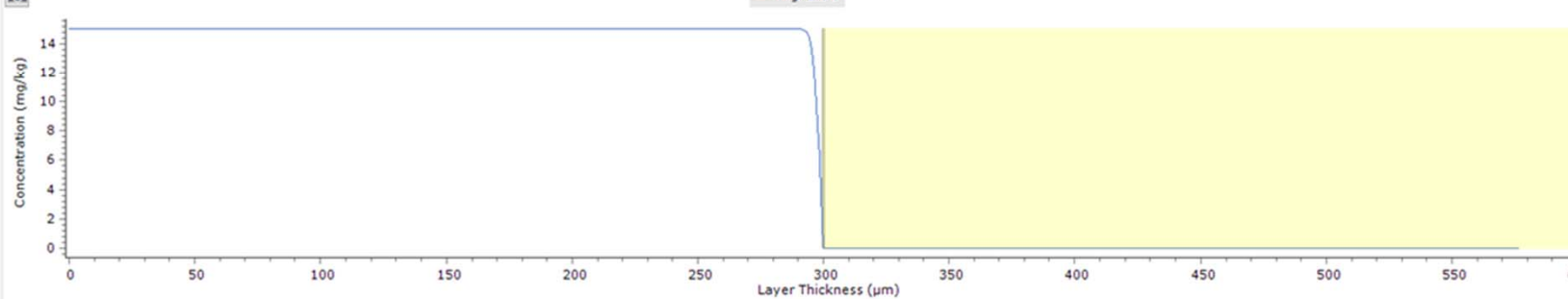
Temperature : 40 (°C) Display unit mg/kg c(t) : draw mean concentration c(t) : draw concentration at 0 % of thickness from surface

Article	Layer 1	Contact Med...
	ACRYLONIT...	Acetic acid 3%
	Thickness (µm)	1.667E04
	300	
<input checked="" type="checkbox"/> Migrant 1	ACRYLONIT...	14.89
		0.002171

c(t) - Article 1 - Iso(40°C, 1d) Migrant 1 - Contact Medium 0



c(x,t) - Article 1 - Iso(40°C, 1d) Migrant 1



Package SAN 24h at 40C

Geometry

Contact Surface (cm²): 600

Volume of Contact Medium (cm³): 1000

Width (cm):

Height (cm):

Length (cm):

Surface and mass of contact medium by article

Articles	Surfaces (cm ²)	Mass (g)
Article 1	600	1000

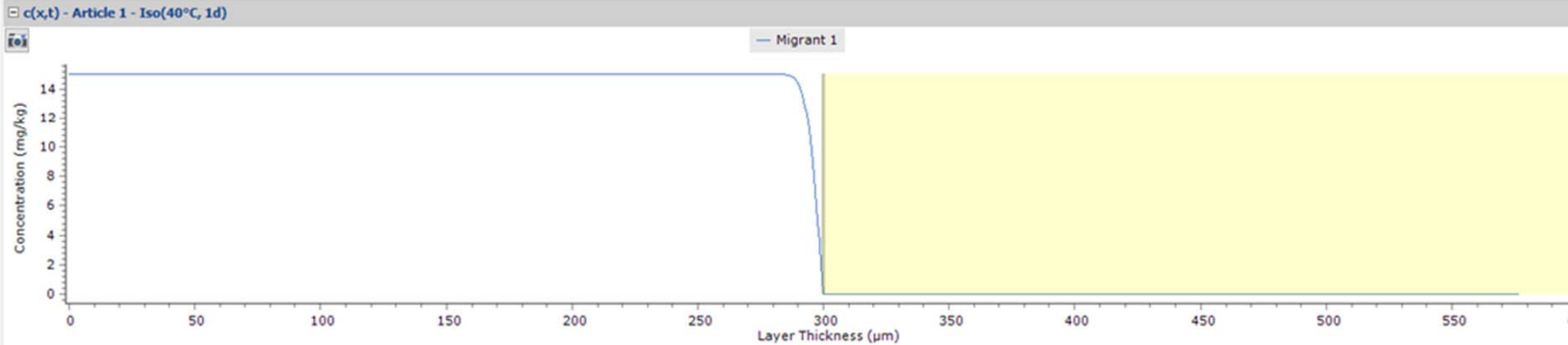
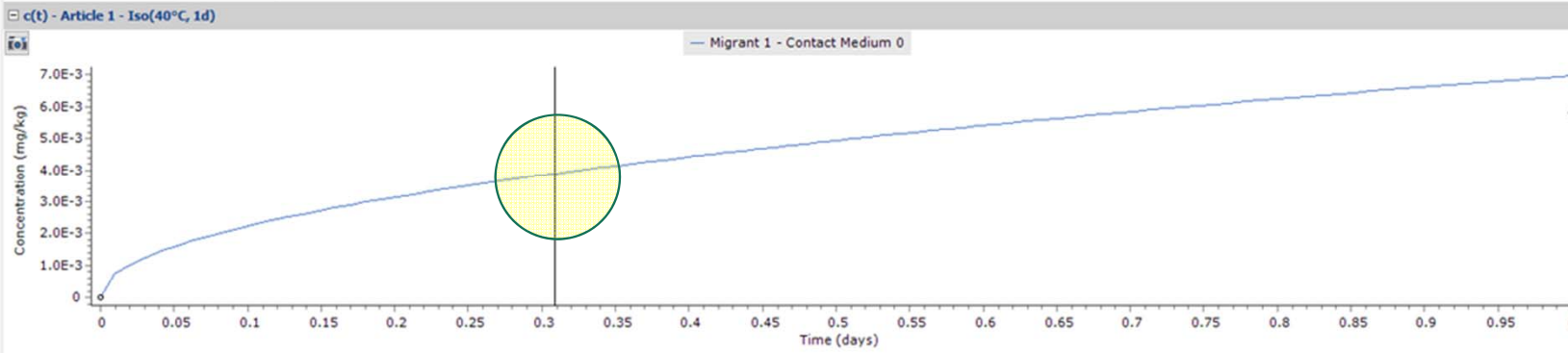
Total surface of all articles (cm²): 600

Package Properties Output Calculation

- Package SAN 24h at 40C
 - Article 1
 - Iso(40°C, 1d)

Temperature : 40 (°C) Display unit mg/kg c(t) : draw mean concentration c(t) : draw concentration at 0 % of thickness from surface

Article	Layer 1	Contact Med...
ACRYLONIT...	ACRYLONIT...	Acetic acid 3%
Thickness (µm)	300	1.667E04
Migrant 1	ACRYLONIT...	14.8
		0.003888



Package SAN 24h at 40C

Geometry: Rectangular

Contact Surface (cm²): 600

Volume of Contact Medium (cm³): 1000

Width (cm):

Height (cm):

Length (cm):

Surface and mass of contact medium by article

Articles	Surfaces (cm ²)	Mass (g)
Article 1	600	1000

Total surface of all articles (cm²): 600

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

Prediction

- Prediction on This Article
- Prediction on All Articles

File

- Close All Articles
- Delete All Article Outputs
- Close All

- Package SAN 24h at 40C
 - Article 1
 - Iso(40°C, 1d)

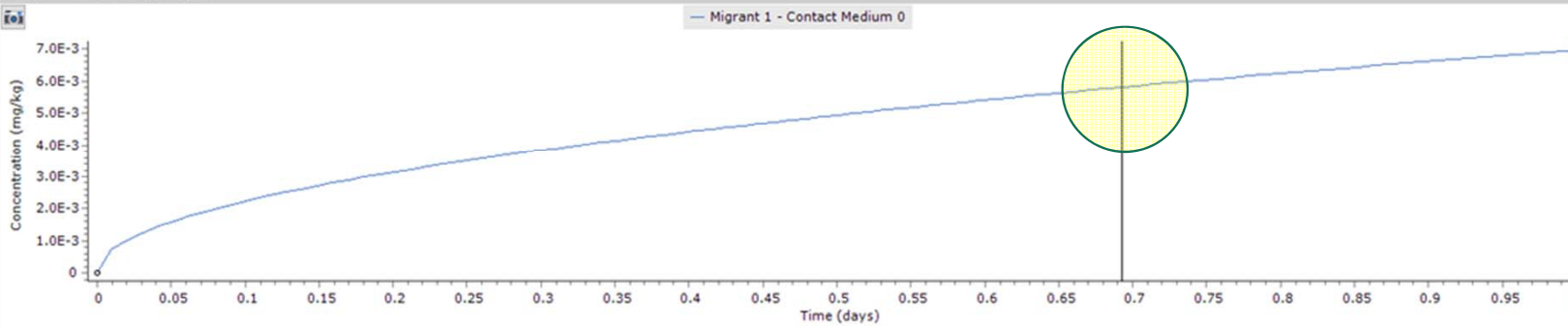
Temperature : 40 (°C) Display unit mg/kg c(t) : draw mean concentration c(t) : draw concentration at 0 % of thickness from surface

Grid

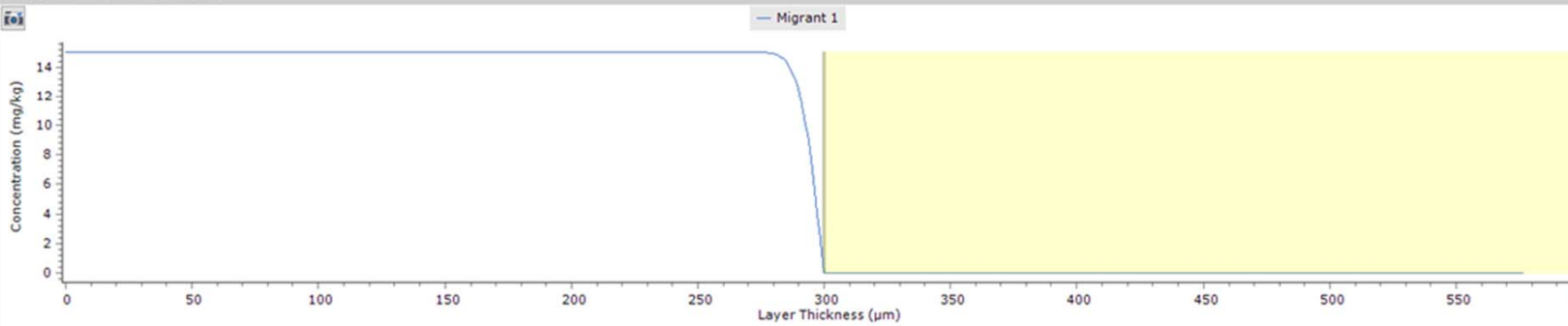
Article	Layer 1	Contact Med...
	ACRYLONIT...	Acetic acid 3%
	Thickness (µm)	1.667E04
<input checked="" type="checkbox"/> Migrant 1	ACRYLONIT...	14.7
		0.005816

Concentration Diffusion Coefficient Partition Coefficient Solubility

c(t) - Article 1 - Iso(40°C, 1d)



c(x,t) - Article 1 - Iso(40°C, 1d)



Package SAN 24h at 40C

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

Total surface of all articles (cm²): 600

Switch Package in Fitting Mode

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

Prediction

- Prediction on This Article
- Prediction on All Articles

File

- Close All Articles
- Delete All Article Outputs
- Close All

- Package SAN 24h at 40C
 - Article 1
 - Iso(40°C, 1d)

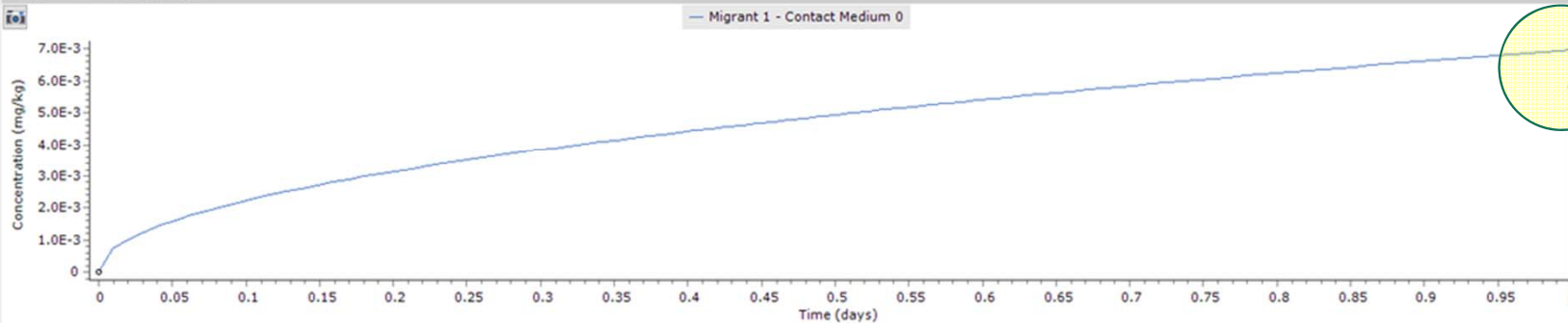
Temperature : 40 (°C) Display unit mg/kg c(t) : draw mean concentration c(t) : draw concentration at 0 % of thickness from surface

Grid

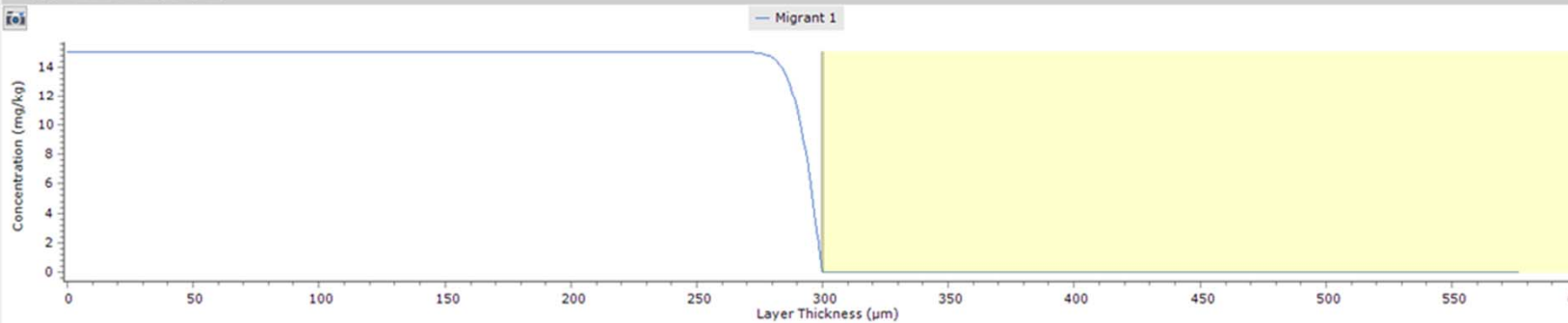
Article	Layer 1	Contact Med...
	ACRYLONIT...	Acetic acid 3%
	Thickness (µm)	1.667E04
<input checked="" type="checkbox"/> Migrant 1	ACRYLONIT...	0.006981
	14.64	

Concentration Diffusion Coefficient Partition Coefficient Solubility

c(t) - Article 1 - Iso(40°C, 1d)



c(x,t) - Article 1 - Iso(40°C, 1d)



Package SAN 24h at 40C

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

Total surface of all articles (cm²): 600

Switch Package in Fitting Mode

Package Properties Output Calculation

Package SAN 24h at 40C

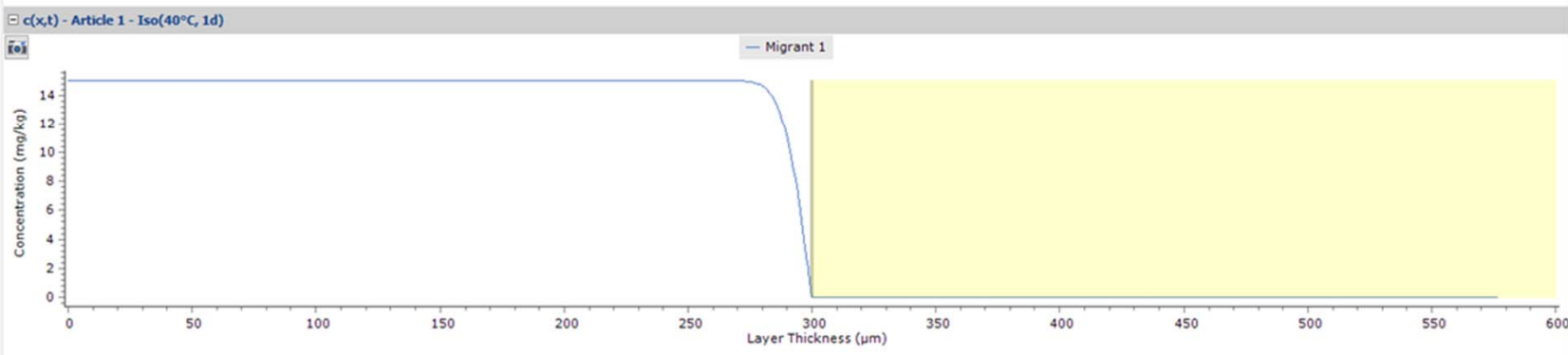
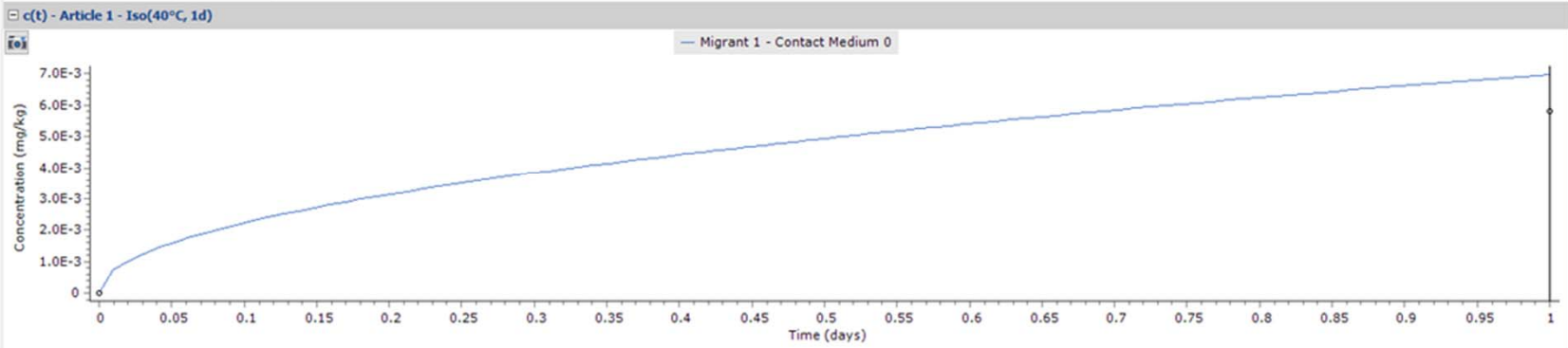
- Article 1
 - Iso(40°C, 1d)

Temperature : 40 (°C) Display unit mg/kg c(t) : draw mean concentration c(t) : draw concentration at 0 % of thickness from surface

Grid

Article	Layer 1	Contact Med...
	ACRYLONIT...	Acetic acid 3%
	Thickness (µm)	1.667E04
	300	0.006981
<input checked="" type="checkbox"/> Migrant 1	ACRYLONIT...	14.64
	Thickness (µm)	0.006981

31:このコマンドにより回帰計算モードになります。



Package SAN 24h at 40C

Geometry

Rectangular

Contact Surface (cm²): 600

Volume of Contact Medium (cm³): 1000

Width (cm): 10

Height (cm): 10

Length (cm): 10

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

Package Properties Output Calculation

Package

Article

Prediction

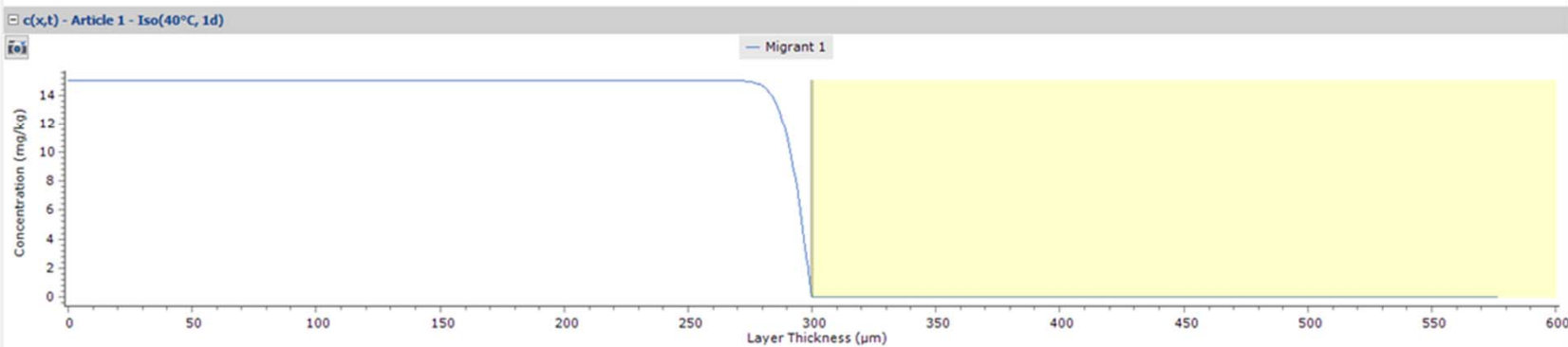
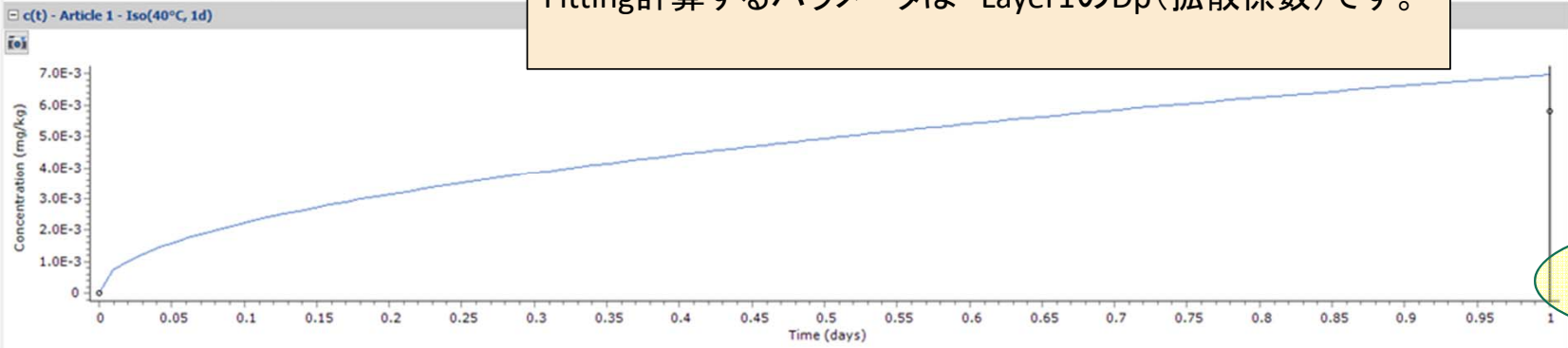
File

- Package SAN 24h at 40C
- Article 1
- Iso(40°C, 1d)

Temperature : 40 (°C) Display unit mg/kg c(t) : draw mean concentration c(t) : draw concentration at 0 % of thickness from surface

Grid	Article	Layer 1	Contact Med...
<input checked="" type="checkbox"/>	Migrant 1	ACRYLONIT...	Acetic acid 3%
		Thickness (µm)	
		300	1.667E04
		14.64	0.006981

32: Refreshをクリックします。
 Dp既知値は 4.6E-12 になっています。
 Fitting計算するパラメータは Layer1のDp(拡散係数)です。



Fitting Mode

RSS

Loops

Loops per serie 20

Optimize

Refresh

Correlation

mtau 1

mtolg 1E-6

mtolx 1E-6 mrealstep 1E-2

Parameter Name	Value
Layer 1-Dp-Known(cm^2/s)	4.6E-12

Close Fitting Mode for This Package

Create Global Package

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
- Close Article
- Save Article
- Duplicate Article
- Import Initial Concentration

Prediction

- Prediction on This Article
- Prediction on All Articles

File

- Close All Articles
- Delete All Article Outputs
- Close All

Package SAN 24h at 40C

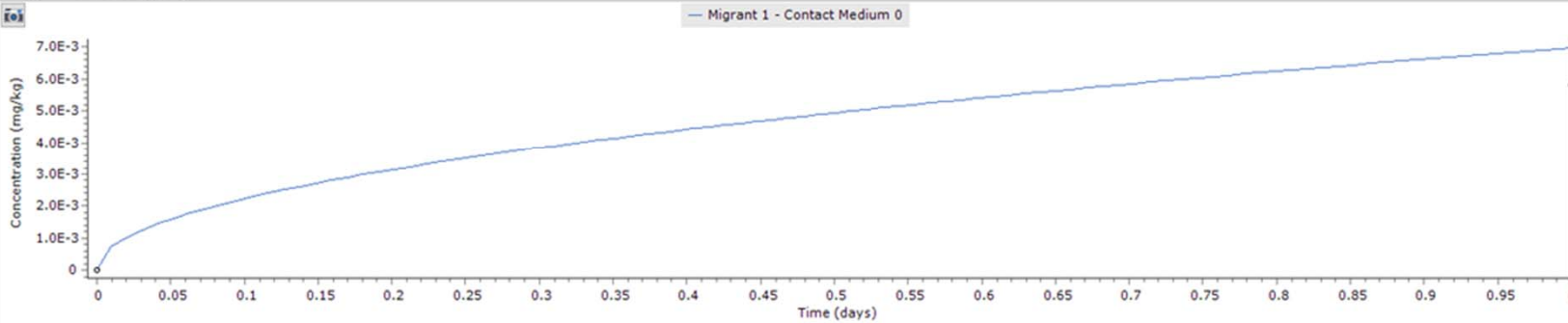
- Article 1
- Iso(40°C, 1d)

Temperature : 40 (°C) Display unit mg/kg c(t) : draw mean concentration c(t) : draw concentration at 0 % of thickness from surface

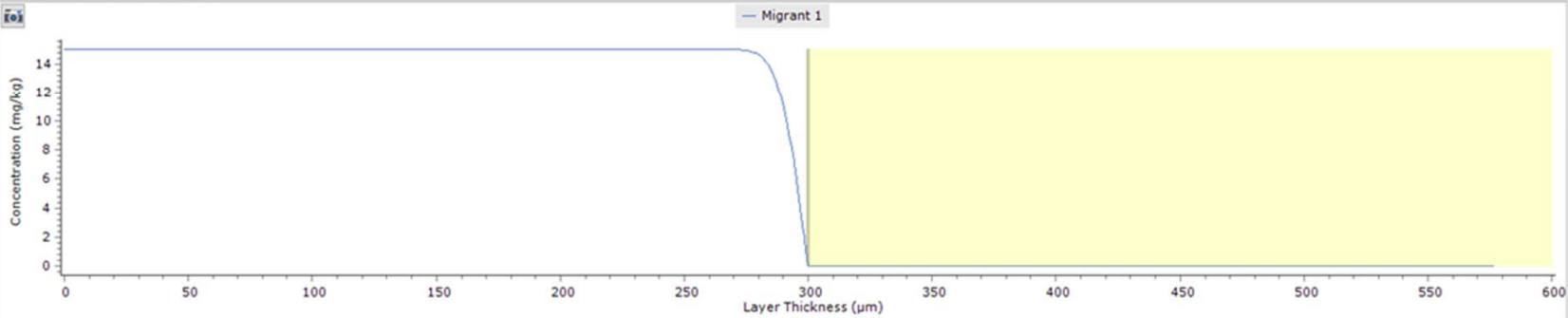
Article	Layer 1	Contact Med...
	ACRYLONIT...	Acetic acid 3%
	Thickness (µm)	1.667E04
<input checked="" type="checkbox"/> Migrant 1	ACRYLONIT...	0.006981

33: Optimize (回帰計算を開始)をクリックします。

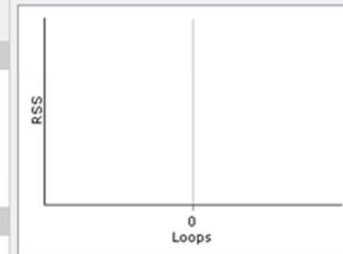
c(t) - Article 1 - Iso(40°C, 1d)



c(x,t) - Article 1 - Iso(40°C, 1d)



Fitting Mode



Loops per serie 20

mtau 1
mtolg 1E-6
mtolx 1E-6 mrealstep 1E-3

Parameter Name	Value
Layer 1-Dp-Known(cm^2/s)	4.6E-12

Package Properties Output Calculation

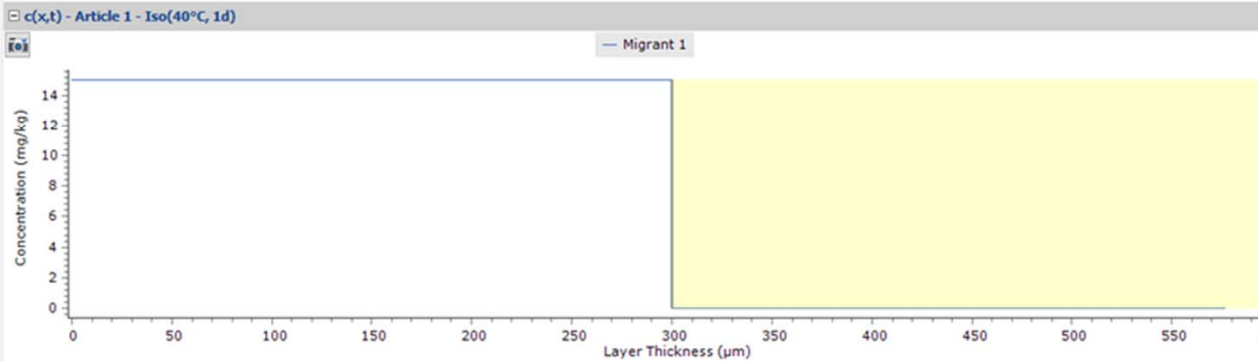
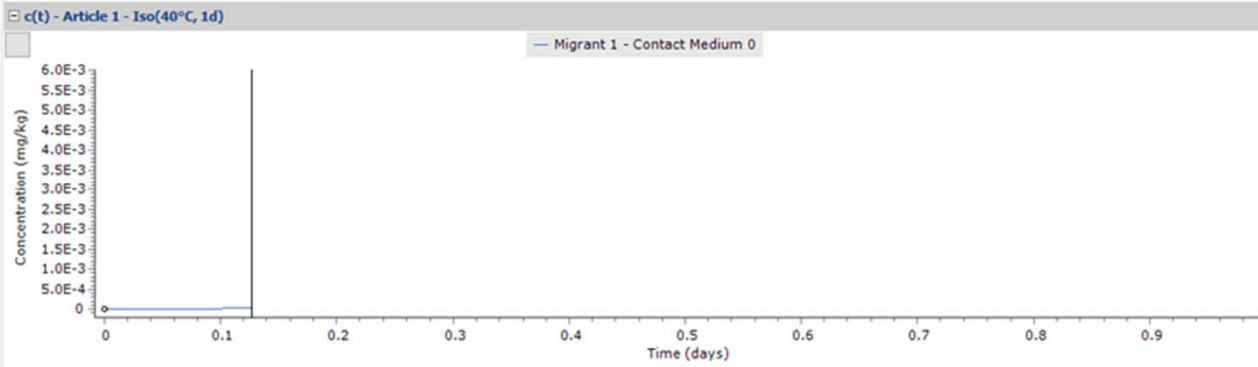
Package SAN 24h at 40C

- Article 1
 - Iso(40°C, 1d)

Temperature : 40 (°C) Display unit mg/kg c(t) : draw mean concentration c(t) : draw concentration at 0 % of thickness from surface

Grid

Article	Layer 1	Contact Med...
	ACRYLONIT...	Acetic acid 3%
	Thickness (µm)	1.667E04
	300	
<input checked="" type="checkbox"/> Migrant 1	ACRYLONIT...	1.565E-05



Package SAN 24h at 40C

Geometry: Rectangular

Contact Surface (cm²): 600

Volume of Contact Medium (cm³): 1000

Width (cm): 10

Height (cm): 10

Length (cm): 10

Surface and mass of contact medium by article

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

Total surface of all articles (cm²): 600

Fitting Mode

Loops per serie: 20 Iterations: 0

mtau: 1

mtolg: 1E-6

mtolx: 1E-6 mrealstep: 1E-3

Parameter Name	Value
Layer 1-Dp-Known(cm ² /s)	2.149E-16

Package Properties

Output Calculation

New Package
Open Package
Close Package

Save Package
Duplicate Package
Close Package

Save Article
Duplicate Article
Close Article

Import Initial Concentration

Prediction on This Article
Prediction on All Articles

Close All Articles
Delete All Article Outputs
Close All

Package SAN 24h at 40C

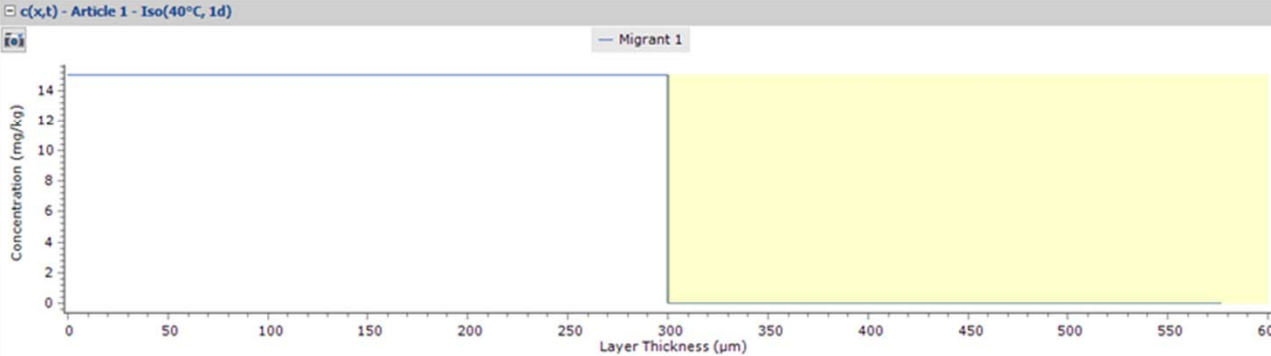
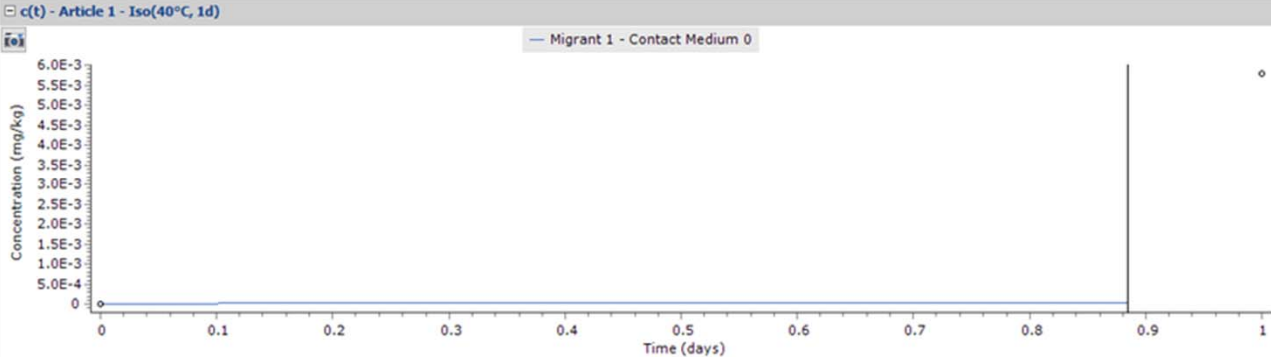
Article 1

Iso(40°C, 1d)

Temperature : 40 (°C) Display unit mg/kg $c(t)$: draw mean concentration $c(t)$: draw concentration at 0 % of thickness from surface

Grid

Article	Layer 1	Contact Med...
	ACRYLONIT...	Acetic acid 3%
	Thickness (µm)	300
		1.667E04
<input checked="" type="checkbox"/> Migrant 1	ACRYLONIT...	15
		4.44E-05



Package SAN 24h at 40C

Geometry: Rectangular

Contact Surface (cm²): 600
Volume of Contact Medium (cm³): 1000

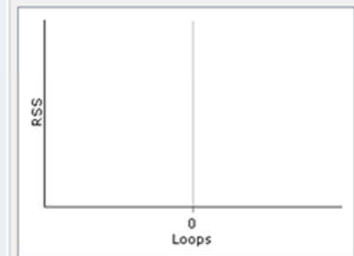
Width (cm): 10
Height (cm): 10
Length (cm): 10

Surface and mass of contact medium by article

Articles	Surfaces (cm ²)	Mass (g)
Article 1	600	1000

Total surface of all articles (cm²): 600

Fitting Mode



Loops per serie: 20 Iterations: 0

Optimize Refresh

Correlation

mtau: 1
mtolg: 1E-6
mtolx: 1E-6 mrealstep: 1E-3

Parameter Name	Value
Layer 1-Op-Known(cm ² /s)	2.149E-16

Close Fitting Mode for This Package

Create Global Package

Package Properties Output Calculation

Save Package Save Package As Duplicate Package Save All Packages Close Package Package Details

New Package Open Package

New Article Open Article Import Article Save Article Duplicate Article Close Article

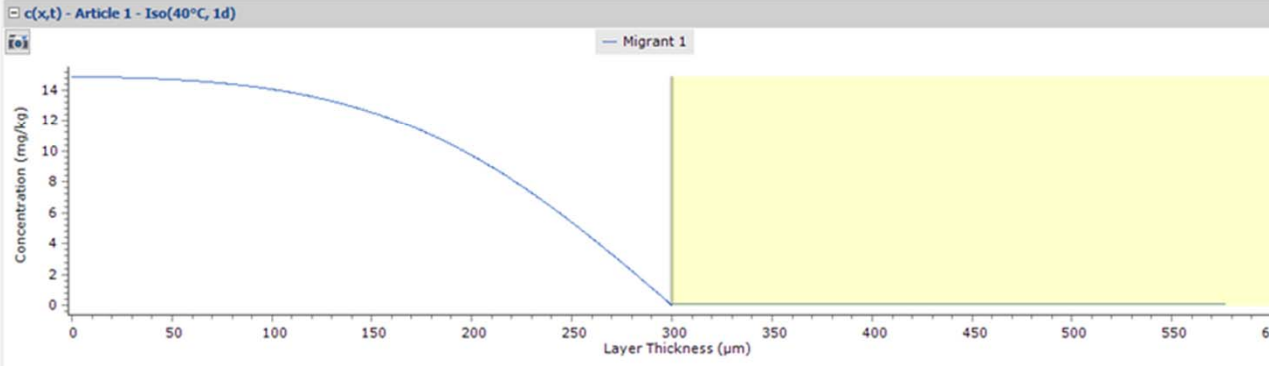
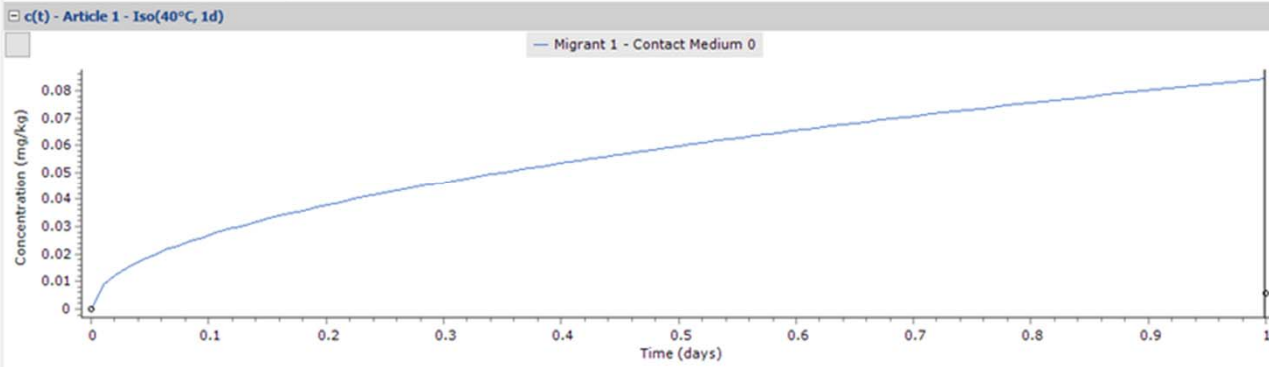
Import Initial Concentration Prediction on This Article Prediction on All Articles Close All Articles Delete All Article Outputs Close All

- Package SAN 24h at 40C
- Article 1
- Iso(40°C, 1d)

Temperature : 40 (°C) Display unit mg/kg c(t) : draw mean concentration c(t) : draw concentration at 0 % of thickness from surface

Article	Layer 1	Contact Med...
	ACRYLONIT...	Acetic acid 3%
	Thickness (µm)	300
		1.667E04
<input checked="" type="checkbox"/> Migrant 1	ACRYLONIT...	10.74
		0.0836

Concentration Diffusion Coefficient Partition Coefficient Solubility



Package SAN 24h at 40C

Geometry Rectangular

Contact Surface (cm²): 600

Volume of Contact Medium (cm³): 1000

Width (cm): 10

Height (cm): 10

Length (cm): 10

Surface and mass of contact medium by article

Articles	Surfaces (cm ²)	Mass (g)
Article 1	600	1000

Total surface of all articles (cm²): 600

Fitting Mode

Loops per serie: 20 Iterations: 1

Optimize Refresh

Correlation

mtau: 1

mtolg: 1E-6

mtolx: 1E-6 mrealstep: 1E-3

Parameter Name	Value
Layer 1-Dp-Known(cm ² /s)	6.729E-10

Close Fitting Mode for This Package

Create Global Package

Package Properties

Output Calculation

Save Package Save Package As Duplicate Package Save All Packages Close Package Package Details

New Article Open Article Import Article Save Article Duplicate Article Close Article

Import Initial Concentration Prediction on This Article Prediction on All Articles Close All Articles Delete All Article Outputs Close All

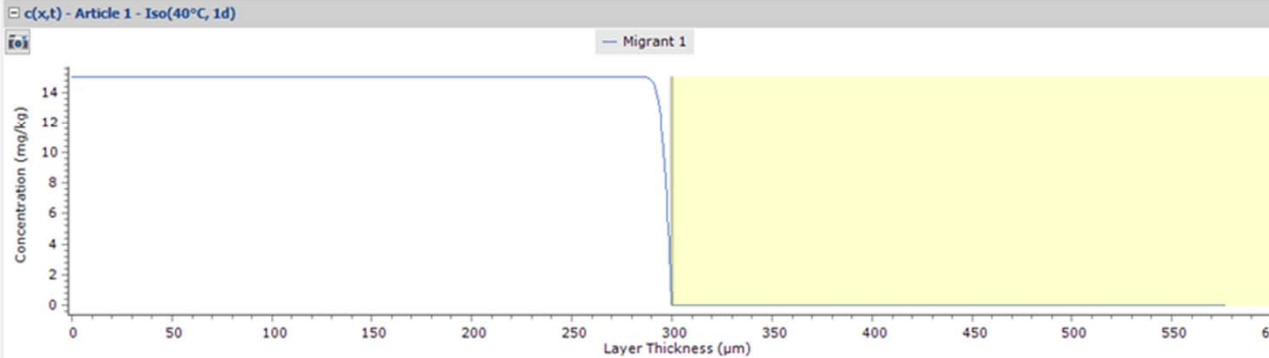
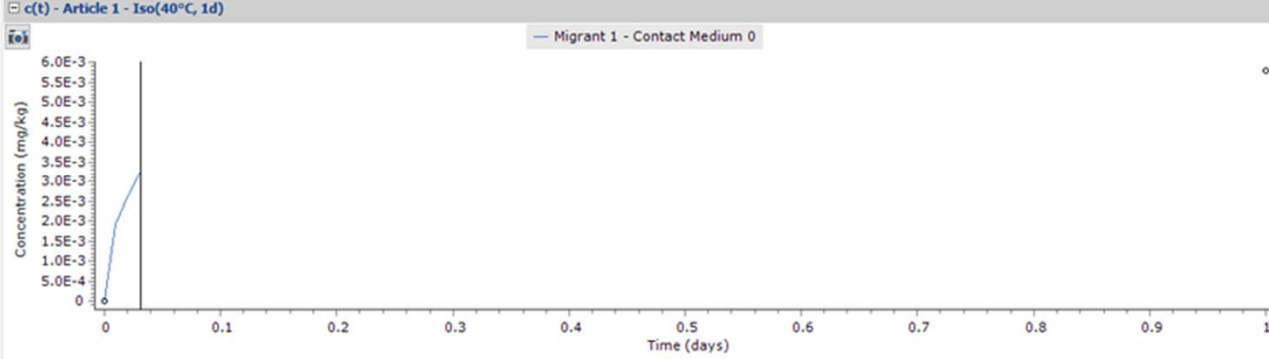
- Package SAN 24h at 40C
- Article 1
- Iso(40°C, 1d)

Temperature : 40 (°C) Display unit mg/kg c(t) : draw mean concentration c(t) : draw concentration at 0 % of thickness from surface

Grid

	Layer 1	Contact Med...
ACRYLONIT...	ACRYLONIT...	Acetic acid 3%
Thickness (µm)	300	1.667E04
Migrant 1	ACRYLONIT...	14.9
		0.001912

Concentration Diffusion Coefficient Partition Coefficient Solubility



Package SAN 24h at 40C

Geometry Rectangular

Contact Surface (cm²): 600

Volume of Contact Medium (cm³): 1000

Width (cm): 10

Height (cm): 10

Length (cm): 10

Add Article

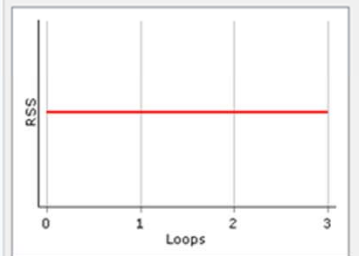
Surface and mass of contact medium by article

Articles	Surfaces (cm ²)	Mass (g)
Article 1	600	1000

Total surface of all articles (cm²): 600

Switch Package in Fitting Mode

Fitting Mode



Loops per serie 20 Iterations: 3

Optimize Refresh

Correlation

mtau 1

mtolg 1E-6

mtolx 1E-6 mrealstep 1E-3

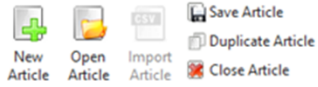
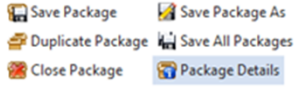
Parameter Name	Value
Layer 1-Dp-Known(cm ² /s)	3.089E-11

Close Fitting Mode for This Package

Create Global Package

Package Properties

Output Calculation



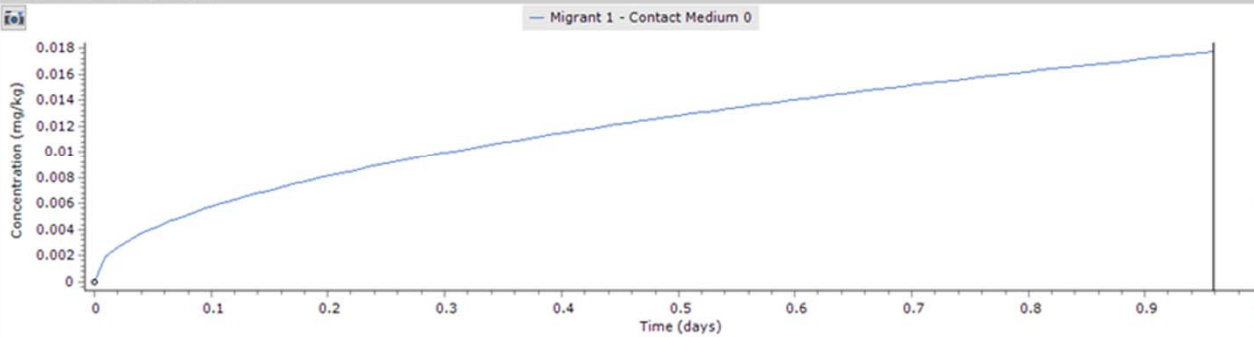
- Package SAN 24h at 40C
- Article 1
- Iso(40°C, 1d)

Temperature : 40 (°C) Display unit mg/kg c(t) : draw mean concentration c(t) : draw concentration at 0 % of thickness from surface

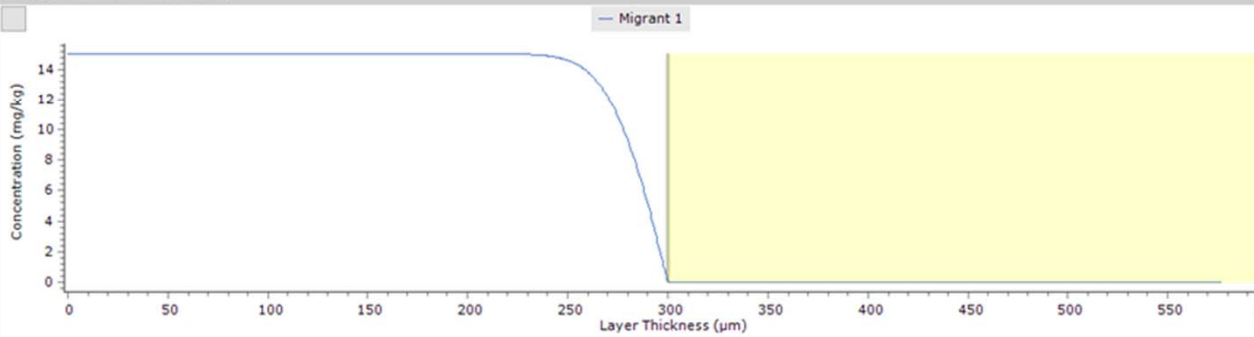
Article	Layer 1	Contact Med...
ACRYLONIT...	ACRYLONIT...	Acetic acid 3%
Thickness (µm)	300	1.667E04
Migrant 1	ACRYLONIT...	14.1
		0.01762

Concentration Diffusion Coefficient Partition Coefficient Solubility

c(t) - Article 1 - Iso(40°C, 1d)



c(x,t) - Article 1 - Iso(40°C, 1d)



Package SAN 24h at 40C

Geometry

Rectangular

Contact Surface (cm²): 600

Volume of Contact Medium (cm³): 1000

Width (cm): 10

Height (cm): 10

Length (cm): 10

Add Article

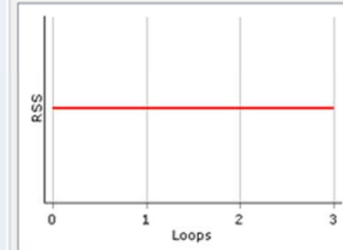
Surface and mass of contact medium by article

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

Fitting Mode



Loops per serie 20 Iterations: 3

Optimize Refresh

Correlation

mtau 1

mtolg 1E-6

mtolx 1E-6 mrealstep 1E-3

Parameter Name	Value
Layer 1-Op-Known(cm ² /s)	3.089E-11

Close Fitting Mode for This Package

Create Global Package

Package Properties Output Calculation

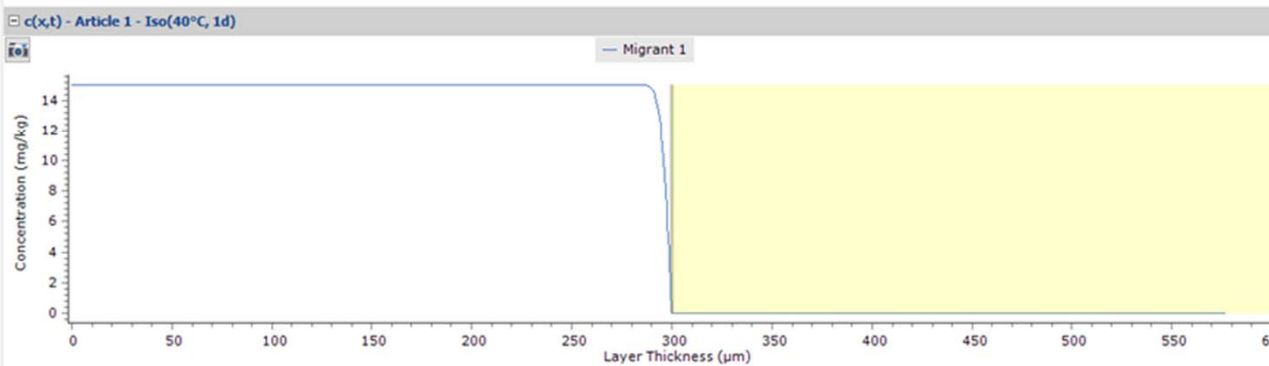
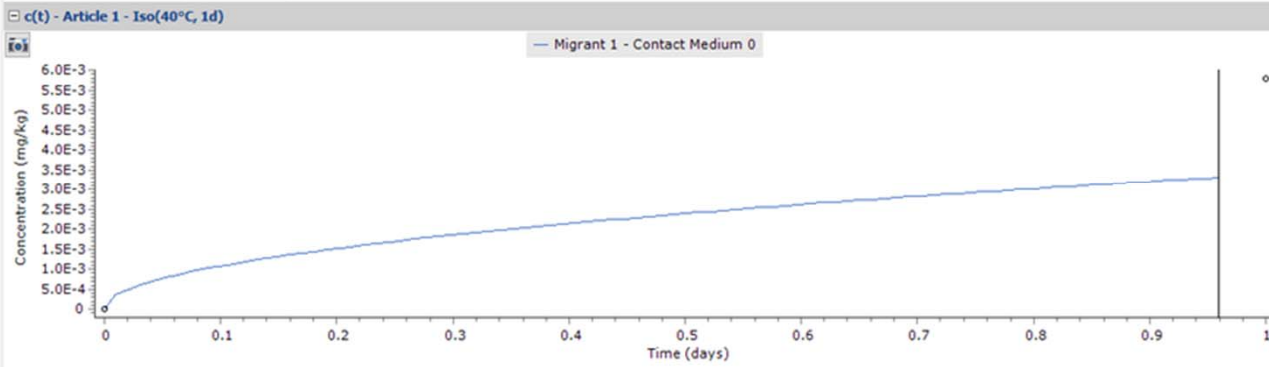
Package SAN 24h at 40C

- Article 1
 - Iso(40°C, 1d)

Temperature : 40 (°C) Display unit mg/kg c(t) : draw mean concentration c(t) : draw concentration at 0 % of thickness from surface

Grid

Article	Layer 1	Contact Med...
	ACRYLONIT...	Acetic acid 3%
	Thickness (µm)	1.667E04
	300	
<input checked="" type="checkbox"/> Migrant 1	ACRYLONIT...	0.003272
	14.83	



Package SAN 24h at 40C

Geometry: Rectangular

Contact Surface (cm²): 600

Volume of Contact Medium (cm³): 1000

Width (cm): 10

Height (cm): 10

Length (cm): 10

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

Total surface of all articles (cm²): 600

Fitting Mode

Loops per serie: 20 Iterations: 4

mtau: 1

mtolg: 1E-6

mtolx: 1E-6 mrealstep: 1E-3

Parameter Name	Value
Layer 1-Op-Known(cm ² /s)	1.074E-12

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Package Properties

Output Calculation

New Package
Open Package

Save Package
Duplicate Package
Close Package
Save Package As
Save All Packages
Package Details

New Article
Open Article
Import Article
Save Article
Duplicate Article
Close Article

Import Initial Concentration

Prediction on This Article
Prediction on All Articles

Close All Articles
Delete All Article Outputs
Close All

Package SAN 24h at 40C

Article 1

Iso(40°C, 1d)

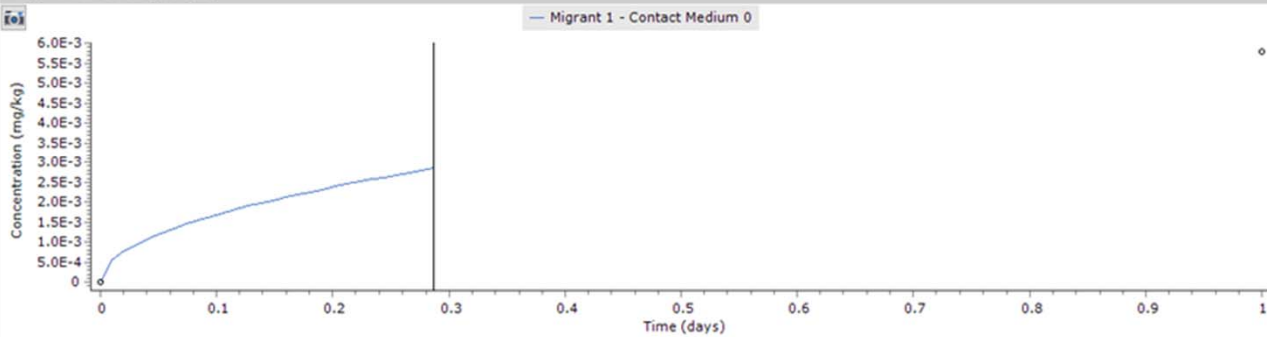
Temperature : 40 (°C) Display unit mg/kg c(t) : draw mean concentration c(t) : draw concentration at 0 % of thickness from surface

Grid

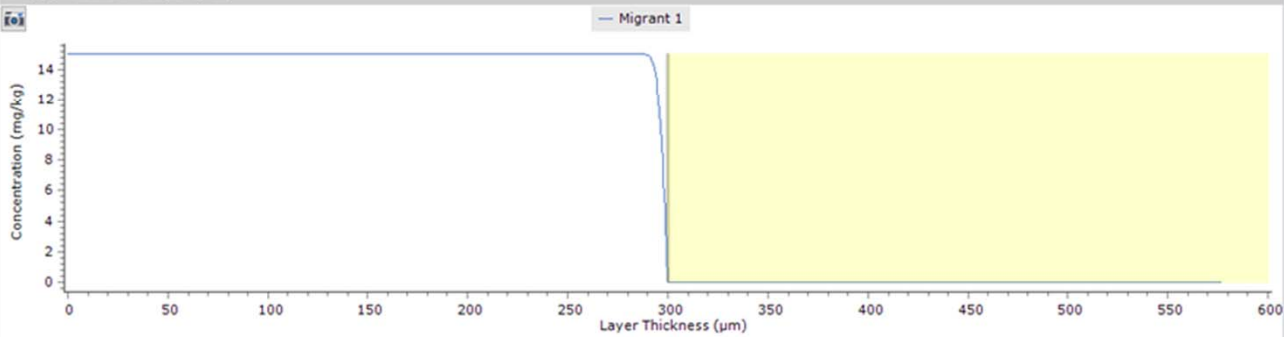
Article	Layer 1	Contact Med...
ACRYLONIT...	<input type="checkbox"/>	<input checked="" type="checkbox"/>
Thickness (µm)	ACRYLONIT...	Acetic acid 3%
	14.86	1.667E04
<input checked="" type="checkbox"/> Migrant 1	ACRYLONIT...	0.002736

Concentration Diffusion Coefficient Partition Coefficient Solubility

c(t) - Article 1 - Iso(40°C, 1d)



c(x,t) - Article 1 - Iso(40°C, 1d)



Package SAN 24h at 40C

Geometry

Rectangular

Contact Surface (cm²): 600

Volume of Contact Medium (cm³): 1000

Width (cm): 10

Height (cm): 10

Length (cm): 10

Add Article

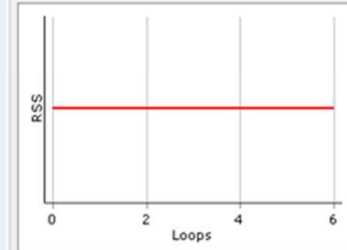
Surface and mass of contact medium by article

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

Total surface of all articles (cm²): 600

Switch Package in Fitting Mode

Fitting Mode



Loops per serie 20 Iterations: 6

Optimize Refresh

Correlation

mtau 1

mtolg 1E-6

mtolx 1E-6 mrealstep 1E-3

Parameter Name	Value
Layer 1-Op-Known(cm ² /s)	2.639E-12

Close Fitting Mode for This Package

Create Global Package

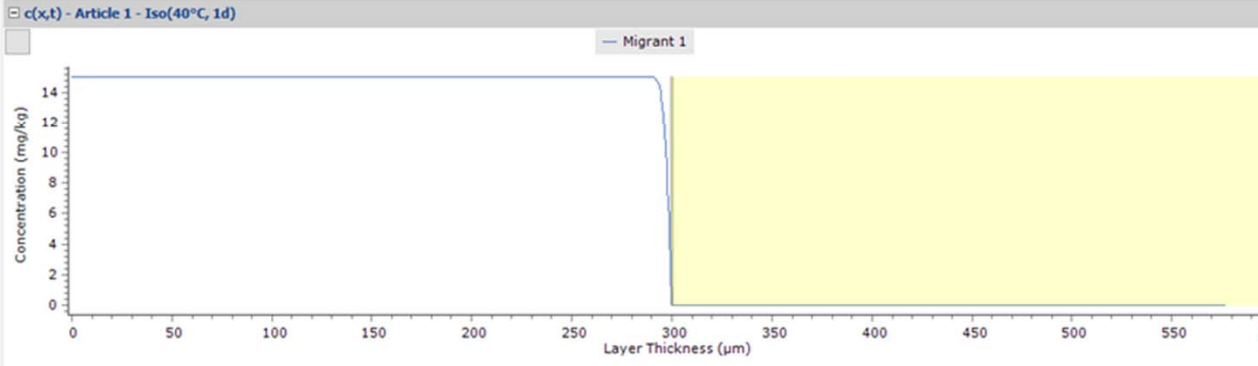
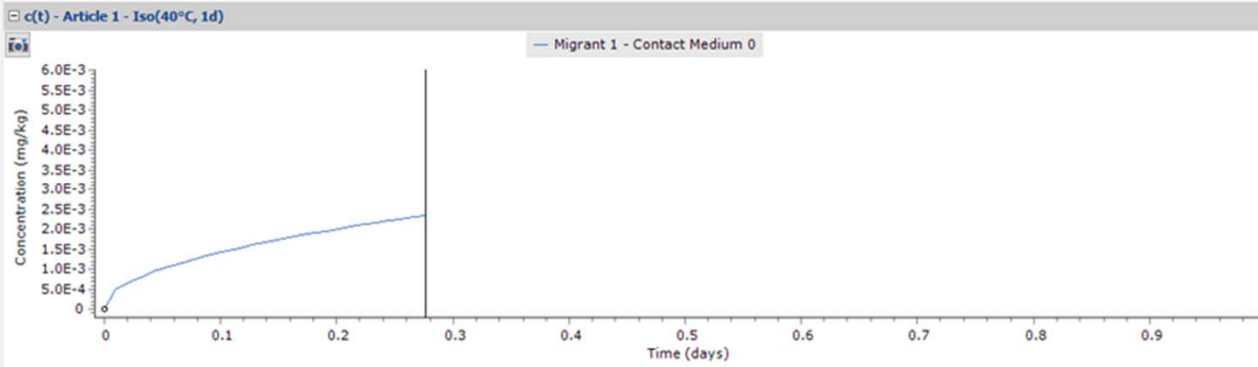
Package Properties Output Calculation

Package SAN 24h at 40C
 Article 1
 Iso(40°C, 1d)

Temperature : 40 (°C) Display unit mg/kg c(t) : draw mean concentration c(t) : draw concentration at 0 % of thickness from surface

Grid

Article	Layer 1	Contact Med...
	ACRYLONIT...	Acetic acid 3%
	Thickness (µm)	1.667E04
	300	
<input checked="" type="checkbox"/> Migrant 1	ACRYLONIT...	0.002305
	14.88	



Package SAN 24h at 40C

Geometry: Rectangular

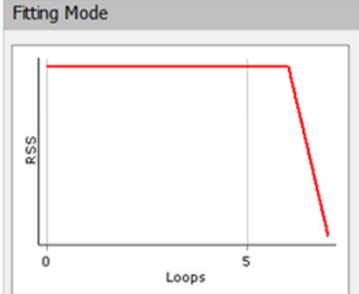
Contact Surface (cm²): 600
 Volume of Contact Medium (cm³): 1000

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

Surface and mass of contact medium by article

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

Total surface of all articles (cm²): 600



Loops per serie: 20 Iterations: 7

mtau: 1
 mtolg: 1E-6
 mtolx: 1E-6 mrealstep: 1E-3

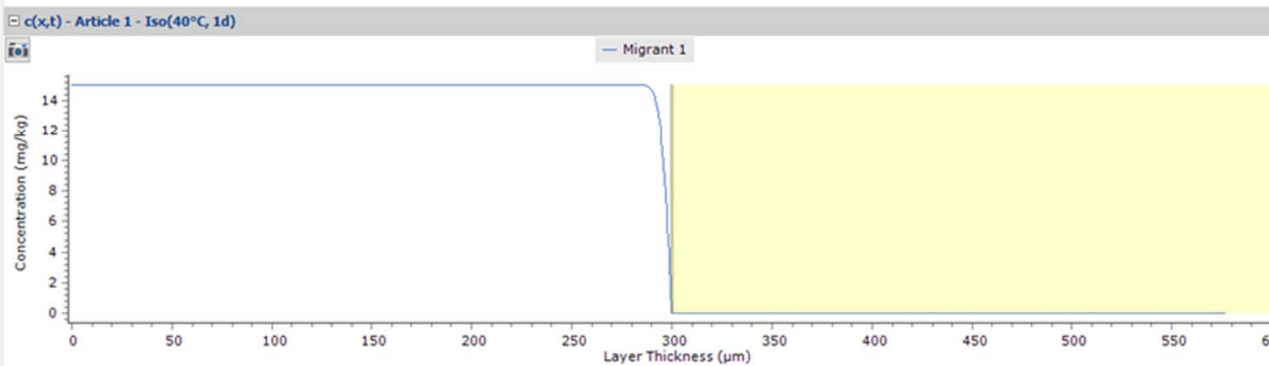
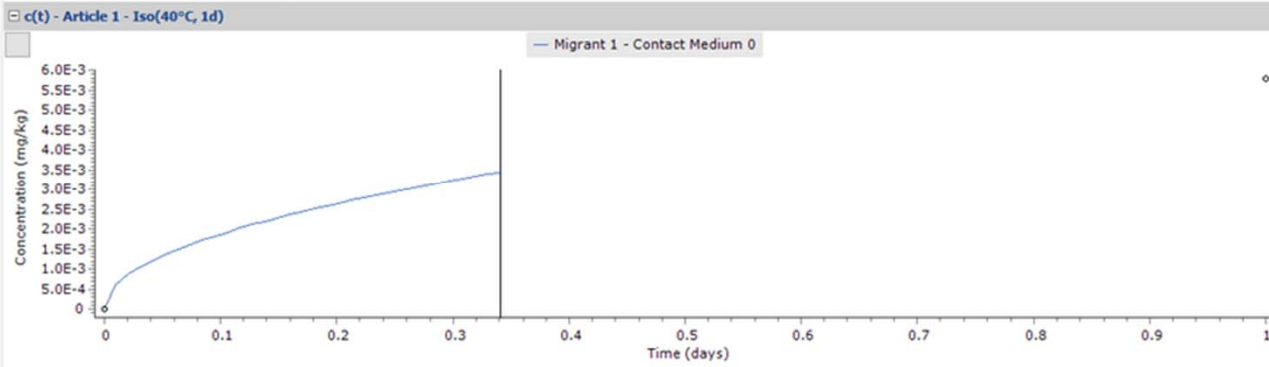
Parameter Name	Value
Layer 1-Op-Known(cm ² /s)	1.872E-12

Package Properties | Output Calculation

- Package SAN 24h at 40C
 - Article 1
 - Iso(40°C, 1d)

Temperature : 40 (°C) Display unit mg/kg c(t) : draw mean concentration c(t) : draw concentration at 0 % of thickness from surface

Article	Layer 1	Contact Med...
	ACRYLONIT...	Acetic acid 3%
	Thickness (µm)	300
		1.667E04
<input checked="" type="checkbox"/> Migrant 1	ACRYLONIT...	14.83
		0.003331



Package SAN 24h at 40C

Geometry: Rectangular

Contact Surface (cm²): 600
Volume of Contact Medium (cm³): 1000

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

Articles	Surfaces (cm ²)	Mass (g)
Article 1	600	1000

Switch Package in Fitting Mode

Fitting Mode

Loops per serie: 20 Iterations: 8

Correlation

mtau: 1
mtolg: 1E-6
mtolx: 1E-6 mrealstep: 1E-3

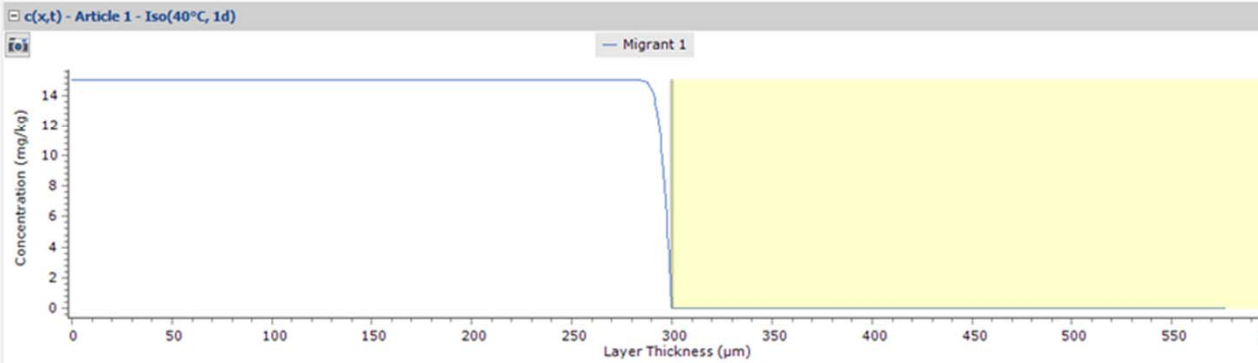
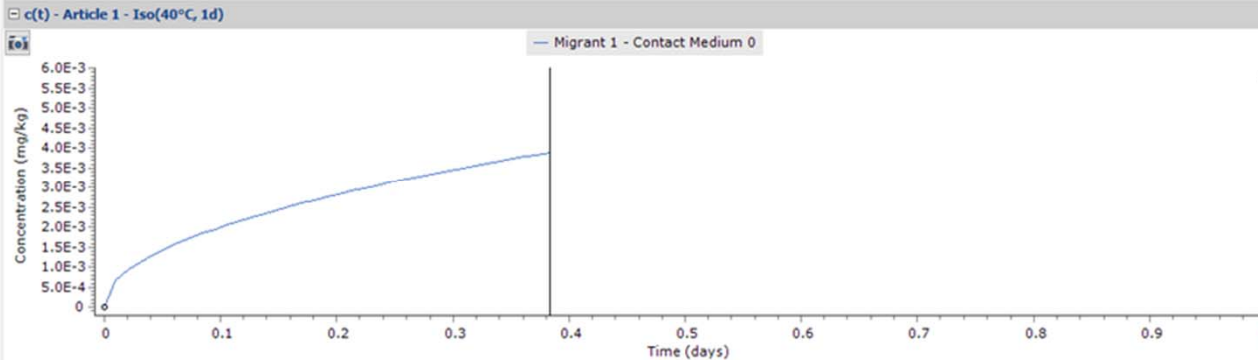
Parameter Name	Value
Layer 1-Op-Known(cm ² /s)	3.263E-12

Package Properties Output Calculation

- Package SAN 24h at 40C
- Article 1
- Iso(40°C, 1d)

Temperature : 40 (°C) Display unit mg/kg c(t) : draw mean concentration c(t) : draw concentration at 0 % of thickness from surface

Article	Layer 1	Contact Med...
	ACRYLONIT...	Acetic acid 3%
	Thickness (µm)	300
		1.667E04
<input checked="" type="checkbox"/> Migrant 1	ACRYLONIT...	14.81
		0.003786



Package SAN 24h at 40C

Geometry: Rectangular

Contact Surface (cm²): 600

Volume of Contact Medium (cm³): 1000

Width (cm): 10

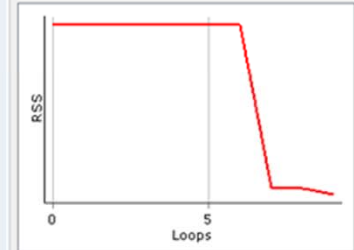
Height (cm): 10

Length (cm): 10

Articles	Surfaces (cm ²)	Mass (g)
Article 1	600	1000

Total surface of all articles (cm²): 600

Fitting Mode



Loops per serie: 20 Iterations: 9

mtau: 1

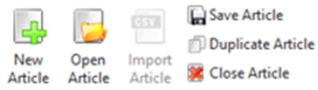
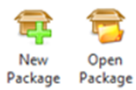
mtolg: 1E-6

mtolx: 1E-6 mrealstep: 1E-3

Parameter Name	Value
Layer 1-Op-Known(cm ² /s)	3.72E-12

Package Properties

Output Calculation



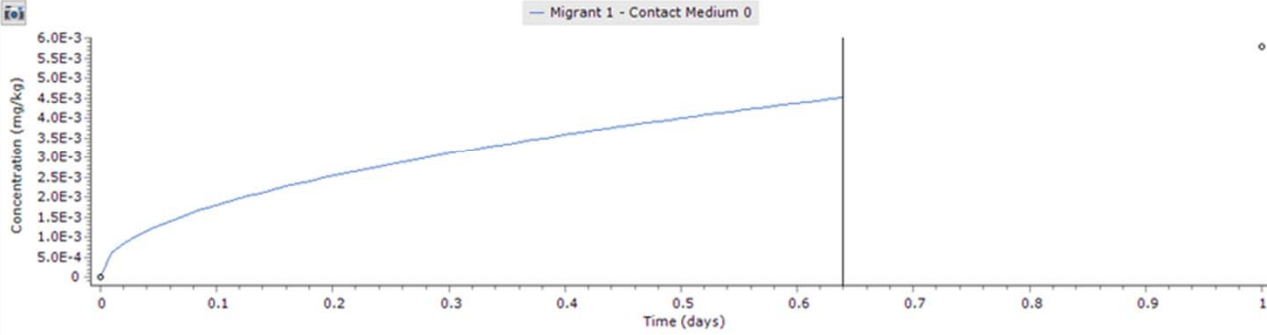
- Package SAN 24h at 40C
- Article 1
- Iso(40°C, 1d)

Temperature : 40 (°C) Display unit mg/kg c(t) : draw mean concentration c(t) : draw concentration at 0 % of thickness from surface

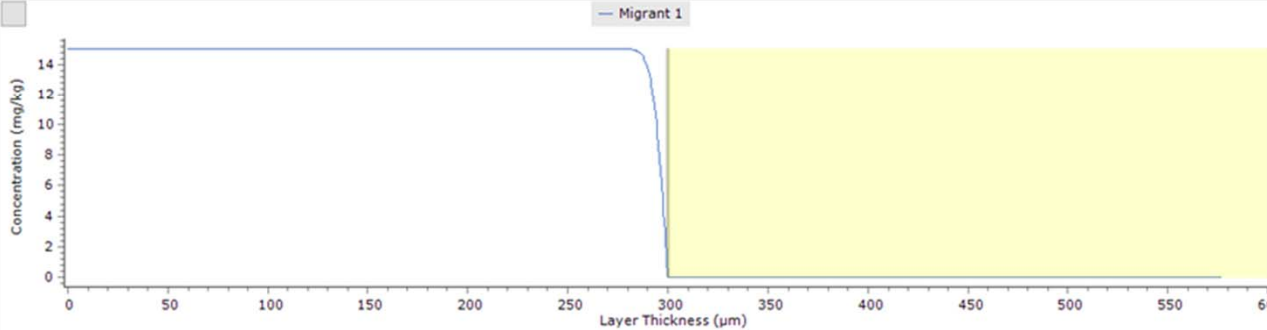
Article	Layer 1	Contact Med...
	ACRYLONIT...	Acetic acid 3%
	Thickness (µm)	1.667E04
	300	0.004483
<input checked="" type="checkbox"/> Migrant 1	ACRYLONIT...	14.77
		0.004483

Concentration Diffusion Coefficient Partition Coefficient Solubility

c(t) - Article 1 - Iso(40°C, 1d)



c(x,t) - Article 1 - Iso(40°C, 1d)



Package SAN 24h at 40C

Geometry: Rectangular

Contact Surface (cm²): 600

Volume of Contact Medium (cm³): 1000

Width (cm): 10

Height (cm): 10

Length (cm): 10

Add Article

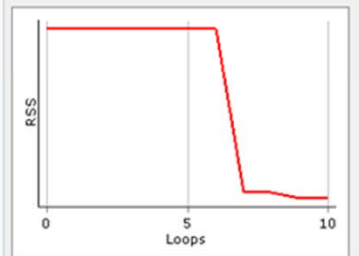
Surface and mass of contact medium by article

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

Total surface of all articles (cm²): 600

Switch Package in Fitting Mode

Fitting Mode



Loops per serie: 20 Iterations: 10

Optimize Refresh

Correlation

mtau: 1

mtolg: 1E-6

mtolx: 1E-6 mrealstep: 1E-3

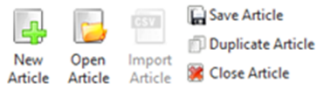
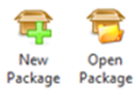
Parameter Name	Value
Layer 1-Op-Known(cm ² /s)	3.009E-12

Close Fitting Mode for This Package

Create Global Package

Package Properties

Output Calculation



Package SAN 24h at 40C

Article 1

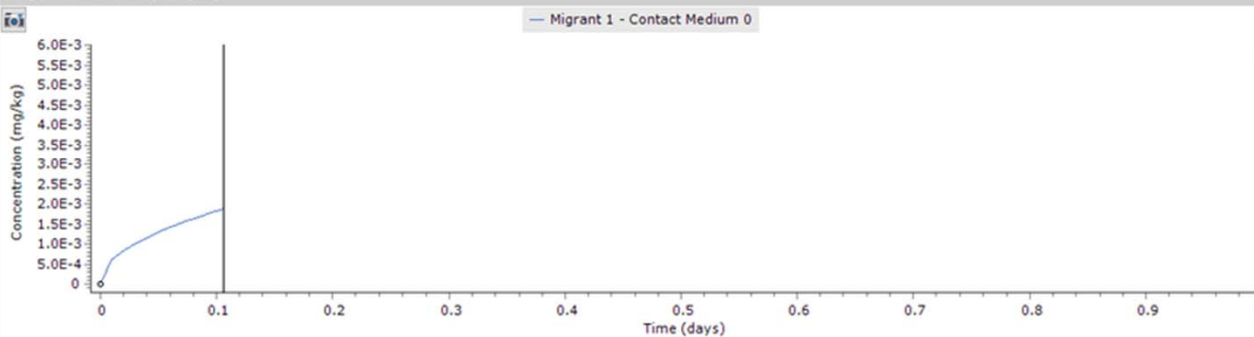
Iso(40°C, 1d)

Temperature : 40 (°C) Display unit mg/kg c(t) : draw mean concentration c(t) : draw concentration at 0 % of thickness from surface

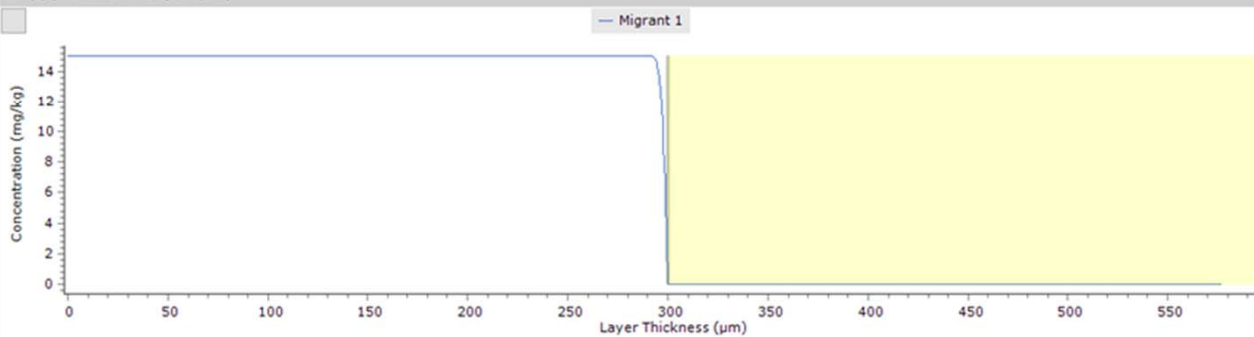
Grid

Article	Layer 1	Contact Med...
ACRYLONIT...	ACRYLONIT...	Acetic acid 3%
Thickness (µm)	300	1.667E04
Migrant 1	ACRYLONIT...	14.91
		0.001784

c(t) - Article 1 - Iso(40°C, 1d)



c(x,t) - Article 1 - Iso(40°C, 1d)



Package SAN 24h at 40C

Geometry

Rectangular

Contact Surface (cm²): 600

Volume of Contact Medium (cm³): 1000

Width (cm): 10

Height (cm): 10

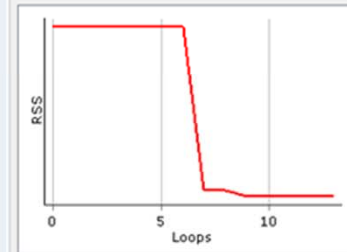
Length (cm): 10

Surface and mass of contact medium by article

Articles	Surfaces (cm ²)	Mass (g)
Article 1	600	1000

Total surface of all articles (cm²): 600

Fitting Mode



Loops per serie 20 Iterations: 13

Optimize Refresh

Correlation

mtau 1

mtolg 1E-6

mtolx 1E-6 mrealstep 1E-3

Parameter Name	Value
Layer 1-Op-Known(cm ² /s)	3.103E-12

Close Fitting Mode for This Package

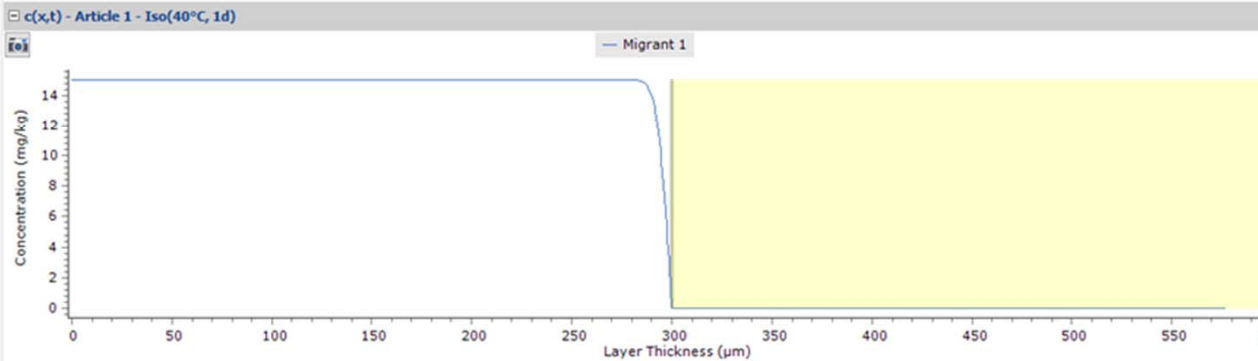
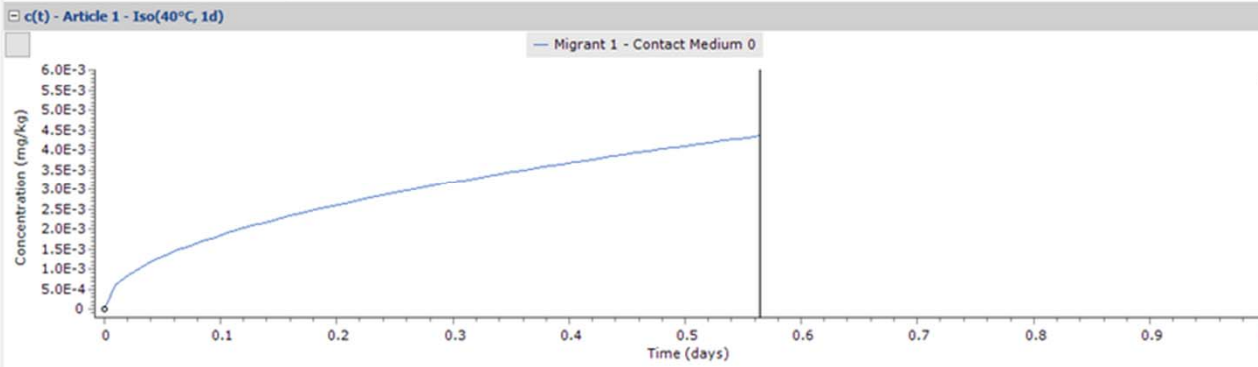
Create Global Package

Package Properties Output Calculation

- Package SAN 24h at 40C
 - Article 1
 - Iso(40°C, 1d)

Temperature : 40 (°C) Display unit mg/kg c(t) : draw mean concentration c(t) : draw concentration at 0 % of thickness from surface

Article	Layer 1	Contact Med...
ACRYLONIT...	ACRYLONIT...	Acetic acid 3%
Thickness (µm)	300	1.667E04
Migrant 1	ACRYLONIT...	14.78
		0.004283



Package SAN 24h at 40C

Geometry

Rectangular

Contact Surface (cm²): 600

Volume of Contact Medium (cm³): 1000

Width (cm): 10

Height (cm): 10

Length (cm): 10

Add Article

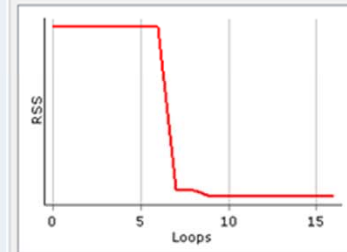
Surface and mass of contact medium by article

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

Fitting Mode



Loops per serie 20 Iterations: 16

Optimize Refresh

Correlation

mtau 1

mtolg 1E-6

mtolx 1E-6 mrealstep 1E-3

Parameter Name	Value
Layer 1-Op-Known(cm ² /s)	3.178E-12

Close Fitting Mode for This Package

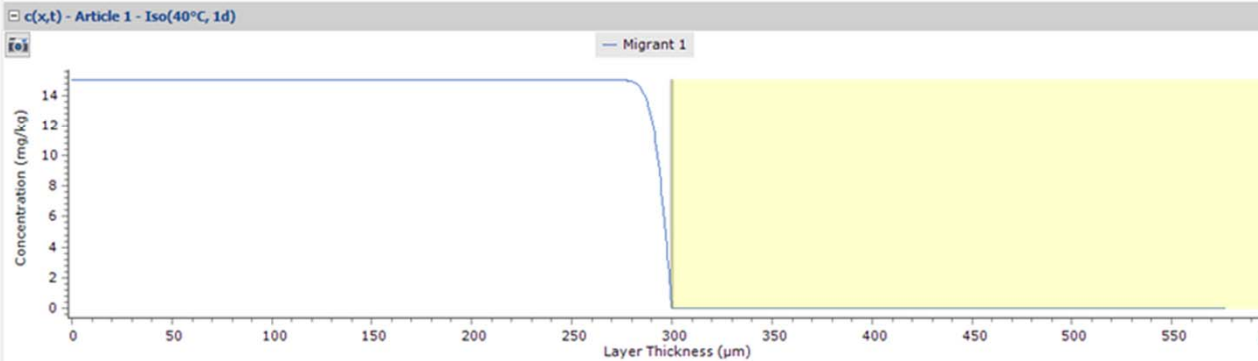
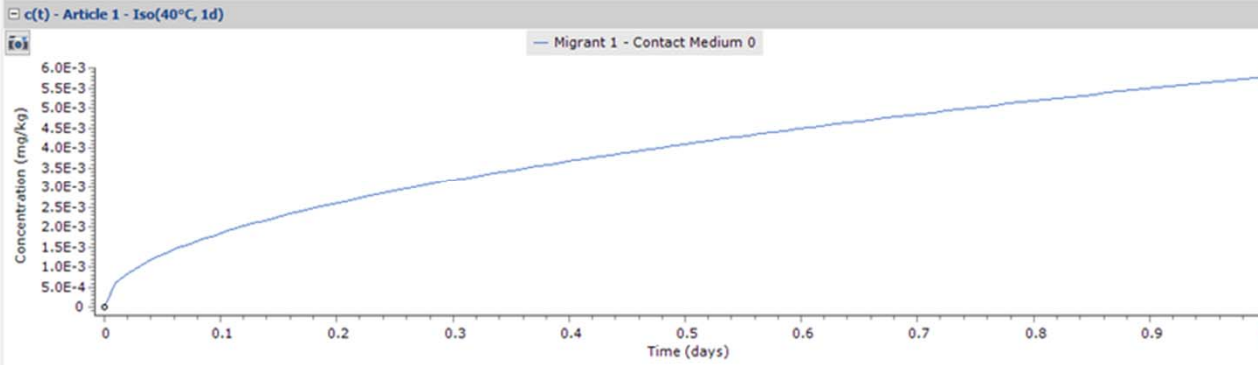
Create Global Package

Package Properties Output Calculation

- Package SAN 24h at 40C
 - Article 1
 - Iso(40°C, 1d)

Temperature : 40 (°C) Display unit mg/kg c(t) : draw mean concentration c(t) : draw concentration at 0 % of thickness from surface

Article	Layer 1	Contact Med...
	ACRYLONIT...	Acetic acid 3%
	Thickness (µm)	1.667E04
	300	
<input checked="" type="checkbox"/> Migrant 1	ACRYLONIT...	0.005776
	14.71	



Package SAN 24h at 40C

Geometry: Rectangular

Contact Surface (cm²): 600

Volume of Contact Medium (cm³): 1000

Width (cm): 10

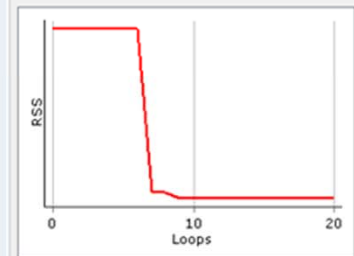
Height (cm): 10

Length (cm): 10

Articles	Surfaces (cm ²)	Mass (g)
Article 1	600	1000

Total surface of all articles (cm²): 600

Fitting Mode



Loops per serie: 20 Iterations: 20

Correlation

mtau: 1

mtolg: 1E-6

mtolx: 1E-6 mrealstep: 1E-3

Parameter Name	Value
Layer 1-Op-Known(cm ² /s)	3.172E-12

Package Properties Output Calculation

Package SAN 24h at 40C

- Article 1
 - Iso(40°C, 1d)

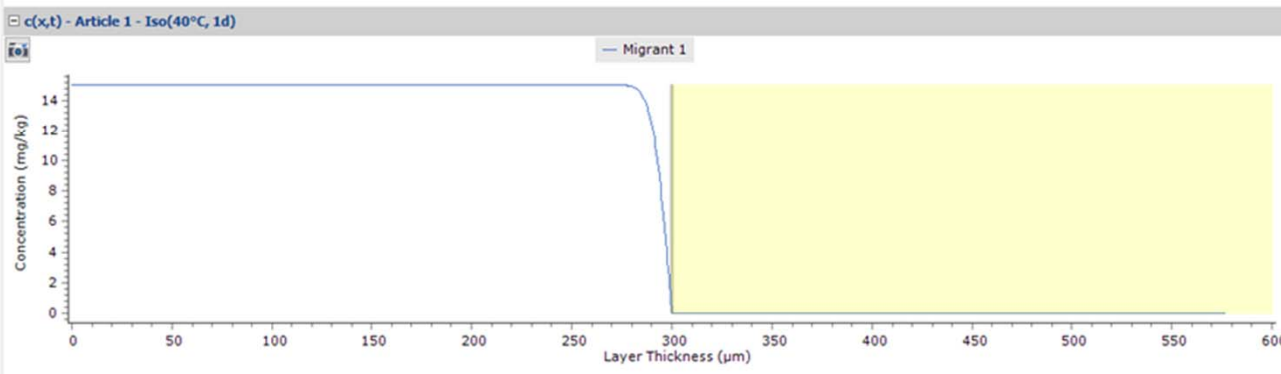
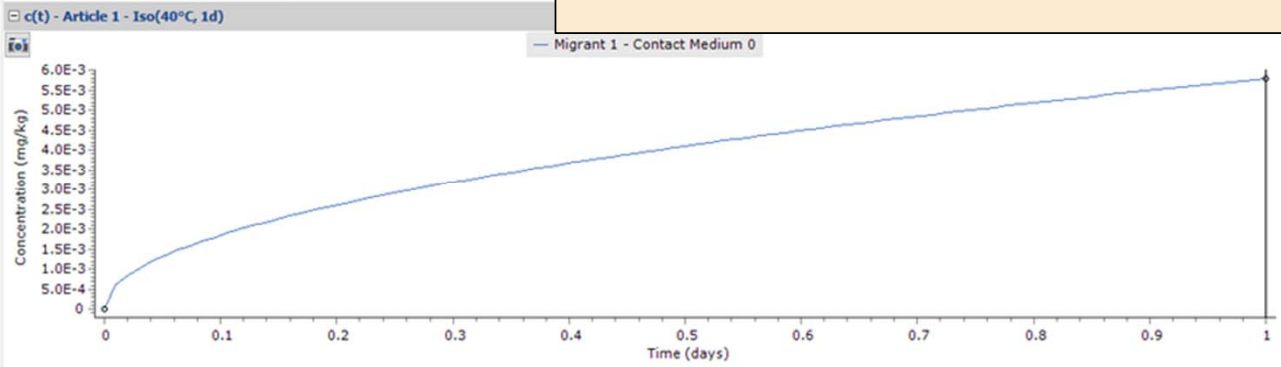
Temperature : 40 (°C) Display unit mg/kg c(t) : draw mean concentration c(t) : draw concentration at 0 % of thickness from surface

Grid

Article	Layer 1	Contact Med...
	ACRYLONIT...	Acetic acid 3%
	Thickness (µm)	1.667E04
	300	
<input checked="" type="checkbox"/> Migrant 1	ACRYLONIT...	0.005776
	14.71	

Concentration Diffusion Coefficient Partition Coefficient

48: Fitting_modeのサムネールの赤曲線が飽和したことで回帰計算が終了したことを示します。



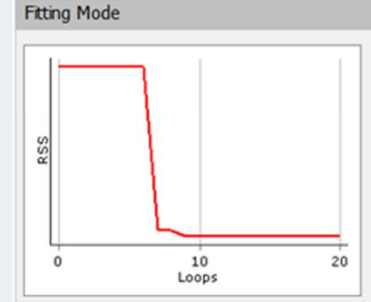
Package SAN 24h at 40C

Geometry: Rectangular

Surface and mass of contact medium by article

Articles	Surfaces (cm ²)	Mass (g)
Article 1	600	1000

Total surface of all articles (cm²): 600



Loops per serie: 20 Iterations: 20

Correlation

mtau: 1 mtol: 1E-6 mtolx: 1E-6 mrealstep: 1E-3

Parameter Name	Value
Layer 1-Dp-Known(cm ² /s)	3.172E-12

Package Properties Output Calculation

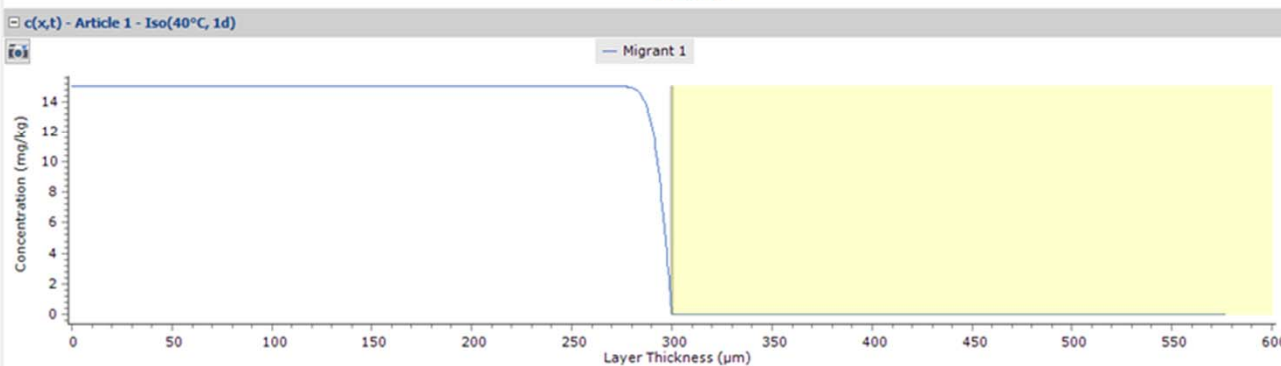
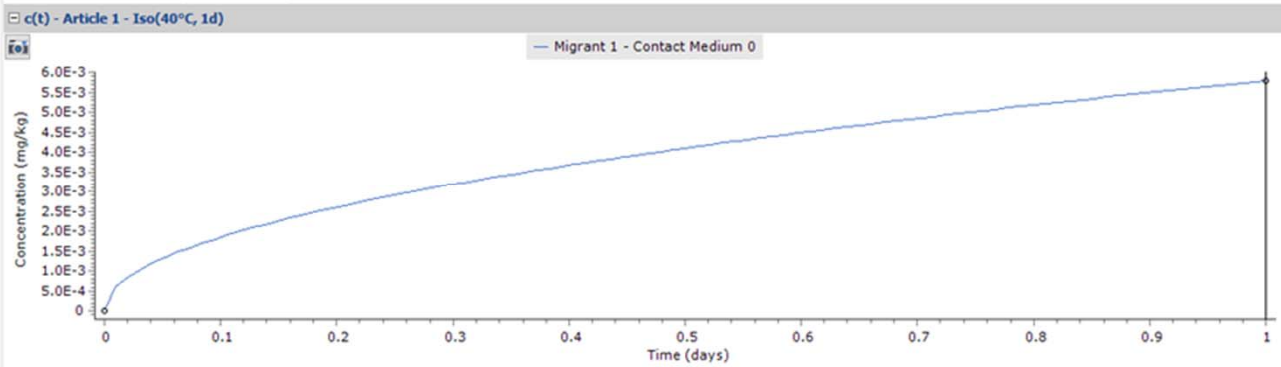
Package SAN 24h at 40C
 Article 1
 Iso(40°C, 1d)

Save currently selected package as a new file name.

Grid

Article	Layer 1	Contact Med...
	ACRYLONIT...	Acetic acid 3%
	Thickness (µm)	1.667E04
	300	0.005776
<input checked="" type="checkbox"/>	Migrant 1	ACRYLONIT...
	Thickness (µm)	14.71

49: 回帰計算が終了したとき、拡散係数が3.17E-12になりました。ここで計算結果をsaveします。



Package SAN 24h at 40C

Geometry: Rectangular

Length (cm): 10

Surface and mass of contact medium by article

Articles	Surfaces (cm ²)	Mass (g)
Article 1	600	1000

Total surface of all articles (cm²): 600

Switch Package in Fitting Mode

Fitting Mode

Loops per serie: 20 Iterations: 20

Optimize Correlation Refresh

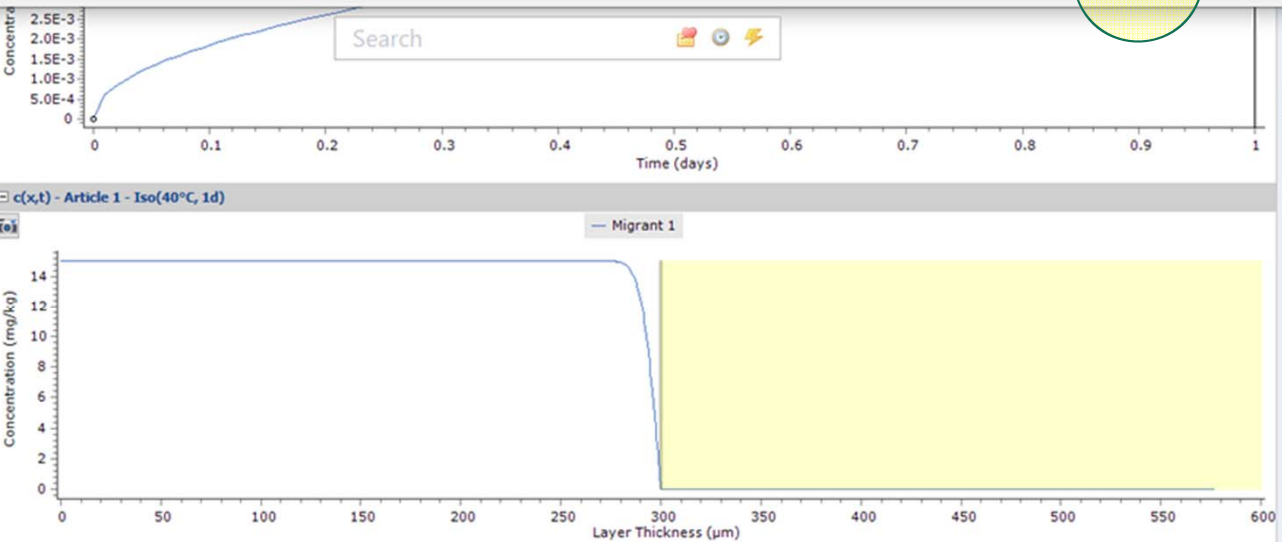
mtau: 1
mtolg: 1E-6
mtolx: 1E-6 mrealstep: 1E-3

Parameter Name: Layer 1-Dp-Known(cm²/s) Value: 3.172E-12

Close Fitting Mode for This Package
Create Global Package

50: saveするファイル名を設定して、saveをクリックします。

Save As dialog box showing file name: Package SAN 24h at 40C optimized.sml and Save as type: SML v5 (*.sml). The Save button is circled in green.



Software interface showing fitting mode parameters and a graph of RSS vs Loops.

Parameters:
Surface (cm²): 600
Contact Medium (cm³): 1000
Surfaces (cm²): 600
Mass (g): 1000

Graph: RSS vs Loops. The curve shows a sharp drop in RSS around 5 loops.

Buttons: Optimize, Refresh, Correlation, Close Fitting Mode for This Package, Create Global Package.

51: All stepsを選択します。

Package Properties Output Calculation

Save Package Save Package As
 Duplicate Package Save All Packages
 Close Package Package Details

New Package Open Package

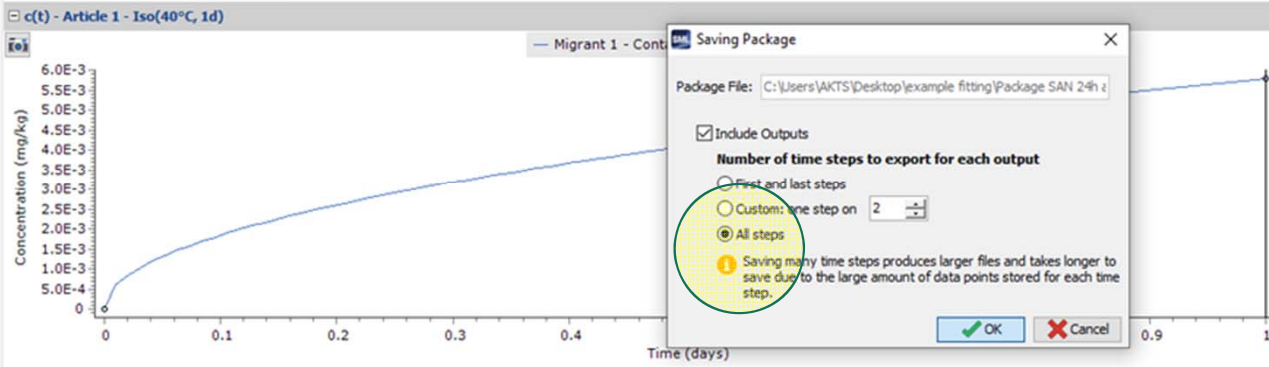
Package SAN 24h at 40°C

- Article 1
- Iso(40°C, 1d)

Temperature : 40 (°C) Display unit mg/kg c(t) : draw mean concentration c(t) : draw concentration at 0 % of thickness from surface

Article	Layer 1	Contact Med...
	ACRYLONIT...	Acetic acid 3%
	Thickness (µm)	1.667E04
	300	
<input checked="" type="checkbox"/> Migrant 1	ACRYLONIT...	0.005776
	14.71	

Concentration Diffusion Coefficient Partition Coefficient Solubility



Saving Package

Package File: C:\Users\AKTS\Desktop\example fitting\Package SAN 24h

Include Outputs

Number of time steps to export for each output

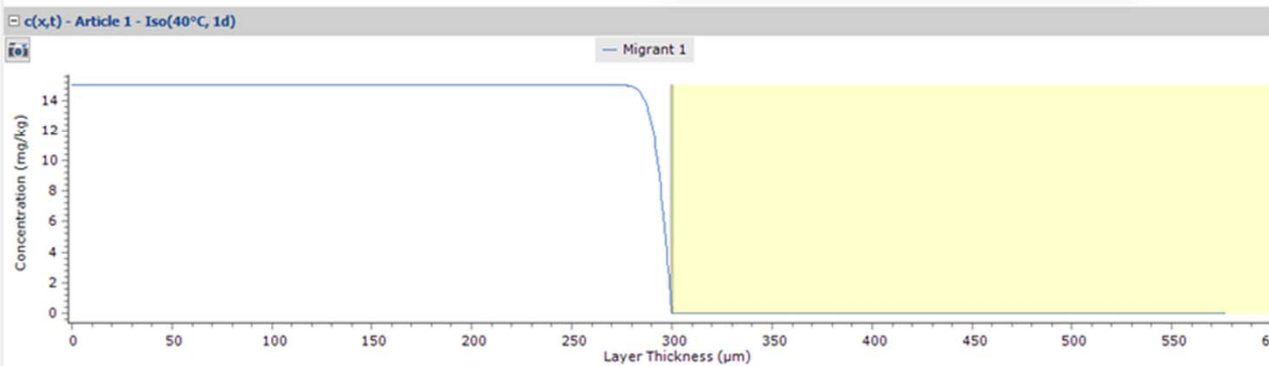
First and last steps

Custom: one step on 2

All steps

Saving many time steps produces larger files and takes longer to save due to the large amount of data points stored for each time step.

OK Cancel



Geometry

Rectangular

Contact Surface (cm²): 600

Volume of Contact Medium (cm³): 1000

Width (cm): 10

Height (cm): 10

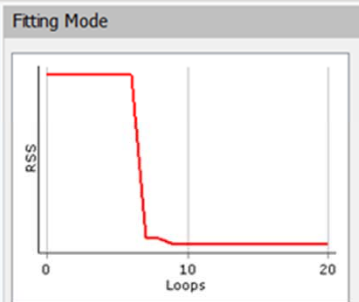
Length (cm): 10

Add Article

Surface and mass of contact medium by article

Articles	Surfaces (cm ²)	Mass (g)
Article 1	600	1000

Total surface of all articles (cm²): 600



Loops per serie 20 Iterations: 20

Optimize Refresh

Correlation

mtau 1

mtolg 1E-6

mtolx 1E-6 mrealstep 1E-3

Parameter Name	Value
Layer 1-Op-Known(cm ² /s)	3.172E-12

Close Fitting Mode for This Package

Create Global Package

52: OK を選択します。

Package Properties Output Calculation

Save Package Save Package As
Duplicate Package Save All Packages
Close Package Package Details

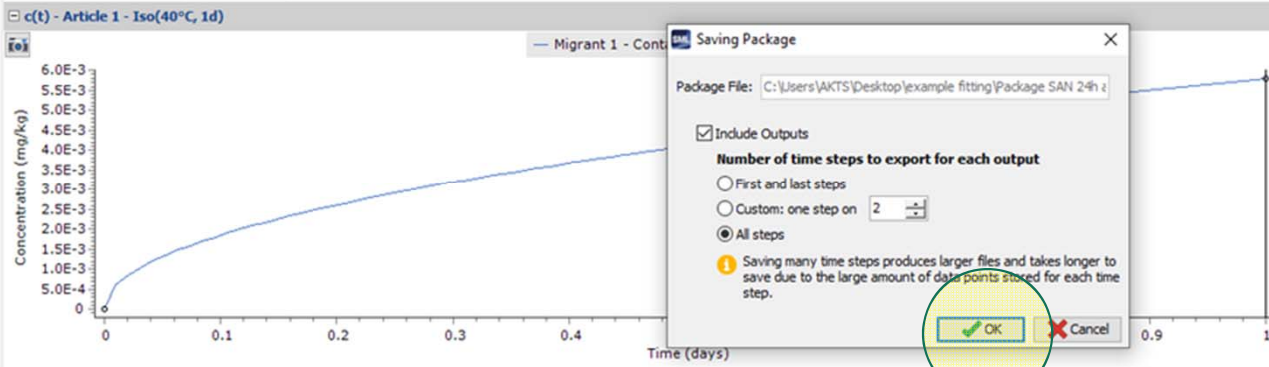
New Package Open Package

Package SAN 24h at 40°C op

- Article 1
 - Iso(40°C, 1d)

Temperature : 40 (°C) Display unit mg/kg c(t) : draw mean concentration c(t) : draw concentration at 0 % of thickness from surface

Article	Layer 1	Contact Med...
	ACRYLONIT...	Acetic acid 3%
	Thickness (µm)	1.667E04
	300	
<input checked="" type="checkbox"/> Migrant 1	ACRYLONIT...	0.005776
	14.71	



Saving Package

Package File: C:\Users\AKTS\Desktop\example fitting\Package SAN 24h

Include Outputs

Number of time steps to export for each output

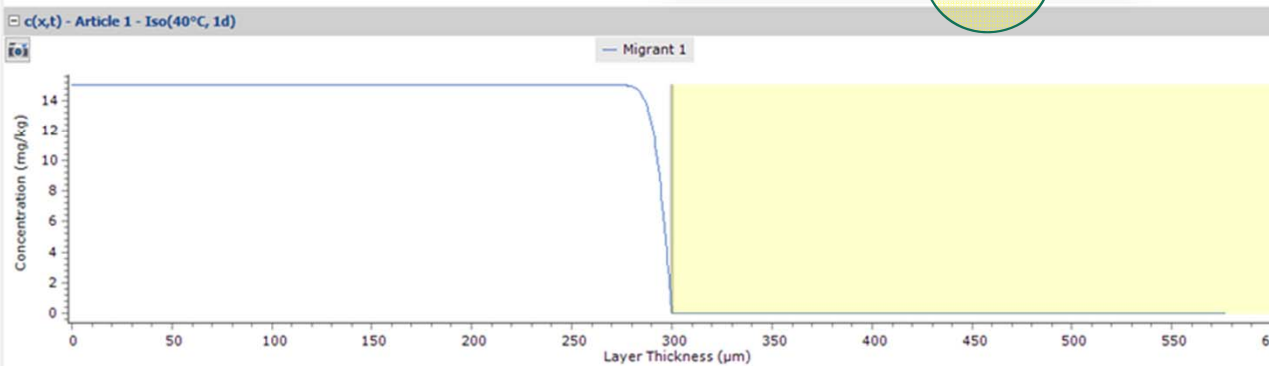
First and last steps

Custom: one step on 2

All steps

1 Saving many time steps produces larger files and takes longer to save due to the large amount of data points stored for each time step.

OK Cancel



Geometry

Rectangular

Contact Surface (cm²): 600

Volume of Contact Medium (cm³): 1000

Width (cm): 10

Height (cm): 10

Length (cm): 10

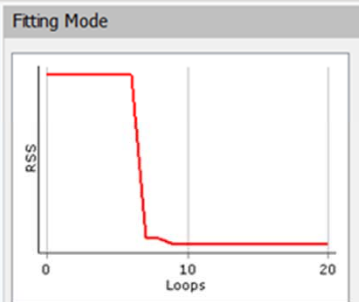
Add Article

Surface and mass of contact medium by article

Articles	Surfaces (cm ²)	Mass (g)
Article 1	600	1000

Total surface of all articles (cm²): 600

Switch Package in Fitting Mode



Loops per serie: 20 Iterations: 20

Optimize Refresh

Correlation

mtau: 1

mtolg: 1E-6

mtolx: 1E-6 mrealstep: 1E-3

Parameter Name	Value
Layer 1-Op-Known(cm ² /s)	3.172E-12

Close Fitting Mode for This Package

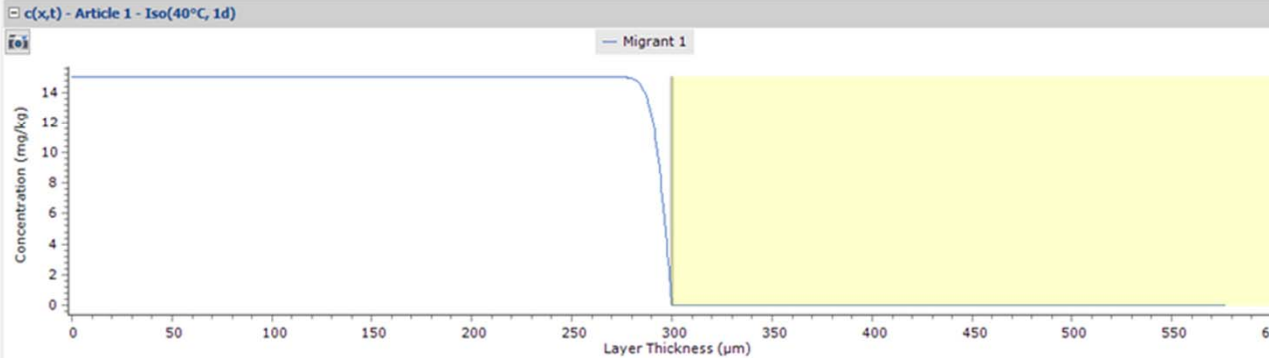
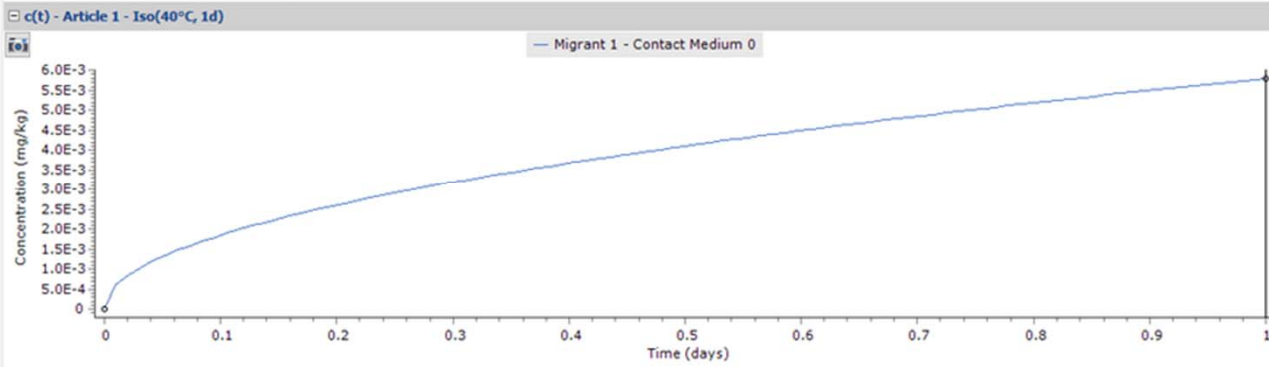
Create Global Package

Package Properties Output Calculation

- Package SAN 24h at 40C op
- Article 1
- Iso(40°C, 1d)

Temperature : 40 (°C) Display unit mg/kg c(t) : draw mean concentration c(t) : draw concentration at 0 % of thickness from surface

Article	Layer 1	Contact Med...
	ACRYLONIT...	Acetic acid 3%
	Thickness (µm)	300
		1.667E04
<input checked="" type="checkbox"/> Migrant 1	ACRYLONIT...	14.71
		0.005776



Package SAN 24h at 40C

Geometry: Rectangular

Contact Surface (cm²): 600

Volume of Contact Medium (cm³): 1000

Width (cm): 10

Height (cm): 10

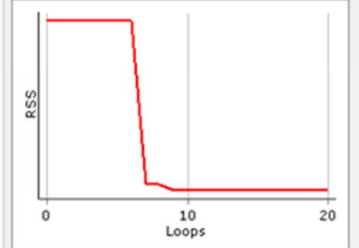
Length (cm): 10

Surface and mass of contact medium by article

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

Total surface of all articles (cm²): 600

Fitting Mode



Loops per serie: 20 Iterations: 20

Correlation

mtau: 1

mtol: 1E-6

mtolx: 1E-6 mrealstep: 1E-3

Parameter Name	Value
Layer 1-Op-Known(cm ² /s)	3.172E-12

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

Prediction

- Prediction on This Article
- Prediction on All Articles

File

- Close All Articles
- Delete All Article Outputs
- Close All

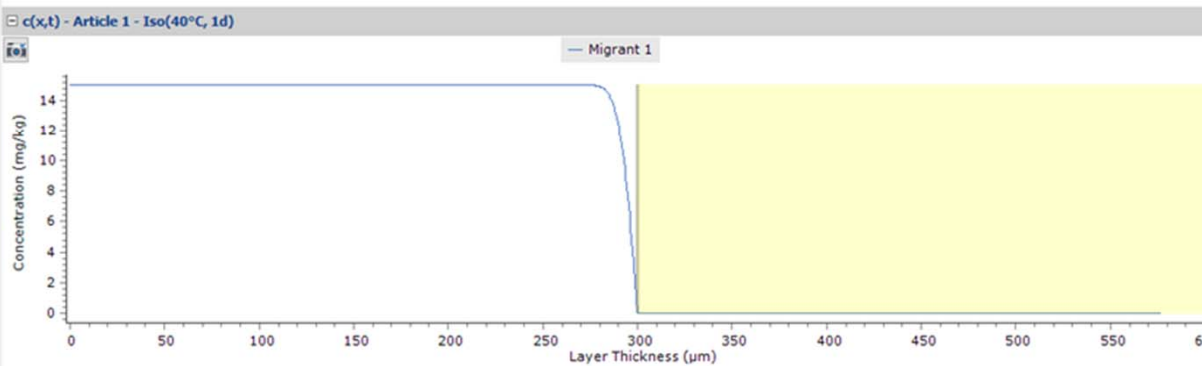
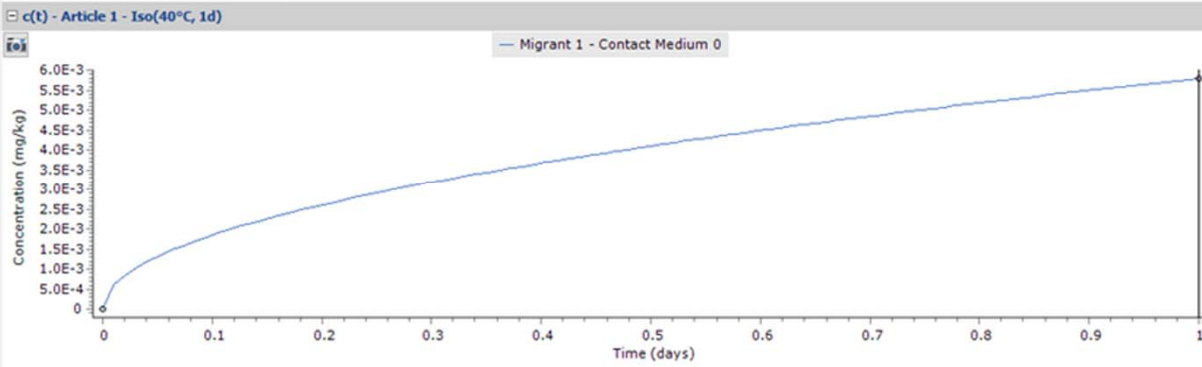
- Package SAN 24h at 40C optimized
 - Article 1
 - Iso(40°C, 1d)

Temperature : 40 (°C) Display unit mg/kg c(t) : draw mean concentration c(t) : draw concentration at 0 % of thickness from surface

Grid

Article	Layer 1	Contact Med...
	ACRYLONIT...	Acetic acid 3%
	Thickness (µm)	1.667E04
<input checked="" type="checkbox"/> Migrant 1	ACRYLONIT...	0.005776

Concentration Diffusion Coefficient Partition Coefficient Solubility



Package SAN 24h at 40C

Geometry

Rectangular

Contact Surface (cm²): 600

Volume of Contact Medium (cm³): 1000

Width (cm): 10

Height (cm): 10

Length (cm): 10

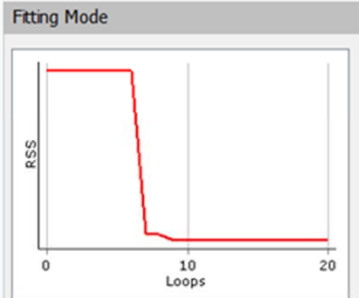
Add Article

Surface and mass of contact medium by article

Articles	Surfaces (cm ²)	Mass (g)
Article 1	600	1000

Total surface of all articles (cm²): 600

Switch Package in Fitting Mode



Loops per serie 20 Iterations: 20

Optimize Refresh

Correlation

mtau 1

mtolg 1E-6

mtolx 1E-6 mrealstep 1E-3

Parameter Name	Value
Layer 1-Op-Known(cm ² /s)	3.172E-12

Close Fitting Mode for This Package

Create Global Package

Package Properties Output Calculation

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

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

Prediction on This Article
 Prediction on All Articles
 Close All Articles
 Delete All Article Outputs
 Close All

Package SAN 24h at 40C optimized

- Article 1
 - Iso(40°C, 1d)

Temperature : 40 (°C) Display unit mg/kg c(t) : draw mean concentration c(t) : draw concentration at 0 % of thickness from surface

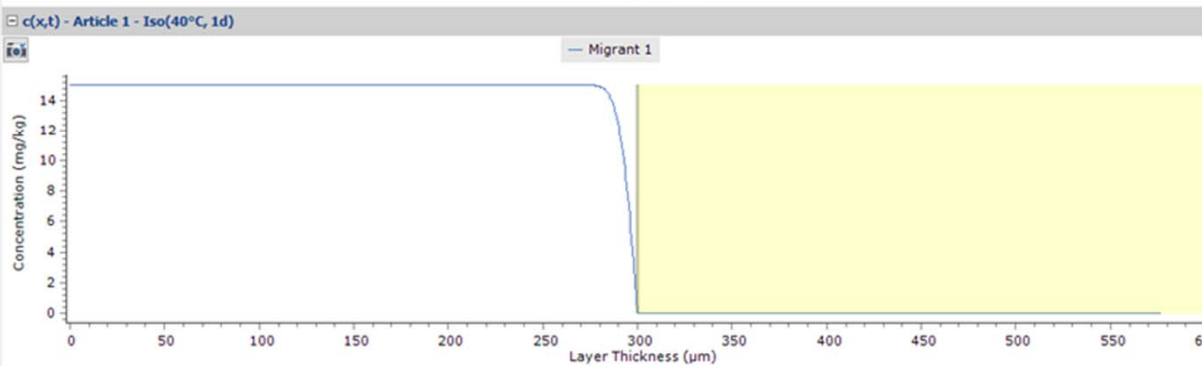
Grid	Article	Layer 1	Contact Med...
		ACRYLONIT...	Acetic acid 3%
		Thickness (µm)	1.667E04
		300	
	Migrant 1	ACRYLONIT...	0.005776
		14.71	

New Package
 Open Package
 New Global Comparison Output
 Close All

Concentration
 Diffusion Coefficient
 Partition Coefficient
 Solubility



55:次に70°Cの実測データを読み込みます。



Package SAN 24h at 40C

Geometry: Rectangular

Contact Surface (cm²): 600

Volume of Contact Medium (cm³): 1000

Width (cm): 10

Height (cm): 10

Length (cm): 10

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

Total surface of all articles (cm²): 600

Fitting Mode

Loops per serie: 20 Iterations: 20

Correlation

mtau: 1
 mtolg: 1E-6
 mtolx: 1E-6
 mrealstep: 1E-3

Parameter Name	Value
Layer 1-Op-Known(cm ² /s)	3.172E-12

Package Properties Output Calculation

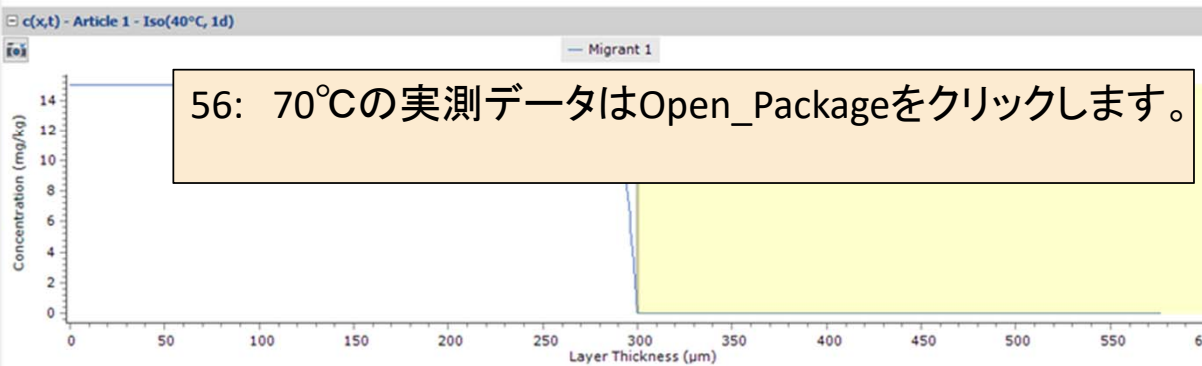
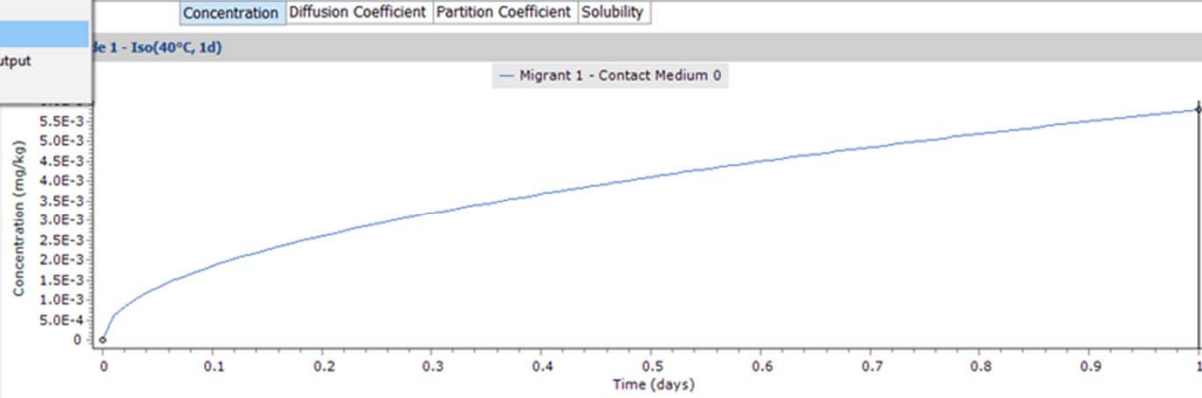
Package SAN 24h at 40C optimized

- Article 1
 - Iso(40°C, 1d)

Temperature : 40 (°C) Display unit mg/kg c(t) : draw mean concentration c(t) : draw concentration at 0 % of thickness from surface

Grid

Article	Layer 1	Contact Med...
	ACRYLONIT...	Acetic acid 3%
	Thickness (µm)	1.667E04
	Migrant 1	ACRYLONIT... 14.71 0.005776



56: 70°Cの実測データはOpen_Packageをクリックします。

Package SAN 24h at 40C

Geometry: Rectangular

Contact Surface (cm²): 600
Volume of Contact Medium (cm³): 1000

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

Surface and mass of contact medium by article

Articles	Surfaces (cm ²)	Mass (g)
Article 1	600	1000

Total surface of all articles (cm²): 600

Fitting Mode

Loops per serie: 20 Iterations: 20

Correlation

mtau: 1
mtolg: 1E-6
mtolx: 1E-6 mrealtstep: 1E-3

Parameter Name	Value
Layer 1-Op-Known(cm ² /s)	3.172E-12

Open

This PC > Desktop > example fitting

Search example fitting

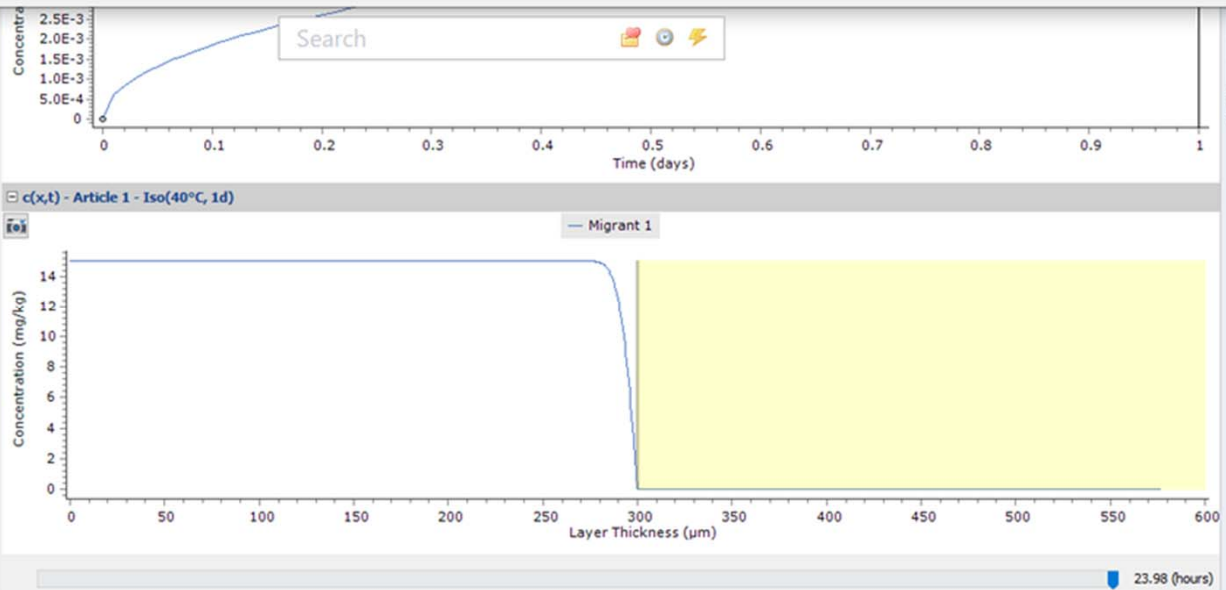
Organise New folder

Name	Date modified	Type	Size
Package SAN 24h at 40C.sml	02.09.2022 14:37	SML File	2 KB
Package SAN 24h at 40C optimized.sml	02.09.2022 15:01	SML File	106 KB

File name: Package SAN 24h at 40C optimized.sml

AKTS SML (*.sml)

Open Cancel



Palmetrics

AN 24h at 40C

Surface (cm²): 600

Contact Medium (cm³): 1000

Surfaces (cm²) Mass (g)

600	1000	<input checked="" type="checkbox"/>
-----	------	-------------------------------------

Total surface of all articles (cm²): 600

Switch Package in Fitting Mode

Fitting Mode

Loops per serie: 20 Iterations: 20

Optimize Refresh

Correlation

mtau: 1

mtolg: 1E-6

mtolx: 1E-6 mrealstep: 1E-3

Parameter Name	Value
Layer 1-Op-Known(cm ² /s)	3.172E-12

Close Fitting Mode for This Package

Create Global Package

57

2023/7/2

58: 70°Cの実測データをopenして読み込みます。

Open

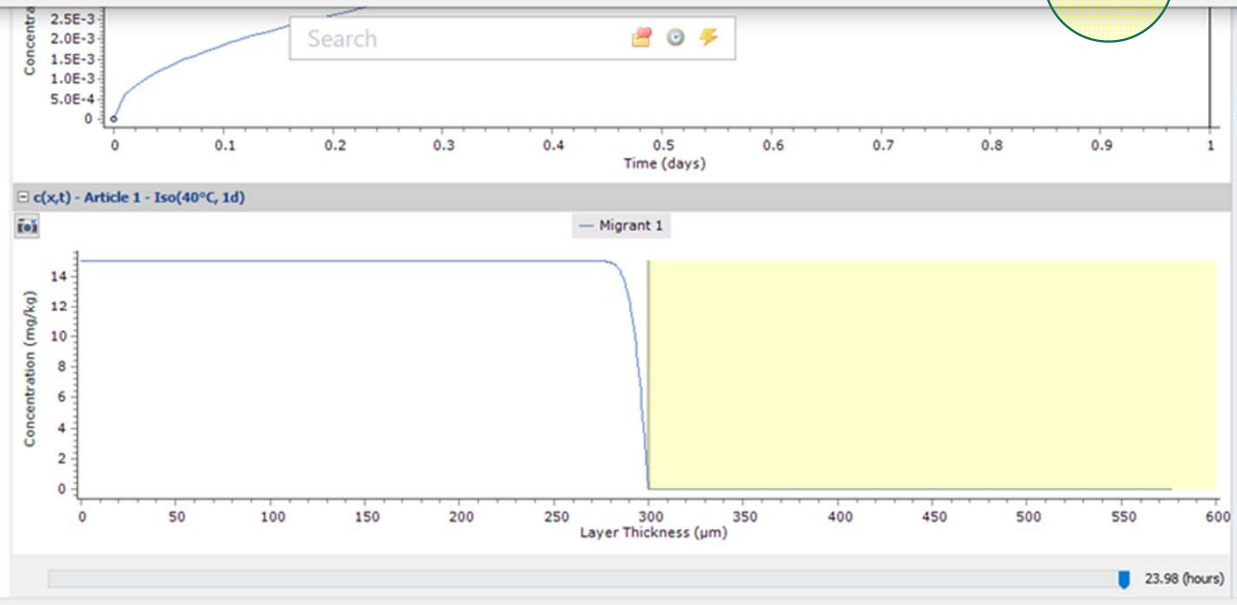
This PC > Desktop > example fitting

Name	Date modified	Type	Size
Package SAN 24h at 40C.sml	02.09.2022 14:37	SML File	2 KB
Package SAN 24h at 40C optimized.sml	02.09.2022 15:01	SML File	106 KB

File name: Package SAN 24h at 40C.sml

AKTS SML (*.sml)

Open Cancel



Palmetrics

AN 24h at 40C

Surface (cm²): 600

Contact Medium (cm³): 1000

Loops per serie: 20

Iterations: 20

Optimize Refresh

Correlation

mtau: 1

mtolg: 1E-6

mtolx: 1E-6 mrealstep: 1E-3

Parameter Name	Value
Layer 1-Op-Known(cm ² /s)	3.172E-12

Total surface of all articles (cm²): 600

Close Fitting Mode for This Package

Create Global Package

58

2023/7/2

Package Properties Output Calculation

New Package
 Open Package
 Save Package
 Save Package As
 Duplicate Package
 Save All Packages
 Package Details

New Article
 Open Article
 Import Article
 Duplicate Article
 Close Article
 Import Initial Concentration

Prediction on This Article
 Prediction on All Articles
 Close All Articles
 Delete All Article Outputs
 Close All

Package SAN 24h at 40C optimized
 Article 1
 Iso(90°C, 1d)
 Package SAN 24h at 40C
 Article 1

Surface (cm²)

Article	Layer 1	Contact Medi...
	ACRYLONIT...	Acetic acid 3%
Thickness (µm)	300	1.667E04
Migrant 1	ACRYLONIT...	0

Concentration Diffusion Coefficient Partition Coefficient Solubility

Add Migrant(s)
 Run Prediction...

Layer (Layer 1) Migrant Data
 Copy From...
 Reset Layer
 Set to User Defined
 Database...

Type: Polymer Contact Medium

Thickness (µm):

Density (g/cm³):

Layer Abbreviation:

Material:

Layer Details

Molecular Weight (g/mol): Glass Transition Temperature (°C):

Log Pow:

Material specific constants for estimation of diffusion coefficients according to Pringer

Upper Limit: A^{*}p: Tau: A^{*}p:
 Realistic Case: A^{*}p: Tau: Ap:

Coefficients for estimation of diffusion coefficients according to Welle

a (K⁻¹): c (A³):
 b (cm²*s⁻¹): d (K⁻¹):

Package SAN 24h at 40C

Add Layer(s)
 Set-Off
 Add Article

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

Surface and mass of contact medium by article

Articles	Surfaces (cm ²)	Mass (g)
Article 1	600	1000

Total surface of all articles (cm²): 600

Switch Package in Fitting Mode

59: 70°Cの実測データを読み込まれました。

Package Properties Output Calculation

- Package SAN 24h at 40C optimized
 - Article 1
 - Iso(40°C, 1d)
 - Package SAN 2h at 70C**
 - Article 1

Surface (cm²)

Article	Layer 1	Contact Medi...
	ACRYLONIT...	Acetic acid 3%
Thickness (µm)	300	1.667E04
Migrant 1	ACRYLONIT...	0

Type: Polymer Contact Medium

Thickness (µm):

Density (g/cm³):

Layer Abbreviation:

Material:

Layer Details

Molecular Weight (g/mol): Glass Transition Temperature (°C):

Log Pow:

Material specific constants for estimation of diffusion coefficients according to Pringer

Upper Limit: A^{*p}: Tau: A^{*p}:

Realistic Case: A^p: Tau: A^p:

Coefficients for estimation of diffusion coefficients according to Welle

a (K⁻¹): c (A³):

b (cm²*s⁻¹): d (K⁻¹):

Package SAN 24h at 40C

Geometry:

Contact Surface (cm²):

Volume of Contact Medium (cm³):

Width (cm):

Height (cm):

Length (cm):

Surface and mass of contact medium by article

Articles	Surfaces (cm ²)	Mass (g)
Article 1	600	1000

Total surface of all articles (cm²):

Package Properties Output Calculation

- Package SAN 24h at 40C optimized
 - Article 1
 - Iso(40°C, 1d)
- Package SAN 2h at 70C
 - Article 1

Surface (cm²)

Article	Layer 1	Contact Medi...
	ACRYLONIT...	Acetic acid 3%
Thickness (µm)	300	1.667E04
Migrant 1	ACRYLONIT...	0

Type: Polymer Contact Medium

Thickness (µm):

Density (g/cm³):

Layer Abbreviation:

Material:

Layer Details

Molecular Weight (g/mol): Glass Transition Temperature (°C):

Log Pow:

Material specific constants for estimation of diffusion coefficients according to Pringer

Upper Limit: A^{*p}: Tau: A^{*p}:
 Realistic Case: A^p: Tau: A^p:

Coefficients for estimation of diffusion coefficients according to Welle

a (K⁻¹): c (A³):
 b (cm²*s⁻¹): d (K⁻¹):

Package SAN 2h at 70C

Geometry:

Contact Surface (cm²):

Volume of Contact Medium (cm³):

Width (cm):

Height (cm):

Length (cm):

Surface and mass of contact medium by article

Articles	Surfaces (cm ²)	Mass (g)
Article 1	600	1000

Total surface of all articles (cm²):

Package Properties Output Calculation

- Package SAN 24h at 40C optimized
 - Article 1
 - Iso(40°C, 1d)
- Package SAN 2h at 70C
 - Article 1

Surface (cm²) 600

Article	Layer 1	Contact Medi...
	ACRYLONIT...	Acetic acid 3%
	Thickness (µm) 300	1.667E-1
Migrant 1	ACRYLONIT...	1E-11
		0.0001

Type: Polymer Contact Medium

Thickness (µm): 300

Density (g/cm³): 1.09

Layer Abbreviation: Layer 1

Material: ACRYLONITRILE-STYRENE, COPOLYMER (AS)

Layer Details

Molecular Weight (g/mol): 471.64 Glass Transition Temperature (°C): 97

Log Pow: N/A

Material specific constants for estimation of diffusion coefficients according to Pringer

Upper Limit: A^{*p}: N/A Tau: N/A A^{*p}: N/A
 Realistic Case: A^p: N/A Tau: N/A A^p: N/A

Coefficients for estimation of diffusion coefficients according to Welle

a (K⁻¹): N/A c (A³): N/A
 b (cm²*s⁻¹): N/A d (K⁻¹): N/A

Package SAN 2h at 70C

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

Surface and mass of contact medium by article

Articles	Surfaces (cm ²)	Mass (g)
Article 1	600	1000

Total surface of all articles (cm²): 600

Package Properties Output Calculation

- Package SAN 24h at 40C optimized
 - Article 1
 - Iso(40°C, 1d)
 - Article 1
- Package SAN 2h at 70C
 - Article 1

Surface (cm²) 600

Article	Layer 1	Contact Medi...
	ACRYLONIT...	Acetic acid 3%
Thickness (µm)	300	1.667E04
Migrant 1	ACRYLONIT...	1E-11 0.0001

Concentration Diffusion Coefficient Partition Coefficient Solubility

Layer (Layer 1) Migrant (Migrant 1) Data (Diffusion Coefficient)

Diffusion Coefficient

- Known
- Interpolation based on Tg
- Pringsheim
- Arrhenius
- Customized Equation
- Brandsch Equation
- Welle Equation
- In-Silico

Known Value

Diffusion Coefficient (cm²/s): 1E-11

Package SAN 2h at 70C

Geometry: Rectangular

Contact Surface (cm²): 600

Volume of Contact Medium (cm³): 1000

Width (cm): 10

Height (cm): 10

Length (cm): 10

Surface and mass of contact medium by article

Articles	Surfaces (cm ²)	Mass (g)
Article 1	600	1000

Total surface of all articles (cm²): 600

63: 70°Cの実測データを読み込まれました。

Package Properties Output Calculation

- Package SAN 24h at 40C optimized
 - Article 1
 - Iso(40°C, 1d)
- Package SAN 2h at 70C
 - Article 1

Surface (cm²) 600

Article	Layer 1	Contact Medi...
	ACRYLONIT...	Acetic acid 3%
	Thickness (µm) 300	1.667E04
Migrant 1	ACRYLONIT...	D(4.60E-12) 0.0001



Diffusion Coefficient

Example Temperature (°C): 40

- Known
- Interpolation based on Tg
- Pringsheim
- Arrhenius
- Customized Equation
- Brandsch Equation
- Welle Equation
- In-Silico

Interpolation Based on Tg Calculation Parameters

Layer Glass Transition Temperature (°C): 97
Migrant Molecular Weight (g/mol): 53.06

Package SAN 2h at 70C

Geometry: Rectangular

Contact Surface (cm²): 600

Volume of Contact Medium (cm³): 1000

Width (cm): 10

Height (cm): 10

Length (cm): 10

Surface and mass of contact medium by article

Articles	Surfaces (cm ²)	Mass (g)
Article 1	600	1000

Total surface of all articles (cm²): 600

64: 70°Cの実測データを読み込まれました。

Package Properties Output Calculation

- Package SAN 24h at 40C optimized
 - Article 1
 - Iso(40°C, 1d)
- Package SAN 2h at 70C
 - Article 1

Surface (cm²) 600

Article	Layer 1	Contact Medi...
	ACRYLONIT...	Acetic acid 3%
	Thickness (µm) 300	1.667E04
Migrant 1	ACRYLONIT...	D(4.60E-12) 0.0001

Concentration Diffusion Coefficient Partition Coefficient Solubility

Layer (Layer 1) Migrant (Migrant 1) **Data (Diffusion Coefficient)**

Diffusion Coefficient Example Temperature (°C):

Known

Interpolation based on Tg

Pringer

Arrhenius

Customized Equation

Brandsch Equation

Welle Equation

In-Silico

Interpolation Based on Tg Calculation Parameters

Layer	Glass Transition Temperature (°C): 97
Migrant	Molecular Weight (g/mol): 53.06

Package SAN 2h at 70C

Geometry: Rectangular

Contact Surface (cm²): 600

Volume of Contact Medium (cm³): 1000

Width (cm):

Height (cm):

Length (cm):

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

63: 40°C ⇒ 70°Cと設定します

Package Properties

Output Calculation

New Package
Open Package

Save Package
Duplicate Package
Close Package

Save Package As
Save All Packages
Package Details

New Article
Open Article
Import Article

Save Article
Duplicate Article
Close Article

Import Initial Concentration

Prediction on This Article
Prediction on All Articles

Close All Articles
Delete All Article Outputs
Close All

Package SAN 24h at 40C optimized
Article 1
Iso(40°C, 1d)

Package SAN 2h at 70C
Article 1

Surface (cm²) 600

Article	Layer 1	Contact Medi...
	ACRYLONIT...	Acetic acid 3%
	Thickness (µm)	1.667E04
Migrant 1	ACRYLONIT...	[R: #[R:1-1]...]
		0.0001

Concentration Diffusion Coefficient Partition Coefficient Solubility

Add Migrant(s)

Run Prediction...

Layer (Layer 1) Migrant (Migrant 1) Data (Diffusion Coefficient)

Diffusion Coefficient

Example Temperature (°C): 70

- Known
- Interpolation based on Tg
- Pringer
- Arrhenius
- Customized Equation
- Brandsch Equation
- Welle Equation
- In-Silico

Interpolation Based on Tg Calculation Parameters

Layer Glass Transition Temperature (°C): 97
Migrant Molecular Weight (g/mol): 53.06

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

Add Layer(s)

Add Layer(s)

Set-Off

Package SAN 2h at 70C

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

Total surface of all articles (cm²): 600

Switch Package in Fitting Mode

66: 70°Cにおける拡散係数を設定するのですが、Interpolation based on Tg ではなく Knownを選択します。

Package Properties Output Calculation

- Package SAN 24h at 40C optimized
 - Article 1
- Package SAN 2h at 70C
 - Article 1

Surface (cm²) 600

Article	Layer 1	Contact Medi...
	ACRYLONIT...	Acetic acid 3%
	Thickness (µm) 300	1.667E04
Migrant 1	ACRYLONIT...	IE-11 0.0001

Diffusion Coefficient

- Known
- Interpolation based on Tg
- Prings
- Arrhenius
- Customized Equation
- Brandsch Equation
- Welle Equation
- In-Silico

Known Value

Diffusion Coefficient (cm²/s): IE-11

Package SAN 2h at 70C

Geometry: Rectangular

Contact Surface (cm²): 600

Volume of Contact Medium (cm³): 1000

Width (cm): 10

Height (cm): 10

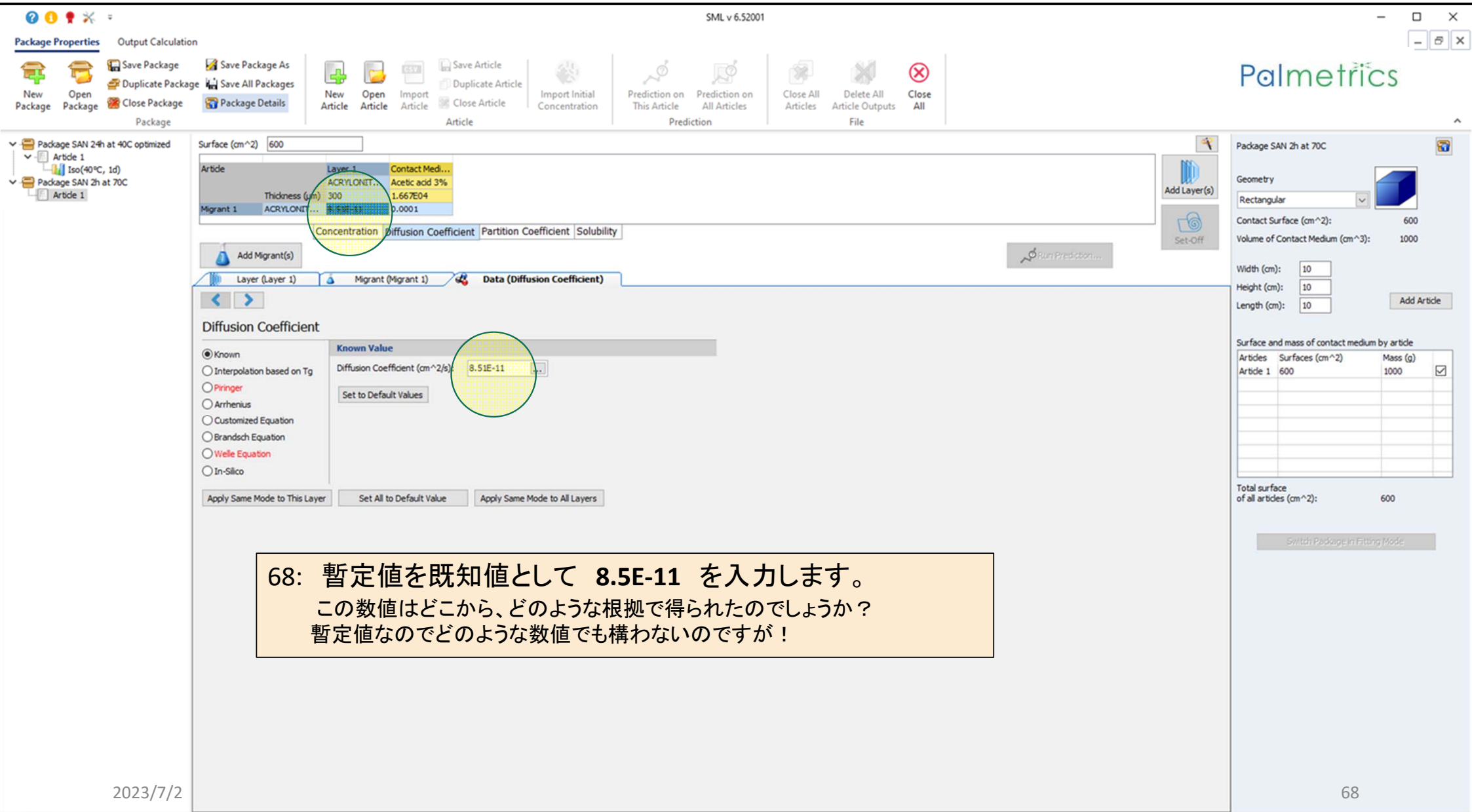
Length (cm): 10

Surface and mass of contact medium by article

Articles	Surfaces (cm ²)	Mass (g)
Article 1	600	1000

Total surface of all articles (cm²): 600

67: 既知値を入力します。



Package Properties

- 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

Prediction

- Prediction on This Article
- Prediction on All Articles

File

- Close All Articles
- Delete All Article Outputs
- Close All

- Package SAN 24h at 40C optimized
 - Article 1
- Package SAN 2h at 70C
 - Article 1

Surface (cm²) 600

Article	Layer 1	Contact Medi...
Thickness (μm)	300	1.667E04
Migrant 1	ACRYLONIT...	Acetic acid 3%
	8.51E-11	0.0001

Concentration Diffusion Coefficient Partition Coefficient Solubility

Add Migrant(s)

Run Prediction...

Layer (Layer 1) Migrant (Migrant 1) Data (Diffusion Coefficient)

Diffusion Coefficient

Known

Interpolation based on Tg

Pringer

Arrhenius

Customized Equation

Bransch Equation

Welle Equation

In-Silico

Known Value

Diffusion Coefficient (cm²/s):

Set to Default Values

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

Package SAN 2h at 70C

Geometry: Rectangular

Contact Surface (cm²): 600

Volume of Contact Medium (cm³): 1000

Width (cm): 10

Height (cm): 10

Length (cm): 10

Surface and mass of contact medium by article

Articles	Surfaces (cm ²)	Mass (g)
Article 1	600	1000

Total surface of all articles (cm²): 600

Switch Package in Fitting Mode

Package Properties Output Calculation

New Package
 Open Package
 Save Package
 Save Package As
 Duplicate Package
 Save All Packages
 Package Details

Package

New Article
 Open Article
 Import Article
 Duplicate Article
 Close Article
 Import Initial Concentration

Article

Prediction on This Article
 Prediction on All Articles

Prediction

Close All Articles
 Delete All Article Outputs
 Close All

File

- Package SAN 2h at 40C optimized
 - Article 1
 - Iso(40°C, 1d)
- Package SAN 2h at 70C
 - Article 1

Surface (cm²)

Article	Layer 1	Contact Medi...
	ACRYLONIT...	Acetic acid 3%
	Thickness (µm)	300
		1.667E04
Migrant 1	ACRYLONIT...	8.51E-11
		0.0001

Diffusion Coefficient

Known
 Interpolation based on Tg
 Pringer
 Arrhenius
 Customized Equation
 Brandsch Equation
 Welle Equation
 In-Silico

Known Value

Diffusion Coefficient (cm²/s):

69:

Package SAN 2h at 70C

Geometry:

Contact Surface (cm²):

Volume of Contact Medium (cm³):

Width (cm):

Height (cm):

Length (cm):

Surface and mass of contact medium by article

Articles	Surfaces (cm ²)	Mass (g)
Article 1	600	1000

Total surface of all articles (cm²):

Package Properties Output Calculation

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

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

Prediction on This Article
 Prediction on All Articles
 Close All Articles
 Delete All Article Outputs
 Close All

Package SAN 24h at 40C optimized

- Article 1
- Iso(90°, 1d)
- Package SAN 2h at 70C
- Article 1

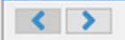
Surface (cm²) 600

Article	Layer 1	Contact Medi...
	ACRYLONIT...	Acetic acid 3%
	Thickness (µm) 300	1.667E04
Migrant 1	ACRYLONIT...	8.51E-11 0.0001

Concentration Diffusion Coefficient Partition Coefficient Solubility

Add Migrant(s)

Layer (Layer 1) Migrant (Migrant 1) **Data (Diffusion Coefficient)**



Diffusion Coefficient

- Known
- Interpolation based on Tg
- Pringer
- Arrhenius
- Customized Equation
- Brandsch Equation
- Welle Equation
- In-Silico

Known Value

Diffusion Coefficient (cm²/s): 8.51E-11

Set to Default Values

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

Run Prediction...

Package SAN 2h at 70C

Add Layer(s)

Set-Off

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

Total surface of all articles (cm²): 600

Switch Package in Fitting Mode

Package Properties Output Calculation

- Package SAN 24h at 40C optimized
 - Article 1
 - Iso(40°C, 1d)
- Package SAN 2h at 70C
 - Article 1

Surface (cm²)

Article	Layer 1	Contact Medi...
	ACRYLONIT...	Acetic acid 3%
	Thickness (µm)	300
		1.667E04
Migrant 1	ACRYLONIT...	8.51E-11
		0.0001

Diffusion Coefficient

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

Predictions

Temperature Profiles

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

Isothermal Conditions

Temperature = °C

ΔT = °C

Number of Isotherms =

Final Temperature = °C

Time Max day

Without Statistics
 Monte Carlo Runs
 Number of Runs

 Include Sobol Runs
 Fast Distribution

Number of steps for this output:

Package SAN 2h at 70C

Geometry

Rectangular

Contact Surface (cm²):

Volume of Contact Medium (cm³):

Width (cm):

Height (cm):

Length (cm):

Surface and mass of contact medium by article

Articles	Surfaces (cm ²)	Mass (g)
Article 1	600	1000

Total surface of all articles (cm²):

Package Properties Output Calculation

- Package SAN 24h at 40C optimized
 - Article 1
 - Iso(40°C, 1d)
- Package SAN 2h at 70C
 - Article 1

Surface (cm²) 600

Article	Layer 1	Contact Medi...
	ACRYLONIT...	Acetic acid 3%
	Thickness (µm) 300	1.667E04
Migrant 1	ACRYLONIT...	8.51E-11 0.0001

Diffusion Coefficient

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

Predictions

Temperature Profiles

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

Isothermal Conditions

Temperature = °C

ΔT = °C

Number of Isotherms =

Final Temperature = °C

Time Max

Without Statistics
 Monte Carlo Runs
 Number of Runs
 Include Sobol Runs
 Fast Distribution

Number of steps for this output:

Package SAN 2h at 70C

Geometry

Rectangular

Contact Surface (cm²): 600

Volume of Contact Medium (cm³): 1000

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

Surface and mass of contact medium by article

Articles	Surfaces (cm ²)	Mass (g)
Article 1	600	1000

Total surface of all articles (cm²): 600

Switch Package in Fitting Mode

Package Properties Output Calculation

- Package SAN 24h at 40C optimized
 - Article 1
 - Iso(40°C, 1d)
- Package SAN 2h at 70C
 - Article 1

Surface (cm²) 600

Article	Layer 1	Contact Medi...
	ACRYLONIT...	Acetic acid 3%
	Thickness (µm) 300	1.667E04
Migrant 1	ACRYLONIT...	0.0001

Concentration
Diffusion Coefficient
Partition Coefficient
Solubility

Layer (Layer 1) Migrant

Diffusion Coefficient

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

Predictions

Temperature Profiles

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

Isothermal Conditions

Temperature = 70 °C
 ΔT = 20 °C
 Number of Isotherms = 1
 Final Temperature = 70 °C

Without Statistics
 Monte Carlo Runs
 Include Sobol Runs
 Fast Distribution

Time Max: 2 day

Number of Runs: 10

Number of steps for this output: 100

Package SAN 2h at 70C

Geometry: Rectangular

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

Surface and mass of contact medium by article

Articles	Surfaces (cm ²)	Mass (g)
Article 1	600	1000

Total surface of all articles (cm²): 600

Package Properties Output Calculation

- Package SAN 24h at 40C optimized
 - Article 1
 - Iso(40°C, 1d)
- Package SAN 2h at 70C
 - Article 1

Surface (cm²) 600

Article	Layer 1	Contact Medi...
	ACRYLONIT...	Acetic acid 3%
	Thickness (µm) 300	1.667E04
Migrant 1	ACRYLONIT...	8.51E-11 0.0001

Concentration
Diffusion Coefficient
Partition Coefficient
Solubility

Layer (Layer 1) Migrant

Diffusion Coefficient

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

Apply Same Mode to This Layer Set A

Predictions

Temperature Profiles

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

Isothermal Conditions

Temperature = 70 °C

ΔT = 20 °C

Number of Isotherms = 1

Final Temperature = 70 °C

Time Max: 2 day

Without Statistics
 Monte Carlo Runs
 Fast Distribution

Number of Runs: [dropdown]

Include Sobol Runs

Save... Load...

Number of steps for this output: 100 OK Cancel

Package SAN 2h at 70C

Geometry: Rectangular

Contact Surface (cm²): 600

Volume of Contact Medium (cm³): 1000

Width (cm): 10

Height (cm): 10

Length (cm): 10

Surface and mass of contact medium by article

Articles	Surfaces (cm ²)	Mass (g)
Article 1	600	1000

Total surface of all articles (cm²): 600

Switch Package in Fitting Mode

Package Properties Output Calculation

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

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

Prediction on This Article
 Prediction on All Articles
 Close All Articles
 Delete All Article Outputs
 Close All

- Package SAN 24h at 40C optimized
 - Article 1
 - Iso(40°C, 1d)
- Package SAN 2h at 70C
 - Article 1

Surface (cm²) 600

Article	Layer 1	Contact Medi...
	ACRYLONIT...	Acetic acid 3%
	Thickness (µm) 300	1.667E04
Migrant 1	ACRYLONIT...	8.51E-11 0.0001

Concentration
 Diffusion Coefficient
 Partition Coefficient
 Solubility

Add Migrant(s)

Layer (Layer 1) Migrant

Diffusion Coefficient

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

Predictions

Temperature Profiles

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

Isothermal Conditions

Temperature = 70 °C

ΔT = 20 °C

Number of Isotherms = 1

Final Temperature = 70 °C

Time Max 2 hour

Without Statistics
 Monte Carlo Runs
 Include Sobol Runs
 Fast Distribution

Number of Runs 10

Save... Load...

Number of steps for this output: 100

OK Cancel

Package SAN 2h at 70C

Geometry: Rectangular

Contact Surface (cm²): 600

Volume of Contact Medium (cm³): 1000

Width (cm): 10

Height (cm): 10

Length (cm): 10

Surface and mass of contact medium by article

Articles	Surfaces (cm ²)	Mass (g)
Article 1	600	1000

Total surface of all articles (cm²): 600

Switch Package in Fitting Mode

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

Prediction

- Prediction on This Article
- Prediction on All Articles

File

- Close All Articles
- Delete All Article Outputs
- Close All

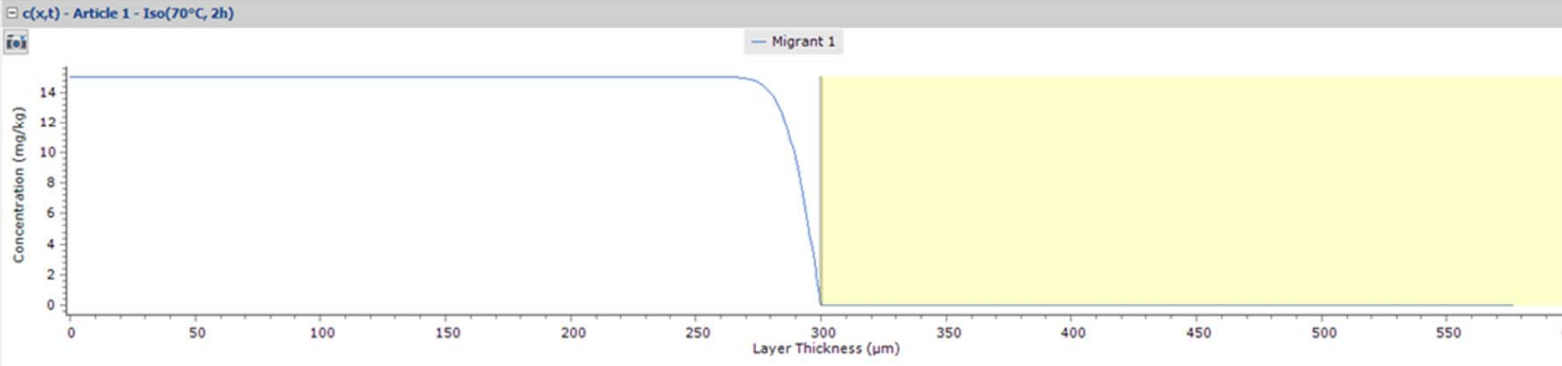
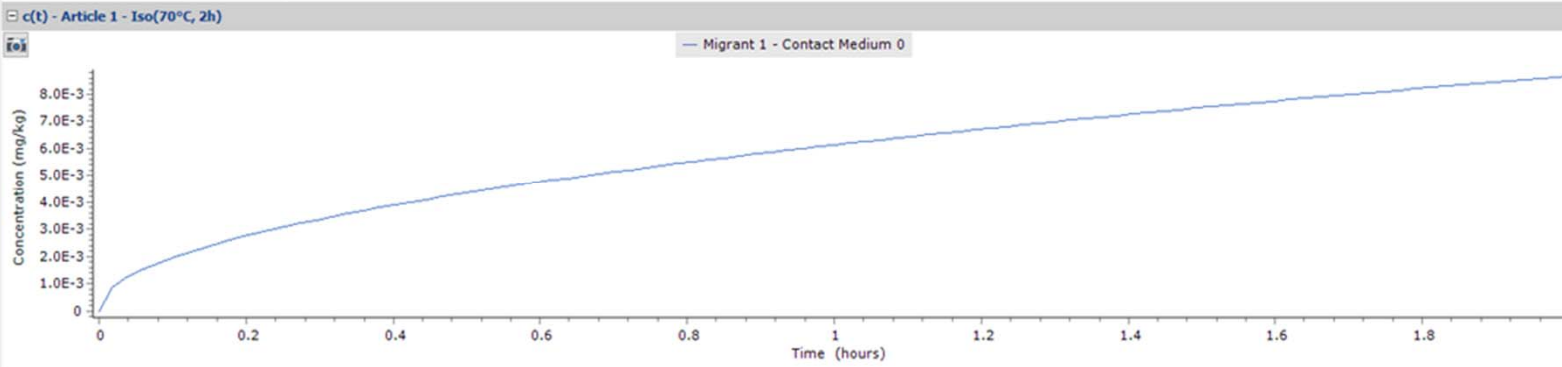
- Package SAN 24h at 40C optimized
 - Article 1
 - Iso(40°C, 1d)
- Package SAN 2h at 70C
 - Article 1
 - Iso(70°C, 2h)

Temperature : 70 (°C) Display unit mg/kg c(t) : draw mean concentration c(t) : draw concentration at 0 % of thickness from surface

Grid

Article	Layer 1	Contact Med...
	ACRYLONIT...	Acetic acid 3%
	Thickness (µm)	1.667E04
<input checked="" type="checkbox"/> Migrant 1	ACRYLONIT...	0.008666
	Thickness (µm)	14.56

Concentration Diffusion Coefficient Partition Coefficient Solubility



Package SAN 2h at 70C

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

Total surface of all articles (cm²): 600

Switch Package in Fitting Mode

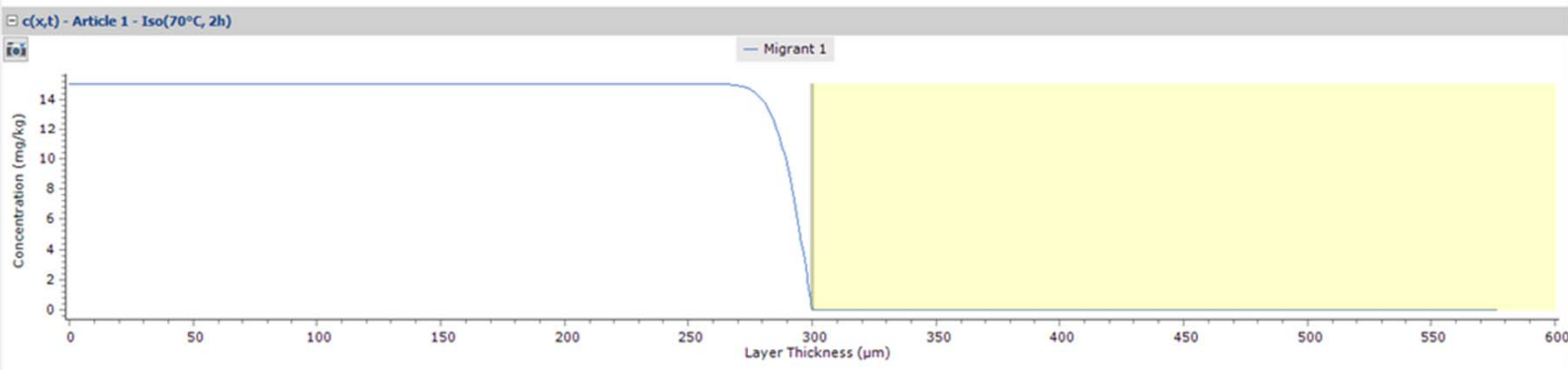
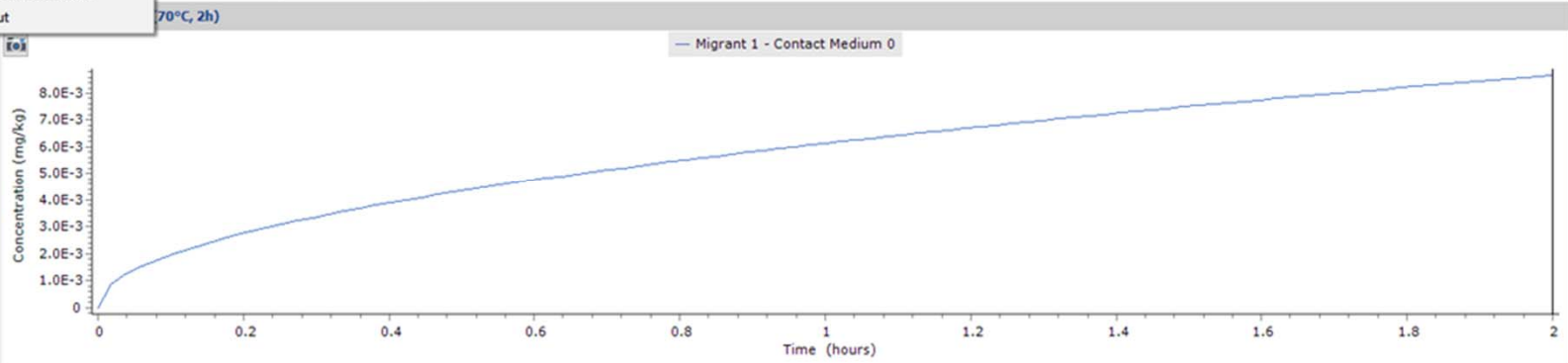
Package Properties Output Calculation

- Package SAN 24h at 40C optimized
 - Article 1
 - Iso(40°C, 1d)
- Package SAN 2h at 70C
 - Article 1
 - Iso(70°C, 2h)

Temperature: 70 (°C) Display unit mg/kg c(t) : draw mean concentration c(t) : draw concentration at 0 % of thickness from surface

- Save Output
- Export Migration c(t)
- Export Concentration c(x,t)
- Import Migration c(t)
- Import Concentration c(x,t)
- Delete Output

Layer	Material	Thickness (µm)	Diffusion Coefficient	Partition Coefficient	Solubility
Layer 1	ACRYLONIT...	300	1.667E04	0.0001	
	Contact Med...				
	Acetic acid 3%				



Package SAN 2h at 70C

Geometry: Rectangular

Contact Surface (cm²): 600

Volume of Contact Medium (cm³): 1000

Width (cm): 10

Height (cm): 10

Length (cm): 10

Surface and mass of contact medium by article

Articles	Surfaces (cm ²)	Mass (g)
Article 1	600	1000

Total surface of all articles (cm²): 600

Switch Package in Fitting Mode

Package Properties Output Calculation

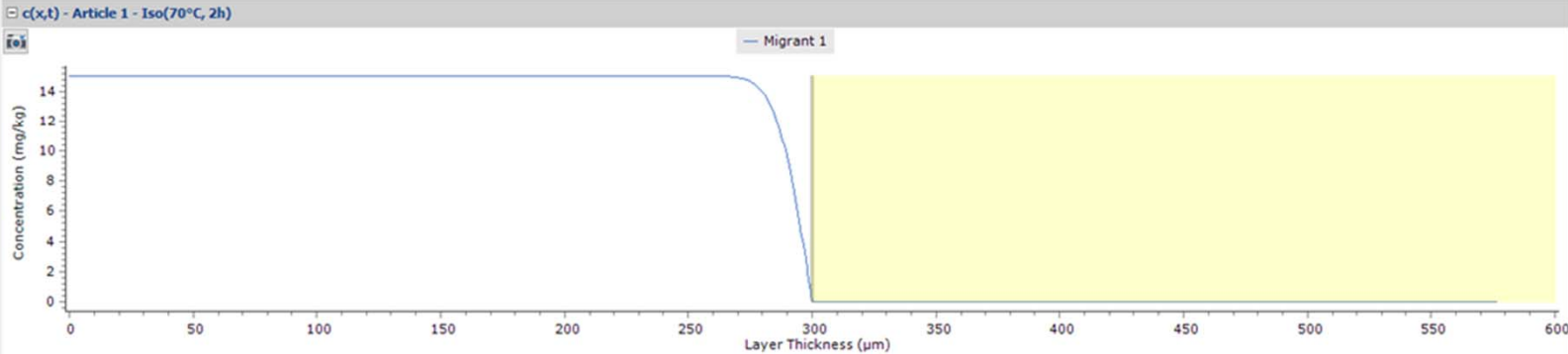
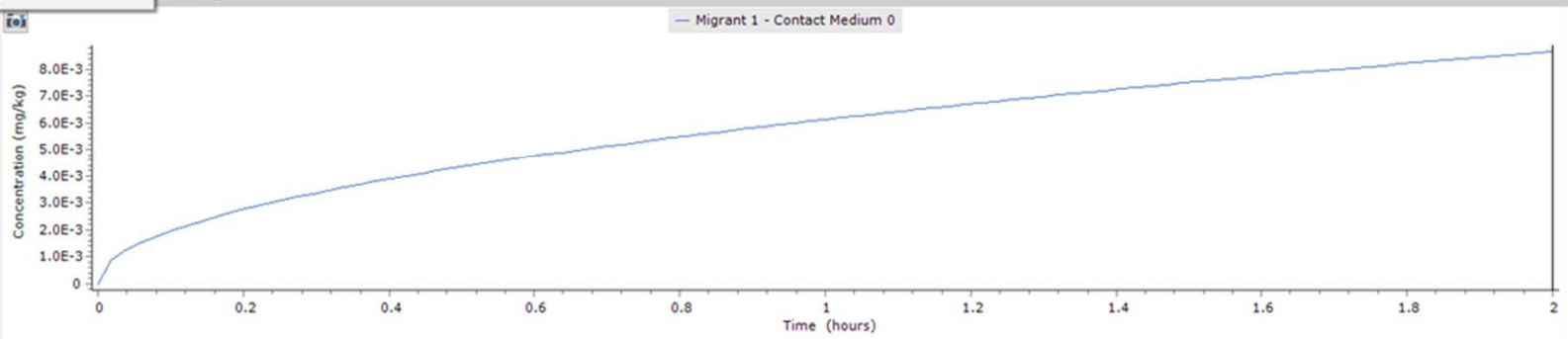
- Package SAN 24h at 40C optimized
 - Article 1
 - Iso(40°C, 1d)
- Package SAN 2h at 70C
 - Article 1
 - Iso(70°C, 2h)

Temperature: 70 (°C) Display unit: mg/kg c(t) : draw mean concentration c(t) : draw concentration at 0 % of thickness from surface

- Save Output
- Export Migration c(t)
- Export Concentration c(x,t)
- Import Migration c(t)**
- Import Concentration c(x,t)
- Delete Output

Layer	Material	Thickness (µm)	Acetic acid 3%
Layer 1	ACRYLONIT...	300	1.667E04
	ACRYLONIT...		0.0001

Concentration Diffusion Coefficient Partition Coefficient Solubility



Package SAN 2h at 70C

Geometry: Rectangular

Contact Surface (cm²): 600

Volume of Contact Medium (cm³): 1000

Width (cm): 10

Height (cm): 10

Length (cm): 10

Surface and mass of contact medium by article

Articles	Surfaces (cm ²)	Mass (g)
Article 1	600	1000

Total surface of all articles (cm²): 600

Switch Package in Fitting Mode

2023/7/2

2 (hours)

Package Properties Output Calculation

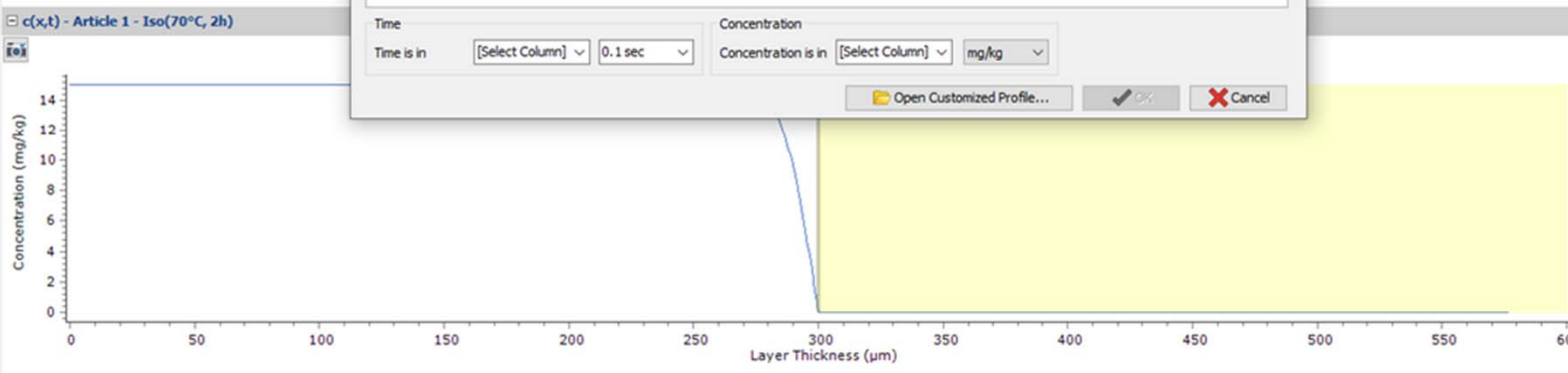
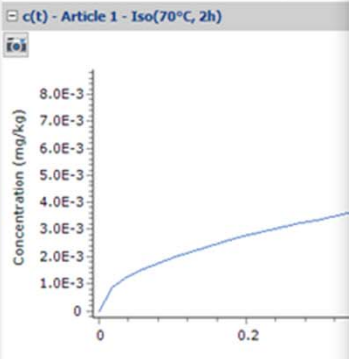
- Package SAN 24h at 40C optimized
 - Article 1
 - Iso(40°C, 1d)
- Package SAN 2h at 70C
 - Article 1
 - Iso(70°C, 2h)

Temperature: 70 (°C) Display unit: mg/kg c(t) : draw mean concentration c(t) : draw concentration at 0 % of thickness from surface

Grid

Article	Layer 1	Material	Thickness (µm)
	ACRYL...	ACRYL...	300
<input checked="" type="checkbox"/>	Migrant 1	ACRYLONT...	

Concentration Diffusion



Import Experimental Migration Profile

Import

t(h) T(°C) S(mg/kg)

	column 1	column 2	column 3
1	0	40	0
2	24	40	0.0058

Time is in: [Select Column] 0.1 sec Concentration is in: [Select Column] mg/kg

Package SAN 2h at 70C

Geometry: Rectangular

Contact Surface (cm²): 600

Volume of Contact Medium (cm³): 1000

Width (cm): 10

Height (cm): 10

Length (cm): 10

Surface and mass of contact medium by article

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

Total surface of all articles (cm²): 600

Package Properties Output Calculation

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

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

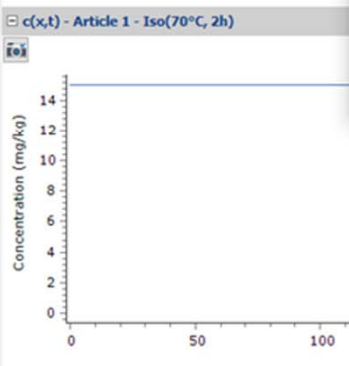
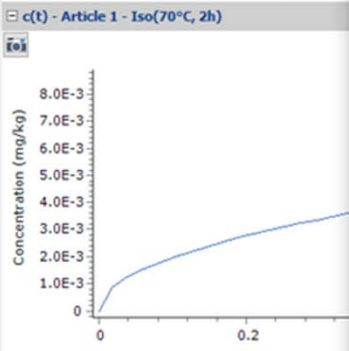
Prediction on This Article
 Prediction on All Articles
 Close All Articles
 Delete All Article Outputs
 Close All

- Package SAN 24h at 40C optimized
 - Article 1
 - Iso(40°C, 1d)
- Package SAN 2h at 70C
 - Article 1
 - Iso(70°C, 2h)

Temperature : 70 (°C) Display unit : mg/kg c(t) : draw mean concentration c(t) : draw concentration at 0 % of thickness from surface

Grid

Article	Layer 1	Material	Thickness (µm)
	ACRYL...	ACRYL...	300
<input checked="" type="checkbox"/>	Migrant 1	ACRYLONT...	



Import Experimental Migration Profile

Import

t(h) T(°C) S(mg/kg)

	column 1	column 2	column 3
1	0	40	0
2	24	40	0.0058

Time is in: [Select Column] 0.1 sec Concentration is in: [Select Column] mg/kg

Package SAN 2h at 70C

Geometry

Rectangular

Contact Surface (cm²): 600

Volume of Contact Medium (cm³): 1000

Width (cm): 10

Height (cm): 10

Length (cm): 10

Surface and mass of contact medium by article

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

Total surface of all articles (cm²): 600

Open

This PC > Desktop > example fitting

Organise New folder

Name	Date modified	Type	Size
24h at 40C.txt	02.09.2022 14:13	Text Document	1 KB
2h at 70C.txt	02.09.2022 14:15	Text Document	1 KB

File name: 2h at 70C.txt

Text files (*.txt)

Open Cancel

Palmetrics

Package SAN 2h at 70C

Geometry

Rectangular

Contact Surface (cm²): 600

Volume of Contact Medium (cm³): 1000

Width (cm): 10

Height (cm): 10

Length (cm): 10

Add Article

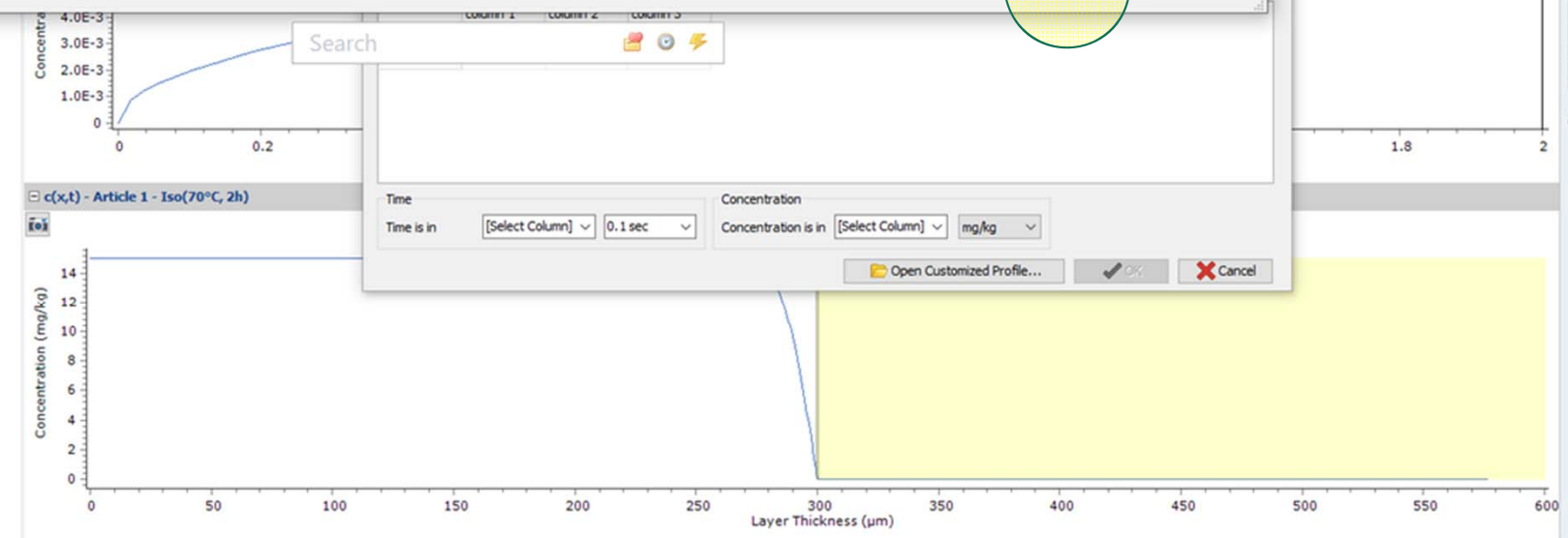
Surface and mass of contact medium by article

Articles	Surfaces (cm ²)	Mass (g)
Article 1	600	1000

Total surface of all articles (cm²): 600

Switch Package in Fitting Mode

2 (hours)

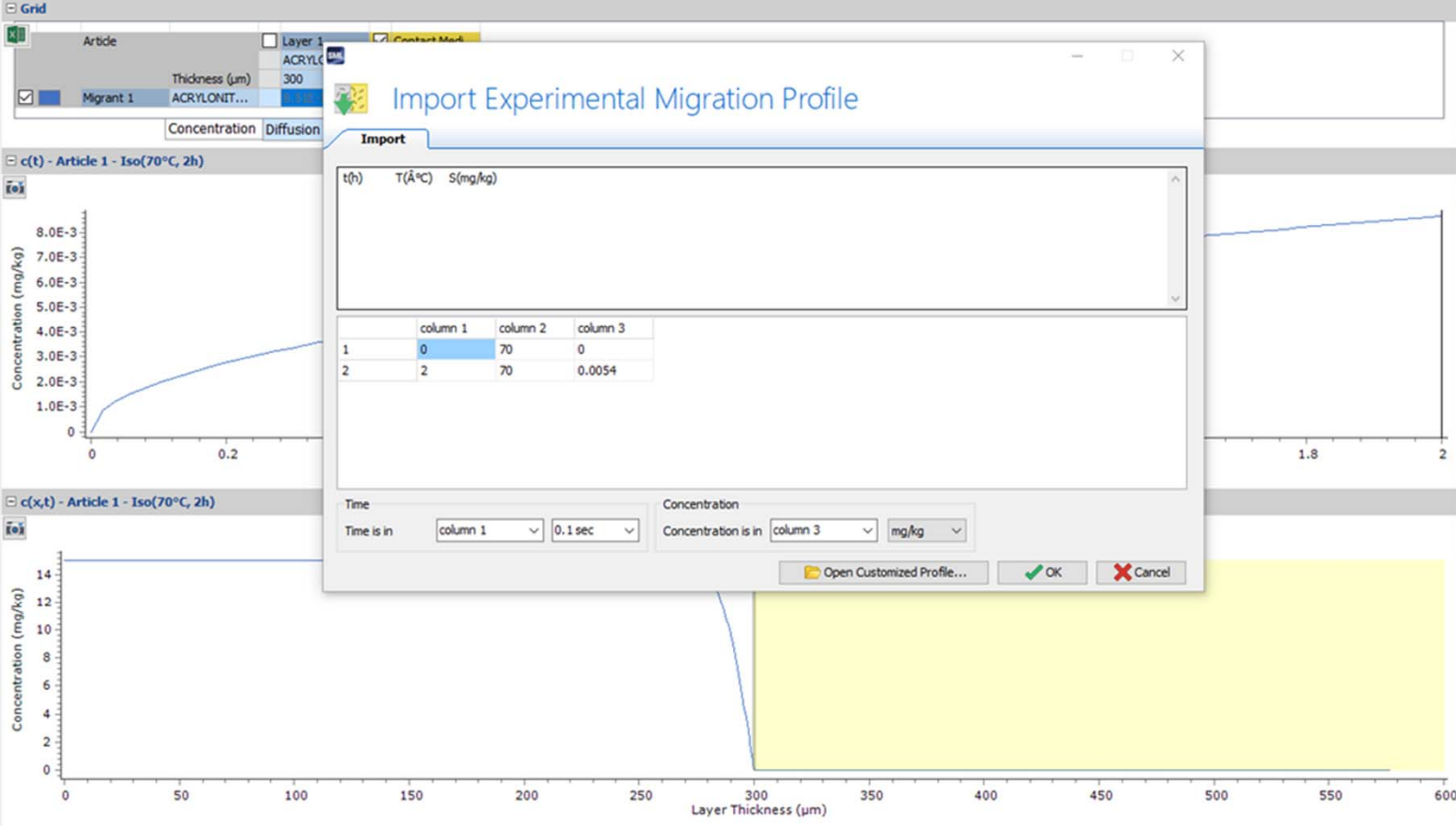


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Package Properties Output Calculation

- Package SAN 24h at 40C optimized
 - Article 1
 - Iso(40°C, 1d)
- Package SAN 2h at 70C
 - Article 1
 - Iso(70°C, 2h)

Temperature: 70 (°C) Display unit: mg/kg c(t) : draw mean concentration c(t) : draw concentration at 0 % of thickness from surface



Import Experimental Migration Profile

Import

t(h) T(°C) S(mg/kg)

	column 1	column 2	column 3
1	0	70	0
2	2	70	0.0054

Time is in: Time unit: Concentration is in: Unit:

Package SAN 2h at 70C

Geometry: Rectangular

Contact Surface (cm²): 600

Volume of Contact Medium (cm³): 1000

Width (cm): 10

Height (cm): 10

Length (cm): 10

Surface and mass of contact medium by article

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

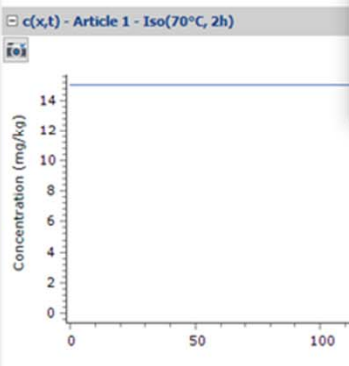
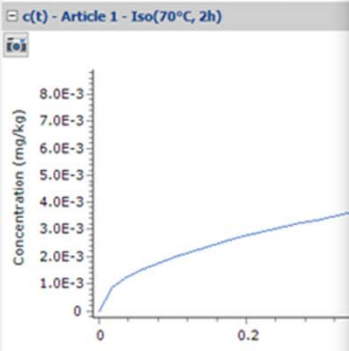
Total surface of all articles (cm²): 600

Package Properties Output Calculation

- Package SAN 24h at 40C optimized
 - Article 1
 - Iso(40°C, 1d)
- Package SAN 2h at 70C
 - Article 1
 - Iso(70°C, 2h)

Temperature: 70 (°C) Display unit: mg/kg c(t) : draw mean concentration c(t) : draw concentration at 0 % of thickness from surface

Article	Layer 1	Material	Thickness (µm)
		ACRYLONITRILE	300
<input checked="" type="checkbox"/>		ACRYLONITRILE...	



Import Experimental Migration Profile

Import

t(h) T(°C) S(mg/kg)

	column 1	column 2	column 3
1	0	70	0
2	2	70	0.0054

Time is in:

Concentration is in:

Package SAN 2h at 70C

Geometry: Rectangular

Contact Surface (cm²): 600

Volume of Contact Medium (cm³): 1000

Width (cm): 10

Height (cm): 10

Length (cm): 10

Surface and mass of contact medium by article

Articles	Surfaces (cm ²)	Mass (g)
Article 1	600	1000

Total surface of all articles (cm²): 600

Package Properties Output Calculation

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

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

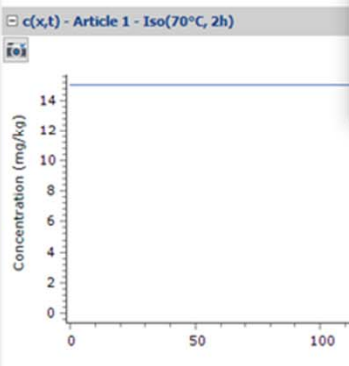
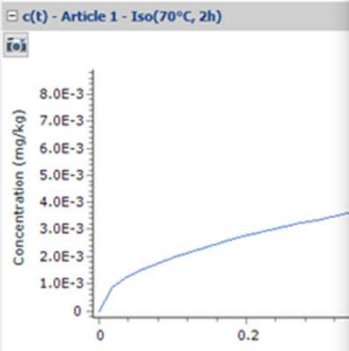
Prediction on This Article
 Prediction on All Articles
 Close All Articles
 Delete All Article Outputs
 Close All

- Package SAN 24h at 40C optimized
 - Article 1
 - Iso(40°C, 1d)
- Package SAN 2h at 70C
 - Article 1
 - Iso(70°C, 2h)

Temperature: 70 (°C) Display unit: mg/kg c(t) : draw mean concentration c(t) : draw concentration at 0 % of thickness from surface

Grid

Article	Layer 1	Material	Thickness (µm)
<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	ACRYLONITRILE	300
<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	Migrant 1	ACRYLONITRILE...



Import Experimental Migration Profile

Import

t(h) T(°C) S(mg/kg)

	column 1	column 2	column 3
1	0	70	0
2	2	70	0.0054

Time is in:

Concentration is in:

Package SAN 2h at 70C

Geometry: Rectangular

Contact Surface (cm²): 600

Volume of Contact Medium (cm³): 1000

Width (cm): 10

Height (cm): 10

Length (cm): 10

Surface and mass of contact medium by article

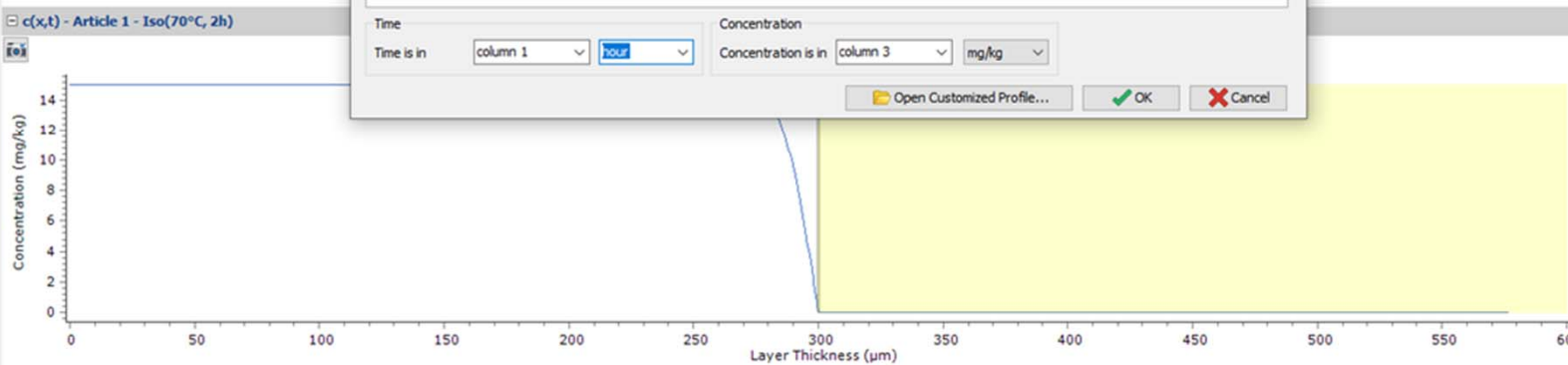
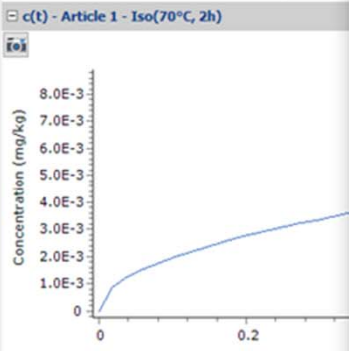
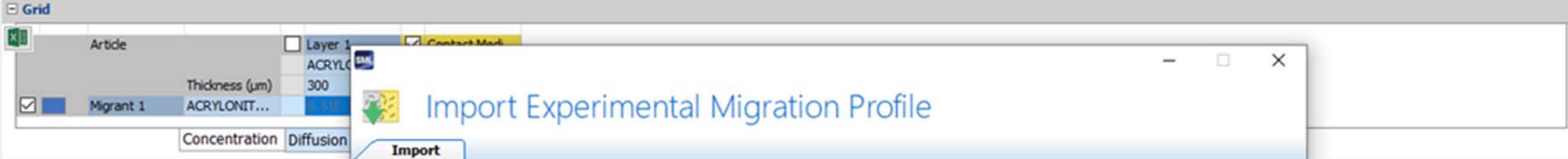
Articles	Surfaces (cm ²)	Mass (g)
Article 1	600	1000

Total surface of all articles (cm²): 600

Package Properties Output Calculation

- Package SAN 24h at 40C optimized
 - Article 1
 - Iso(40°C, 1d)
- Package SAN 2h at 70C
 - Article 1
 - Iso(70°C, 2h)

Temperature: 70 (°C) Display unit: mg/kg c(t) : draw mean concentration c(t) : draw concentration at 0 % of thickness from surface



Import Experimental Migration Profile

Import

t(h) T(°C) S(mg/kg)

	column 1	column 2	column 3
1	0	70	0
2	2	70	0.0054

Time is in: Concentration is in:

Package SAN 2h at 70C

Geometry: Rectangular

Contact Surface (cm²): 600

Volume of Contact Medium (cm³): 1000

Width (cm): 10

Height (cm): 10

Length (cm): 10

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

Package Properties Output Calculation

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

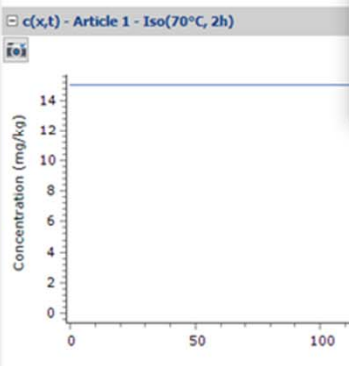
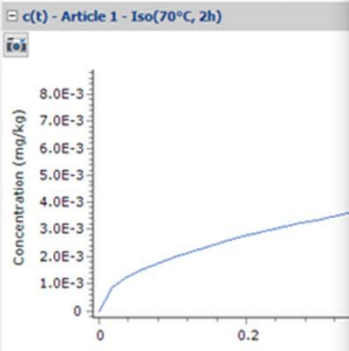
New Article
 Open Article
 Import Article
 Save Article
 Duplicate Article
 Close Article
 Import Initial Concentration

Prediction on This Article
 Prediction on All Articles
 Close All Articles
 Delete All Article Outputs
 Close All

- Package SAN 24h at 40C optimized
 - Article 1
 - Iso(40°C, 1d)
- Package SAN 2h at 70C
 - Article 1
 - Iso(70°C, 2h)

Temperature: 70 (°C) Display unit: mg/kg c(t) : draw mean concentration c(t) : draw concentration at 0 % of thickness from surface

Article	Layer 1	Material	Thickness (µm)
✓ Migrant 1	ACRYLONITRILE	ACRYLONITRILE	300



Import Experimental Migration Profile

Import

t(h) T(°C) S(mg/kg)

	column 1	column 2	column 3
1	0	70	0
2	2	70	0.0054

Time is in: Concentration is in: mg/kg

Package SAN 2h at 70C

Geometry: Rectangular

Contact Surface (cm²): 600

Volume of Contact Medium (cm³): 1000

Width (cm): 10

Height (cm): 10

Length (cm): 10

Surface and mass of contact medium by article

Articles	Surfaces (cm ²)	Mass (g)
Article 1	600	1000

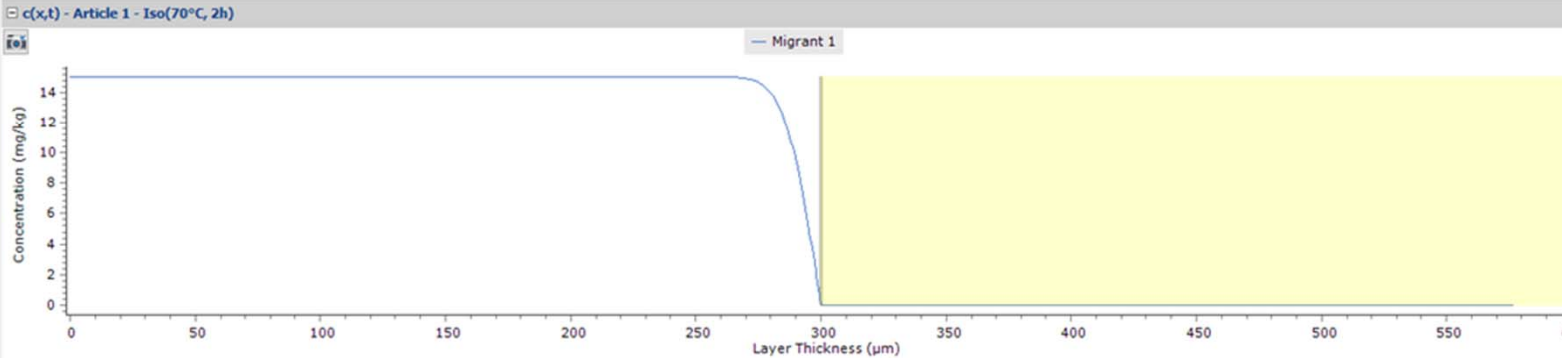
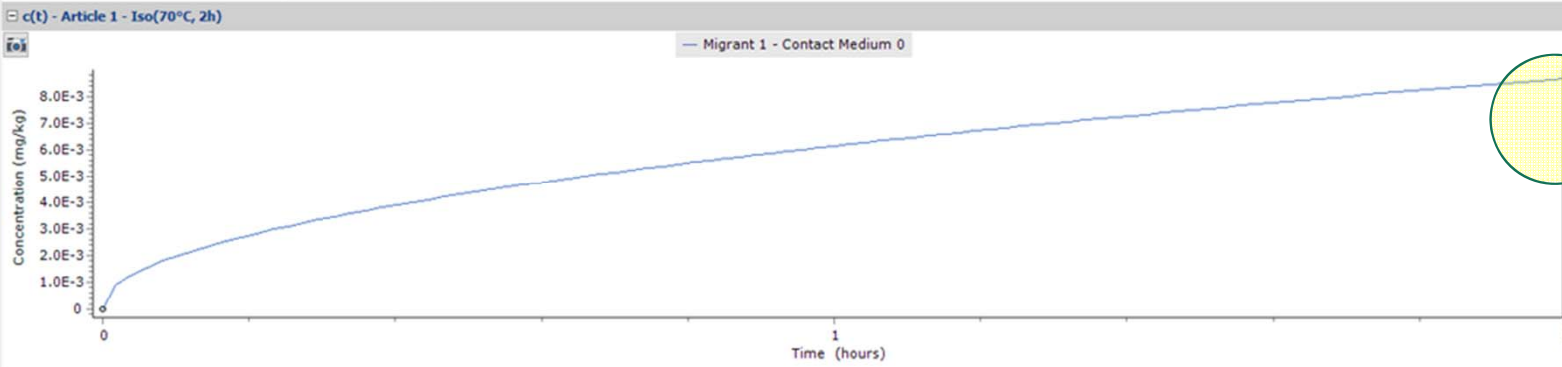
Total surface of all articles (cm²): 600

Package Properties Output Calculation

- Package SAN 24h at 40C optimized
 - Article 1
 - Iso(40°C, 1d)
- Package SAN 2h at 70C
 - Article 1
 - Iso(70°C, 2h)

Temperature: 70 (°C) Display unit mg/kg c(t) : draw mean concentration c(t) : draw concentration at 0 % of thickness from surface

Grid			
Article	Layer	Contact Med...	
	Layer 1	ACRYLONIT...	Acetic acid 3%
		Thickness (µm)	1.667E04
			0.0001
<input checked="" type="checkbox"/>	Migrant 1	ACRYLONIT...	0.0001



Package SAN 2h at 70C

Geometry: Rectangular

Contact Surface (cm²): 600

Volume of Contact Medium (cm³): 1000

Width (cm): 10

Height (cm): 10

Length (cm): 10

Surface and mass of contact medium by article

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

Total surface of all articles (cm²): 600

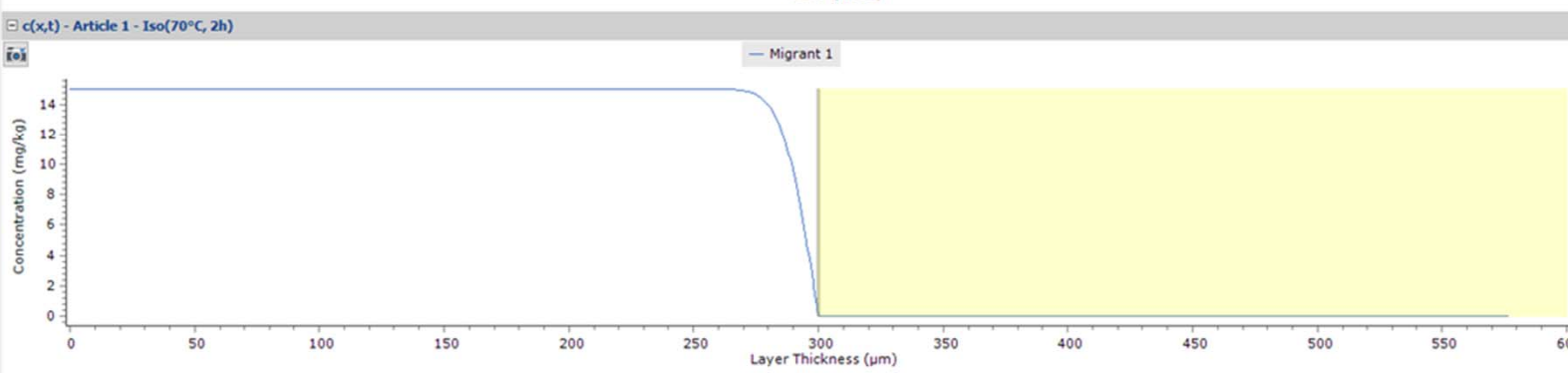
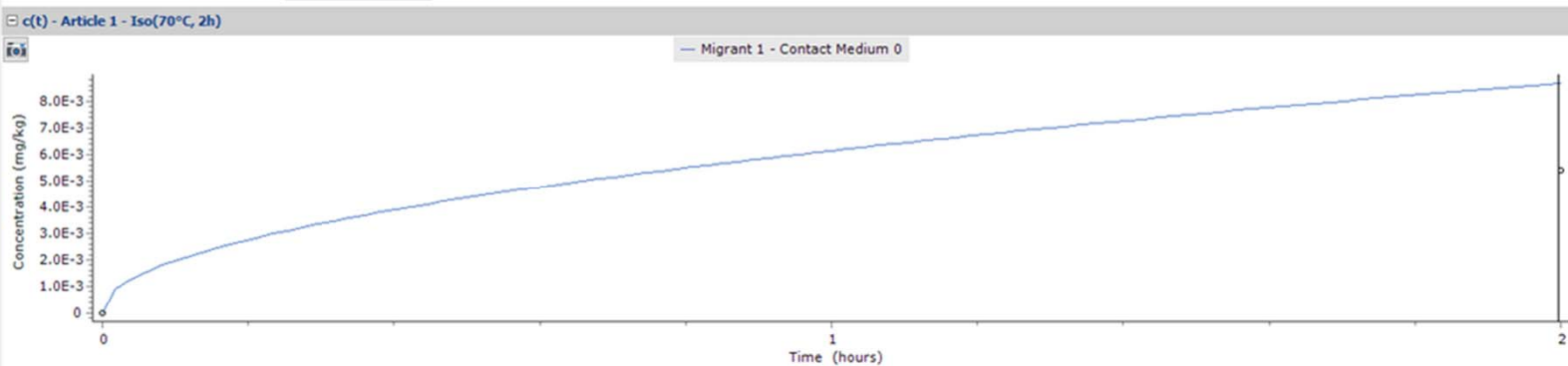
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Package Properties Output Calculation

- Package SAN 2h at 40C optimized
 - Article 1
 - Iso(40°C, 1d)
- Package SAN 2h at 70C
 - Article 1
 - Iso(70°C, 2h)

Temperature: 70 (°C) Display unit: mg/kg c(t) : draw mean concentration c(t) : draw concentration at 0 % of thickness from surface

Article	Layer 1	Contact Medi...
	ACRYLONIT...	Acetic acid 3%
	Thickness (µm): 300	1.667E04
<input checked="" type="checkbox"/> Migrant 1	ACRYLONIT...	0.0001



Package SAN 2h at 70C

Geometry: Rectangular

Contact Surface (cm²): 600

Volume of Contact Medium (cm³): 1000

Width (cm): 10

Height (cm): 10

Length (cm): 10

Surface and mass of contact medium by article

Articles	Surfaces (cm ²)	Mass (g)
Article 1	600	1000

Total surface of all articles (cm²): 600

Package Properties Output Calculation

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

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

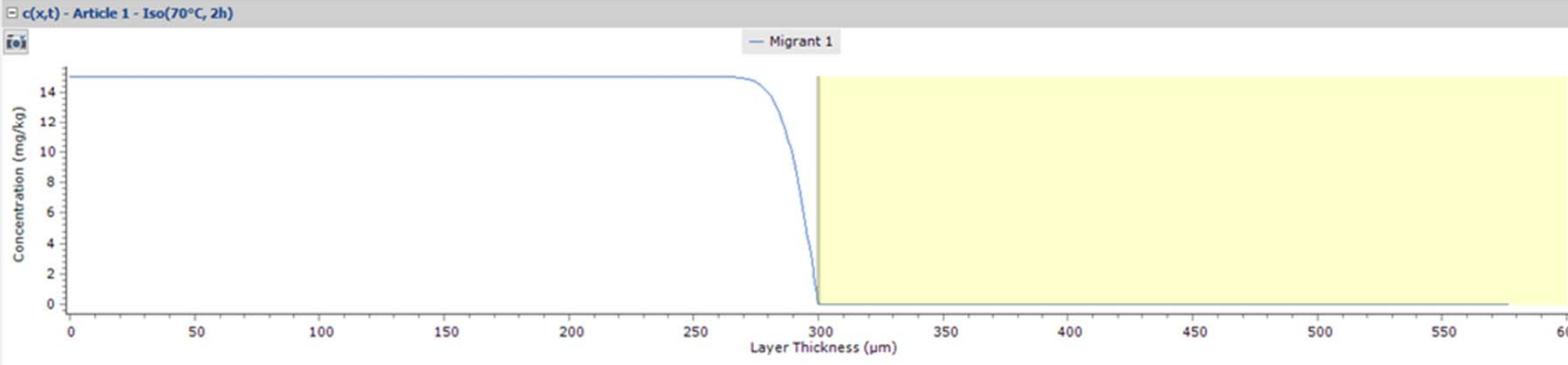
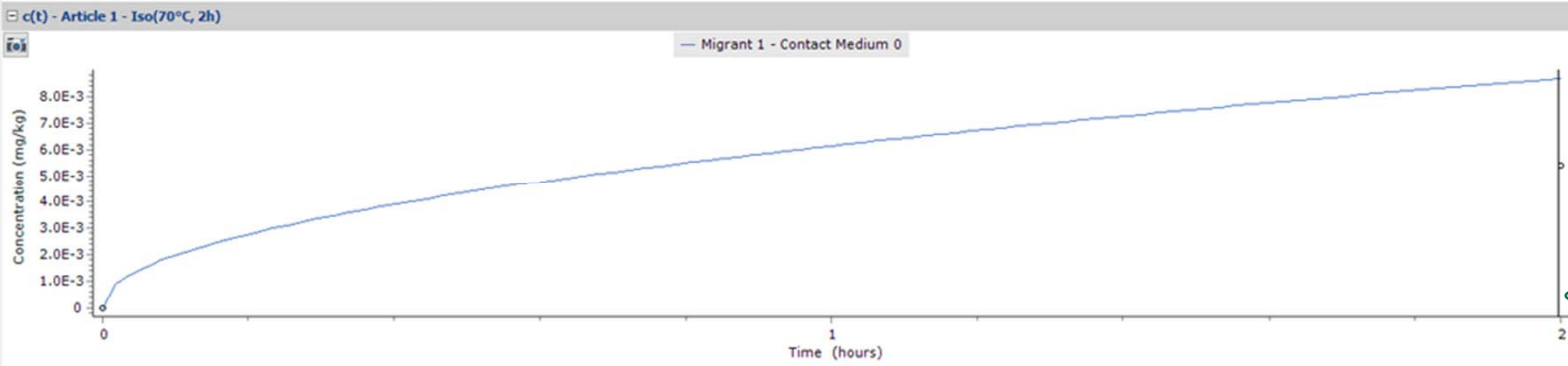
Prediction on This Article Prediction on All Articles Close All Articles Delete All Article Outputs Close All

- Package SAN 24h at 40C optimized
 - Article 1
 - Iso(40°C, 1d)
- Package SAN 2h at 70C
 - Article 1
 - Iso(70°C, 2h)

Temperature: 70 (°C) Display unit: mg/kg c(t): draw mean concentration c(t): draw concentration at 0 % of thickness from surface

Grid	Article	Layer 1	Contact Med...
		ACRYLONIT...	Acetic acid 3%
		Thickness (µm)	1.667E04
<input checked="" type="checkbox"/>	Migrant 1	ACRYLONIT...	0.0001

Concentration Diffusion Coefficient Partition Coefficient Solubility



Fitting Mode

Loops per serie: 20

Optimize Refresh

Correlation

mtau: 1 mtolg: 1E-6 mtolx: 1E-6 mrealstep: 1E-3

Parameter Name	Value
Layer 1-Dp-Known(cm^2/s)	8.51E-11

Close Fitting Mode for This Package Create Global Package

Package Properties Output Calculation

Package SAN 24h at 40C optimized
 Article 1
 Iso(40°C, 1d)
 Package SAN 2h at 70C
 Article 1
 Iso(70°C, 2h)

Surface (cm²) 600

This article is in read-only mode because it has an output or Set-Off

Article	Layer 1	Contact Medi...
	ACRYLONIT...	Acetic acid 3%
	Thickness (µm) 300	1.667E04
Migrant 1	ACRYLONIT...	8.51E-11 0.0001

Layer (Layer 1) Migrant (Migrant 1) **Data (Diffusion Coefficient)**

Diffusion Coefficient

- Known
- Interpolation based on Tg
- Pringer
- Arrhenius
- Customized Equation
- Brandsch Equation
- Welle Equation
- In-Silico

Known Value

Diffusion Coefficient (cm²/s): 8.51E-11 Optimize

Package SAN 2h at 70C

Geometry: Rectangular

Contact Surface (cm²): 600

Volume of Contact Medium (cm³): 1000

Width (cm): 10

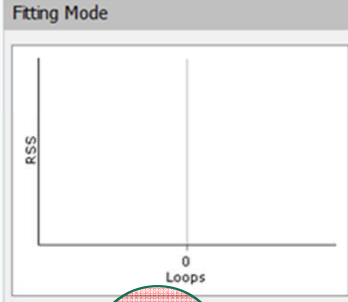
Height (cm): 10

Length (cm): 10

Surface and mass of contact medium by article

Articles	Surfaces (cm ²)	Mass (g)
Article 1	600	1000

Total surface of all articles (cm²): 600



Loops per series: 20

mtau: 1
 mtolg: 1E-6
 mtolx: 1E-6 mrealstep: 1E-3

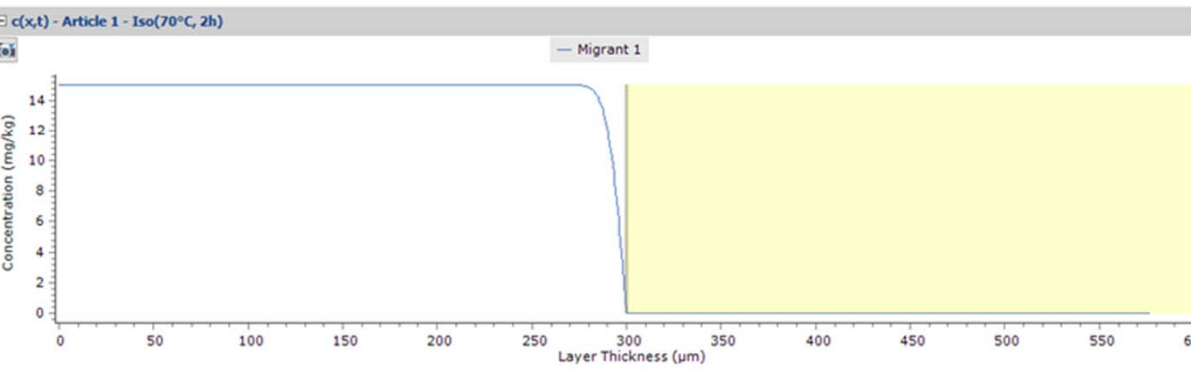
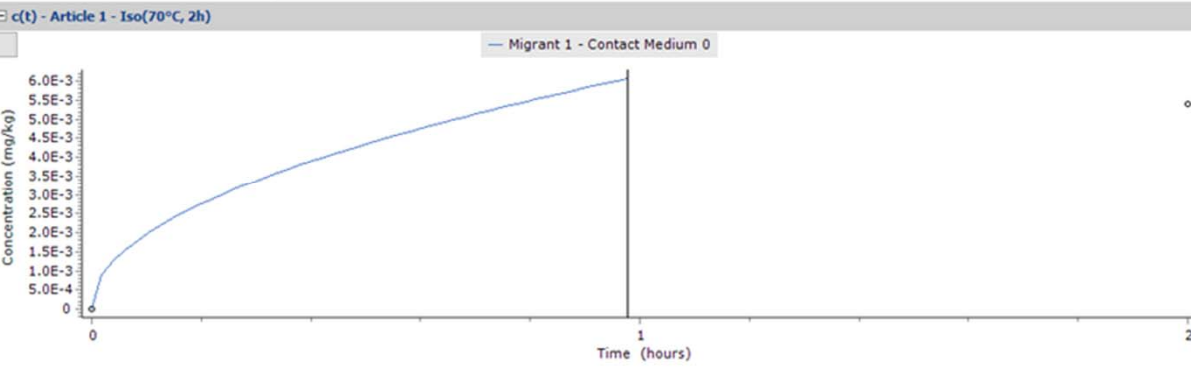
Parameter Name	Value
Layer 1-Dp-Known(cm ² /s)	8.51E-11

Package Properties Output Calculation

- Package SAN 24h at 40C optimized
 - Article 1
 - Iso(40°C, 1d)
- Package SAN 2h at 70C
 - Article 1
 - Iso(70°C, 2h)

Temperature: 70 (°C) Display unit: mg/kg c(t): draw mean concentration c(t): draw concentration at 0 % of thickness from surface

Grid	Article	Layer 1	Contact Med...
		ACRYLONIT...	Acetic acid 3%
		Thickness (µm)	1.667E04
		300	
<input checked="" type="checkbox"/>	Migrant 1	ACRYLONIT...	0.0001



Package SAN 2h at 70C

Geometry: Rectangular

Contact Surface (cm²): 600

Volume of Contact Medium (cm³): 1000

Width (cm): 10

Height (cm): 10

Length (cm): 10

Articles	Surfaces (cm ²)	Mass (g)
Article 1	600	1000

Total surface of all articles (cm²): 600

Fitting Mode

Loops per serie: 20 Initialization

Correlation

mtau: 1

mtolg: 1E-6

mtolx: 1E-6 mrealstep: 1E-3

Parameter Name	Value
Layer 1-Op-Known(cm ² /s)	8.51E-11

2023/7/2

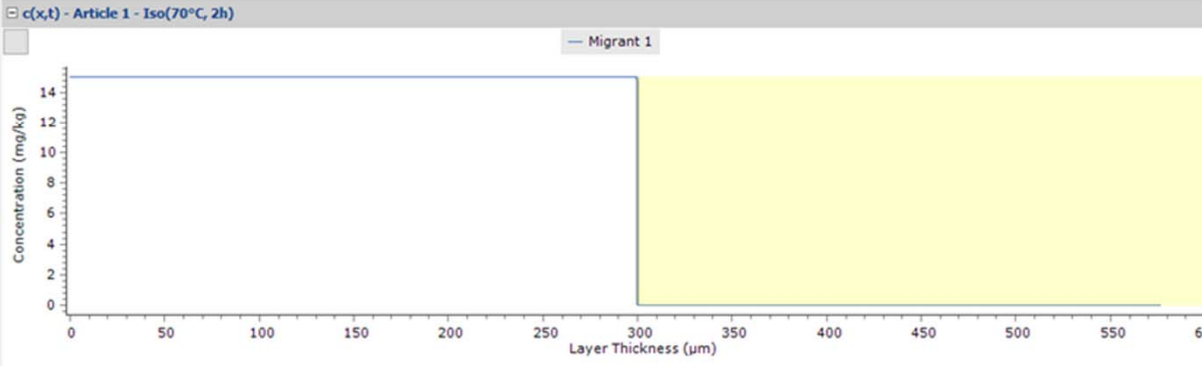
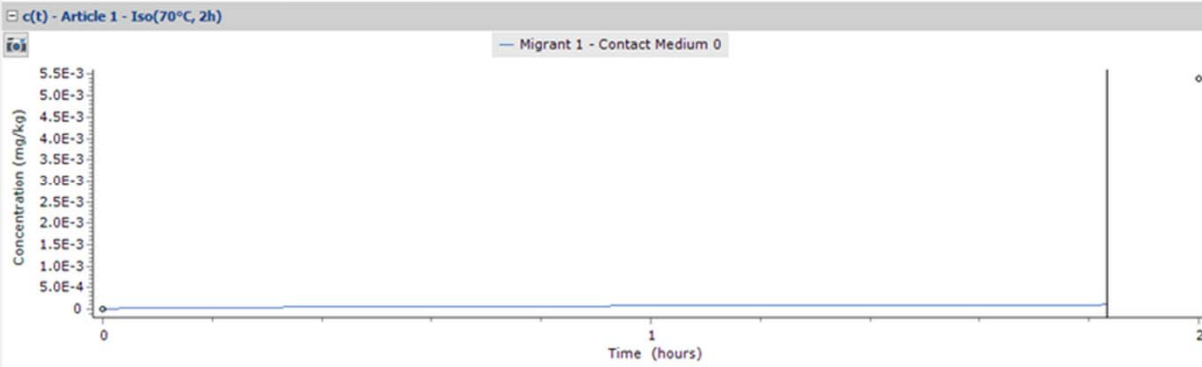
Package Properties | Output Calculation

- Package SAN 24h at 40C optimized
 - Article 1
 - Iso(40°C, 1d)
- Package SAN 2h at 70C
 - Article 1
 - Iso(70°C, 2h)

Temperature: 70 (°C) | Display unit: mg/kg | c(t) : draw mean concentration c(t) : draw concentration at 0 % of thickness from surface

Grid

Article	Layer 1	Contact Med...
	ACRYLONIT...	Acetic acid 3%
	Thickness (µm)	1.667E04
	300	
<input checked="" type="checkbox"/> Migrant 1	ACRYLONIT...	0.0001



Package SAN 2h at 70C

Geometry: Rectangular

Contact Surface (cm²): 600

Volume of Contact Medium (cm³): 1000

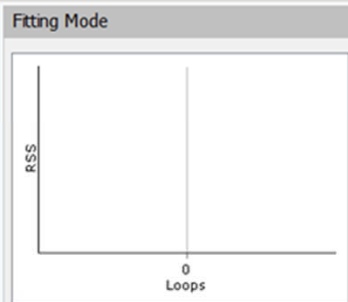
Width (cm): 10

Height (cm): 10

Length (cm): 10

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

Total surface of all articles (cm²): 600



Loops per serie: 20 | Iterations: 0

mtau: 1

mtolg: 1E-6

mtolx: 1E-6 | mrealstep: 1E-3

Parameter Name	Value
Layer 1-Op-Known(cm ² /s)	1.212E-14

2023/7/2

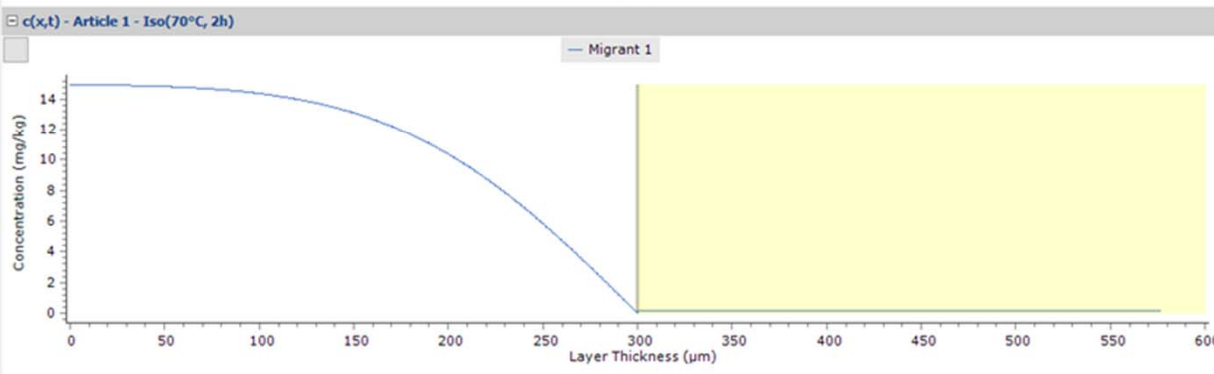
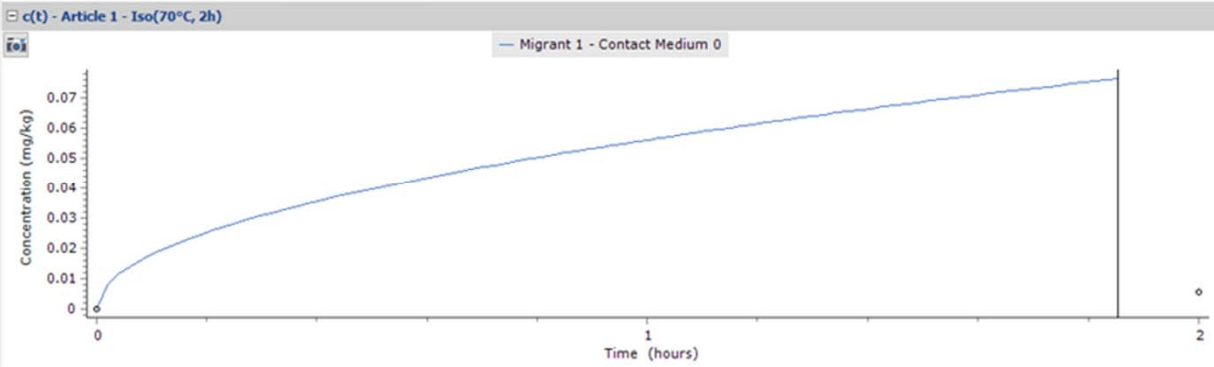
Package Properties Output Calculation

- Package SAN 24h at 40C optimized
 - Article 1
 - Iso(40°C, 1d)
- Package SAN 2h at 70C
 - Article 1
 - Iso(70°C, 2h)

Temperature: 70 (°C) Display unit: mg/kg c(t) : draw mean concentration c(t) : draw concentration at 0 % of thickness from surface

Grid

Article	Layer	Contact Med...
	Layer 1	ACRYLONIT... Acetic acid 3%
	Thickness (µm)	300 1.667E04
<input checked="" type="checkbox"/>	Migrant 1	ACRYLONIT... 0.0001



Package SAN 2h at 70C

Geometry: Rectangular

Contact Surface (cm²): 600

Volume of Contact Medium (cm³): 1000

Width (cm): 10

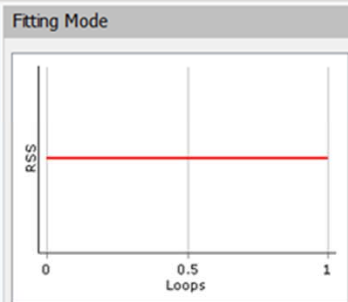
Height (cm): 10

Length (cm): 10

Surface and mass of contact medium by article

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

Total surface of all articles (cm²): 600



Loops per serie: 20 Iterations: 1

mtau: 1

mtolg: 1E-6

mtolx: 1E-6 mrealstep: 1E-3

Parameter Name	Value
Layer 1-Op-Known(cm ² /s)	7.131E-9

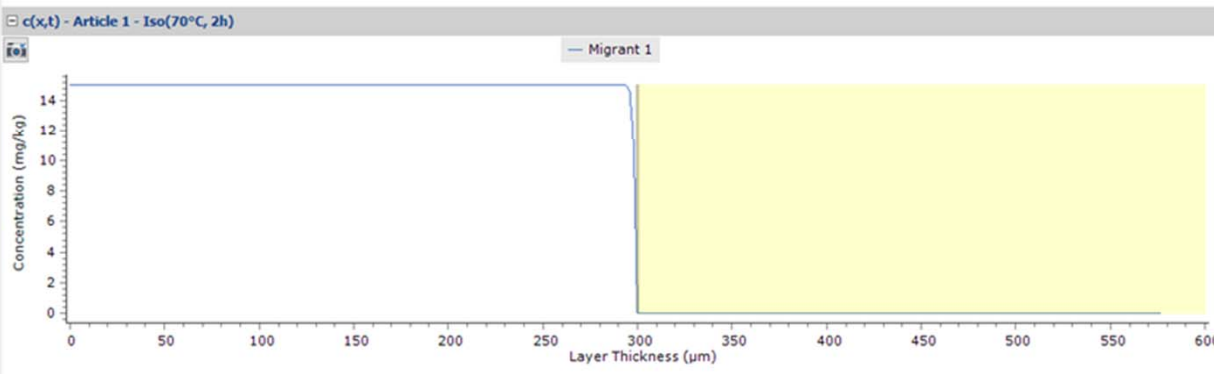
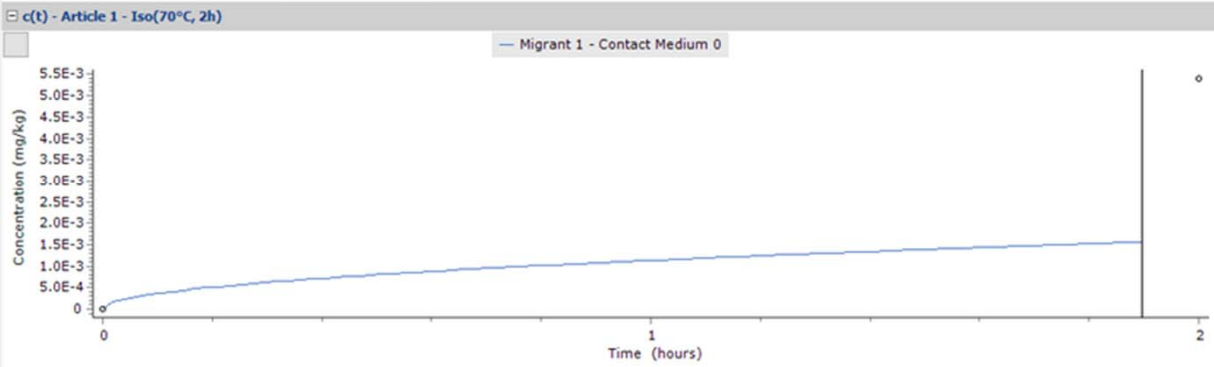
Package Properties Output Calculation

- Package SAN 24h at 40C optimized
 - Article 1
 - Iso(40°C, 1d)
- Package SAN 2h at 70C
 - Article 1
 - Iso(70°C, 2h)

Temperature: 70 (°C) Display unit: mg/kg c(t) : draw mean concentration c(t) : draw concentration at 0 % of thickness from surface

Grid

Article	Layer 1	Contact Med...
	ACRYLONIT...	Acetic acid 3%
	Thickness (µm): 300	1.667E04
<input checked="" type="checkbox"/> Migrant 1	ACRYLONIT...	0.0001



Package SAN 2h at 70C

Geometry: Rectangular

Contact Surface (cm²): 600

Volume of Contact Medium (cm³): 1000

Width (cm): 10

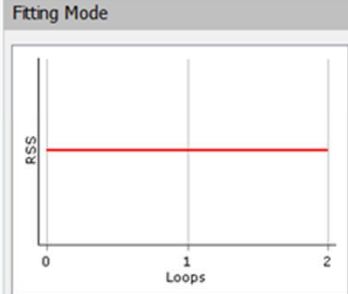
Height (cm): 10

Length (cm): 10

Surface and mass of contact medium by article

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

Total surface of all articles (cm²): 600



Loops per serie: 20 Iterations: 2

mtau: 1

mtolg: 1E-6

mtolx: 1E-6 mrealstep: 1E-3

Parameter Name	Value
Layer 1-Op-Known(cm ² /s)	2.889E-12

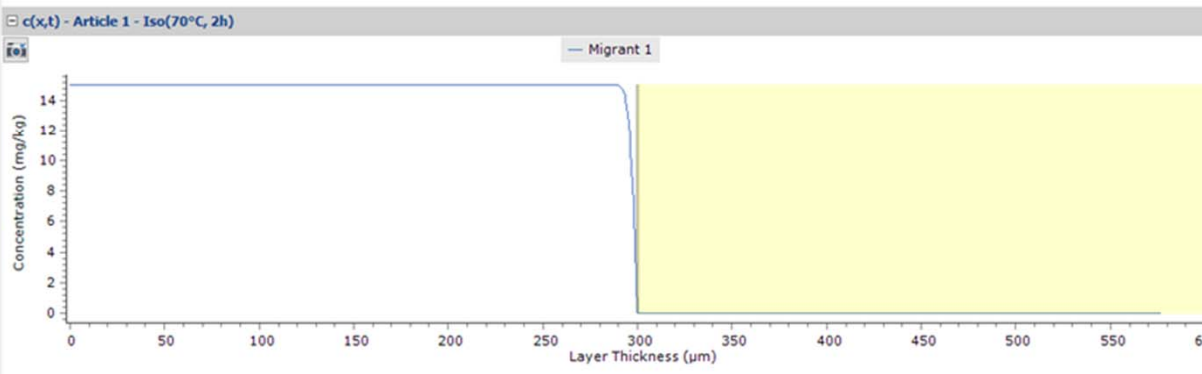
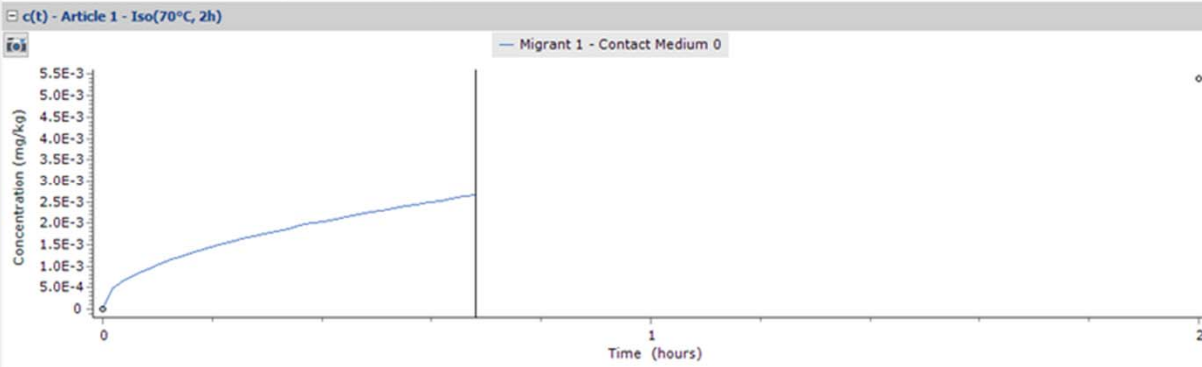
Package Properties | Output Calculation

- Package SAN 24h at 40C optimized
 - Article 1
 - Iso(40°C, 1d)
- Package SAN 2h at 70C
 - Article 1
 - Iso(70°C, 2h)

Temperature: 70 (°C) | Display unit: mg/kg | c(t) : draw mean concentration c(t) : draw concentration at 0 % of thickness from surface

Grid	Article	Layer 1	Contact Med...
		ACRYLONIT...	Acetic acid 3%
		Thickness (µm)	1.667E04
		300	
<input checked="" type="checkbox"/>	Migrant 1	ACRYLONIT...	0.0001

Concentration | Diffusion Coefficient | Partition Coefficient | Solubility



Package SAN 2h at 70C

Geometry: Rectangular

Contact Surface (cm²): 600

Volume of Contact Medium (cm³): 1000

Width (cm): 10

Height (cm): 10

Length (cm): 10

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

Total surface of all articles (cm²): 600

Fitting Mode

Loops per serie: 20 | Iterations: 4

Correlation

mtau: 1

mtolg: 1E-6

mtolx: 1E-6 | mrealstep: 1E-3

Parameter Name	Value
Layer 1-Op-Known(cm ² /s)	2.337E-11

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Package Properties Output Calculation

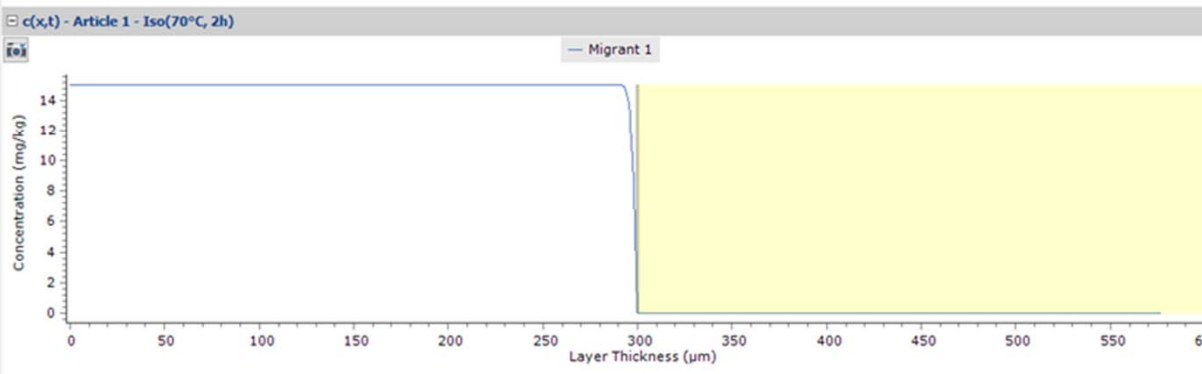
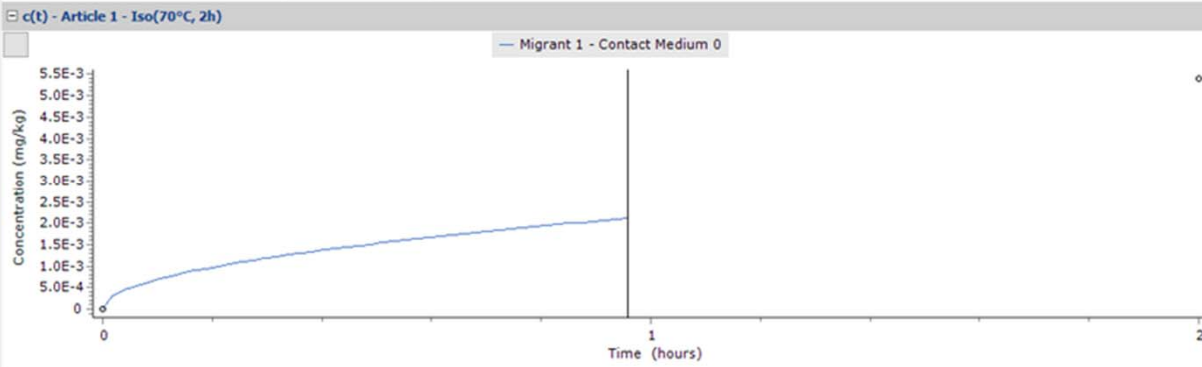
- Package SAN 24h at 40C optimized
 - Article 1
 - Iso(40°C, 1d)
- Package SAN 2h at 70C
 - Article 1
 - Iso(70°C, 2h)

Temperature: 70 (°C) Display unit: mg/kg c(t) : draw mean concentration c(t) : draw concentration at 0 % of thickness from surface

Grid

Article	Layer 1	Contact Med...
	ACRYLONIT...	Acetic acid 3%
	Thickness (µm)	1.667E04
<input checked="" type="checkbox"/>	Migrant 1	ACRYLONIT... 0.0001

Concentration Diffusion Coefficient Partition Coefficient Solubility



Package SAN 2h at 70C

Geometry: Rectangular

Contact Surface (cm²): 600

Volume of Contact Medium (cm³): 1000

Width (cm): 10

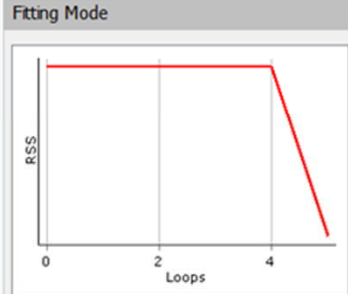
Height (cm): 10

Length (cm): 10

Surface and mass of contact medium by article

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

Total surface of all articles (cm²): 600



Loops per serie: 20 Iterations: 5

mtau: 1

mtolg: 1E-6

mtolx: 1E-6 mrealstep: 1E-3

Parameter Name	Value
Layer 1-Op-Known(cm ² /s)	1.052E-11

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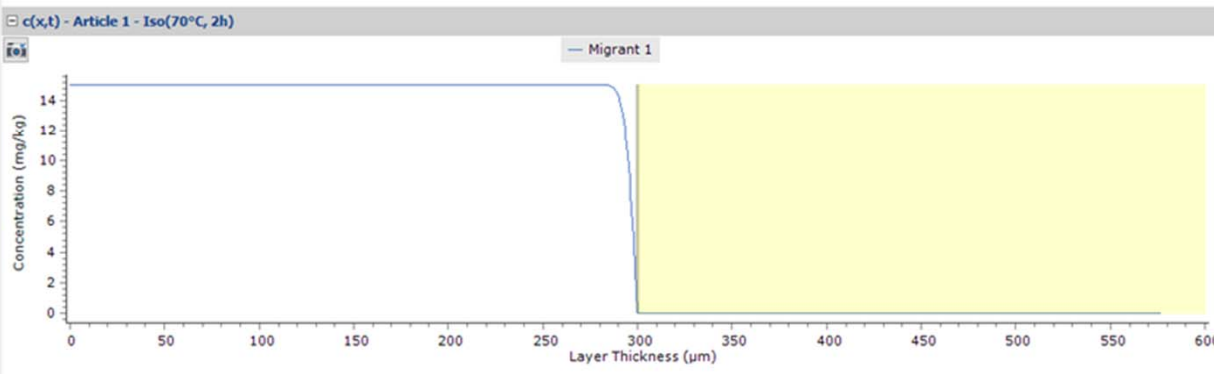
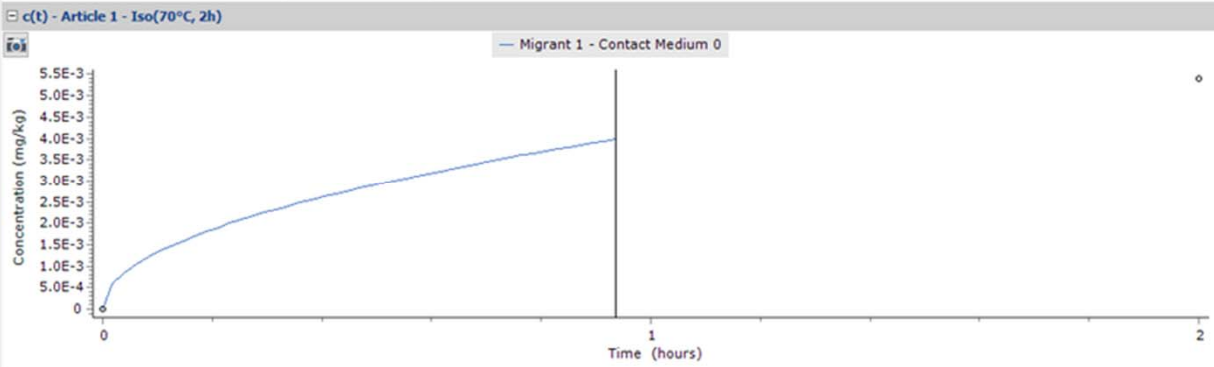
Package Properties Output Calculation

- Package SAN 24h at 40C optimized
 - Article 1
 - Iso(40°C, 1d)
- Package SAN 2h at 70C
 - Article 1
 - Iso(70°C, 2h)

Temperature: 70 (°C) Display unit: mg/kg c(t) : draw mean concentration c(t) : draw concentration at 0 % of thickness from surface

Grid

Article	Layer 1	Contact Med...
	ACRYLONIT...	Acetic acid 3%
	Thickness (µm)	1.667E04
<input checked="" type="checkbox"/>	Migrant 1	ACRYLONIT... 0.0001



Package SAN 2h at 70C

Geometry: Rectangular

Contact Surface (cm²): 600

Volume of Contact Medium (cm³): 1000

Width (cm): 10

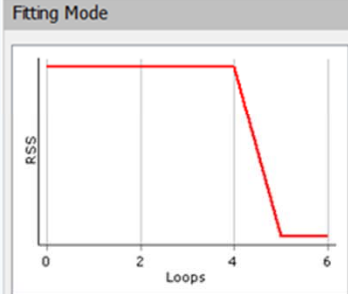
Height (cm): 10

Length (cm): 10

Surface and mass of contact medium by article

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

Total surface of all articles (cm²): 600



Loops per serie: 20 Iterations: 6

mtau: 1

mtolg: 1E-6

mtolx: 1E-6 mrealstep: 1E-3

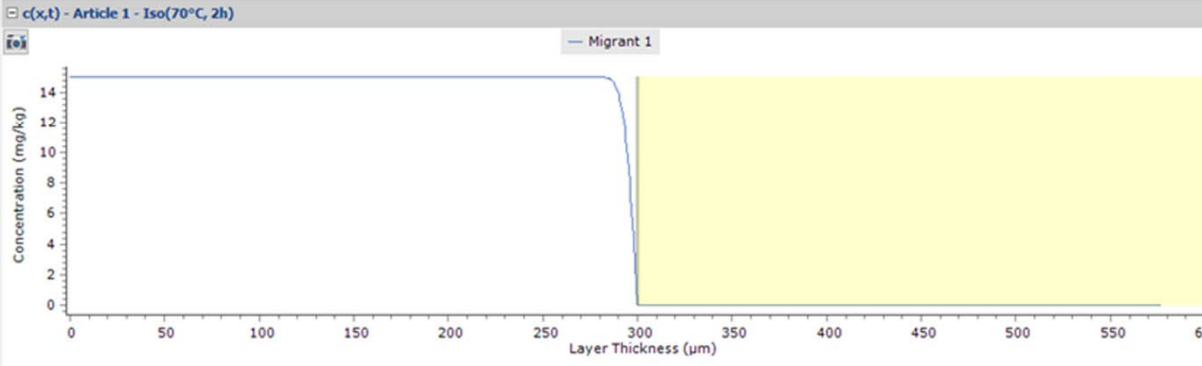
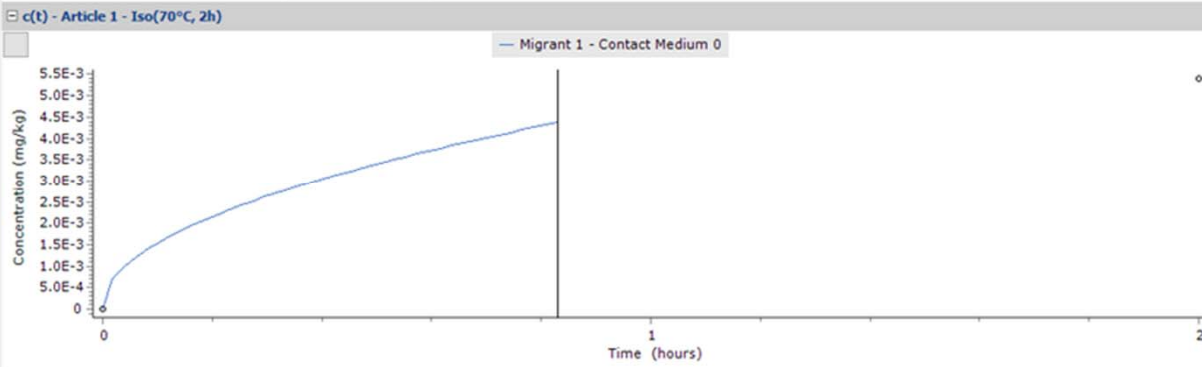
Parameter Name	Value
Layer 1-Op-Known(cm ² /s)	3.829E-11

Package Properties Output Calculation

- Package SAN 24h at 40C optimized
 - Article 1
 - Iso(40°C, 1d)
- Package SAN 2h at 70C
 - Article 1
 - Iso(70°C, 2h)

Temperature : 70 (°C) Display unit mg/kg c(t) : draw mean concentration c(t) : draw concentration at 0 % of thickness from surface

Article	Layer 1	Contact Med...
	ACRYLONIT...	Acetic acid 3%
	Thickness (µm)	1.667E04
<input checked="" type="checkbox"/> Migrant 1	ACRYLONIT...	0.0001



Package SAN 2h at 70C

Geometry: Rectangular

Contact Surface (cm²): 600

Volume of Contact Medium (cm³): 1000

Width (cm): 10

Height (cm): 10

Length (cm): 10

Articles	Surfaces (cm ²)	Mass (g)
Article 1	600	1000

Total surface of all articles (cm²): 600

Fitting Mode

Loops per serie: 20 Iterations: 7

mtau: 1

mtolg: 1E-6

mtolx: 1E-6 mrealstep: 1E-3

Parameter Name	Value
Layer 1-Op-Known(cm ² /s)	5.195E-11

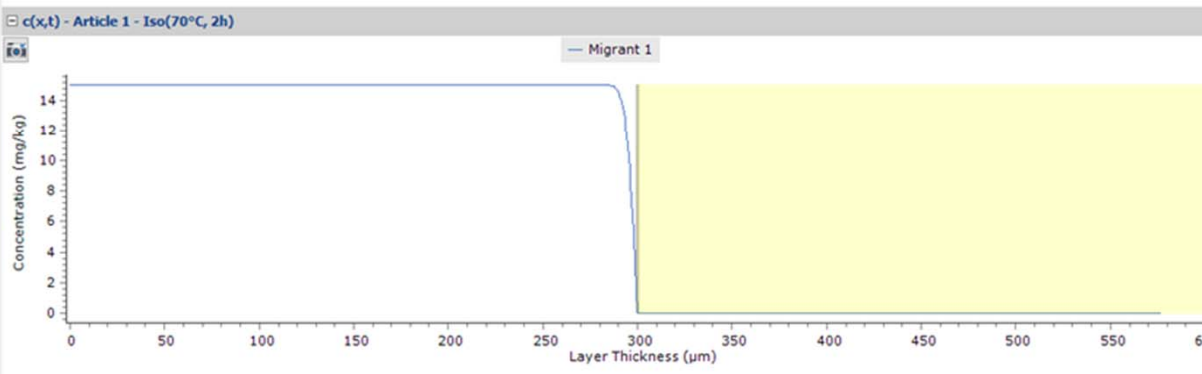
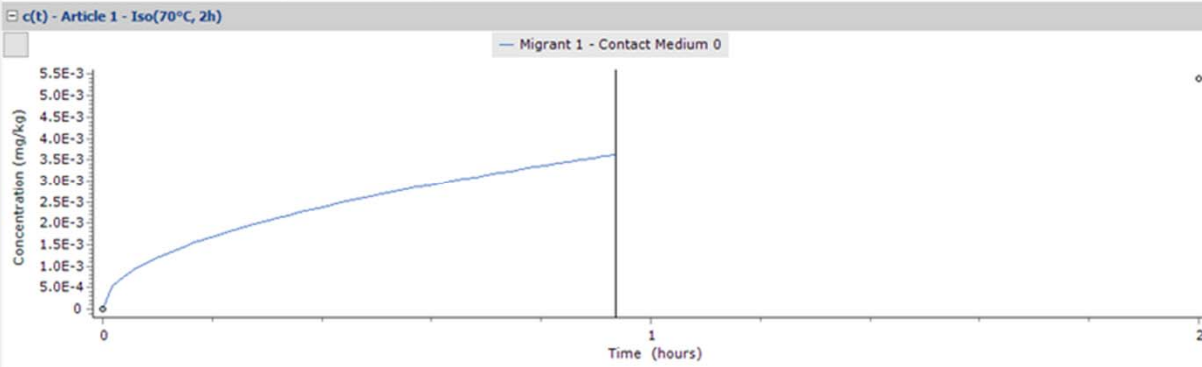
Package Properties Output Calculation

- Package SAN 24h at 40C optimized
 - Article 1
 - Iso(40°C, 1d)
- Package SAN 2h at 70C
 - Article 1
 - Iso(70°C, 2h)

Temperature: 70 (°C) Display unit: mg/kg c(t) : draw mean concentration c(t) : draw concentration at 0 % of thickness from surface

Grid

Article	Layer	Contact Med...
	Layer 1	ACRYLONIT... Acetic acid 3%
	Thickness (µm)	300 1.667E04
<input checked="" type="checkbox"/>	Migrant 1	ACRYLONIT... 0.0001



Package SAN 2h at 70C

Geometry: Rectangular

Contact Surface (cm²): 600

Volume of Contact Medium (cm³): 1000

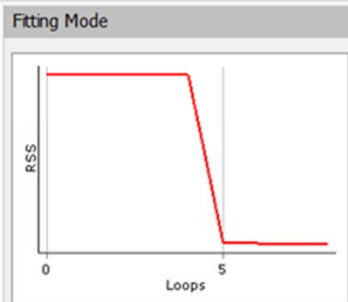
Width (cm): 10

Height (cm): 10

Length (cm): 10

Articles	Surfaces (cm ²)	Mass (g)
Article 1	600	1000

Total surface of all articles (cm²): 600



Loops per serie: 20 Iterations: 8

mtau: 1

mtolg: 1E-6

mtolx: 1E-6 mrealstep: 1E-3

Parameter Name	Value
Layer 1-Op-Known(cm ² /s)	3.171E-11

Package Properties | Output Calculation

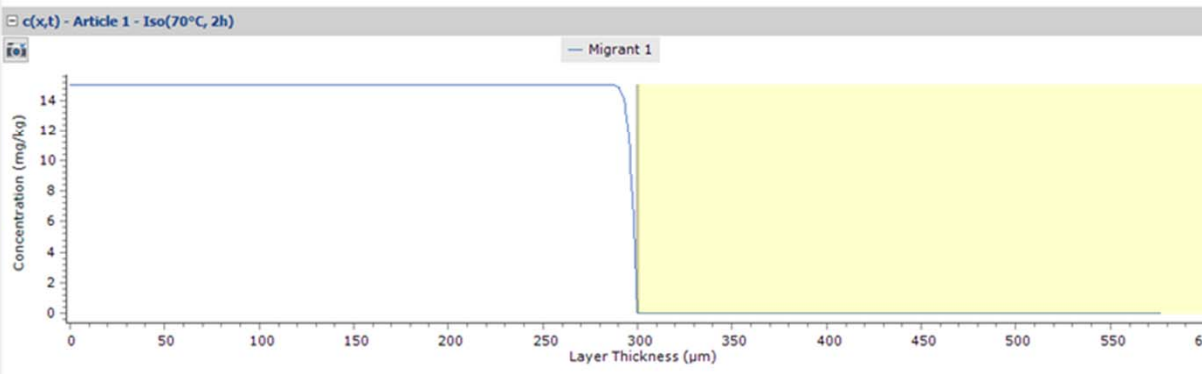
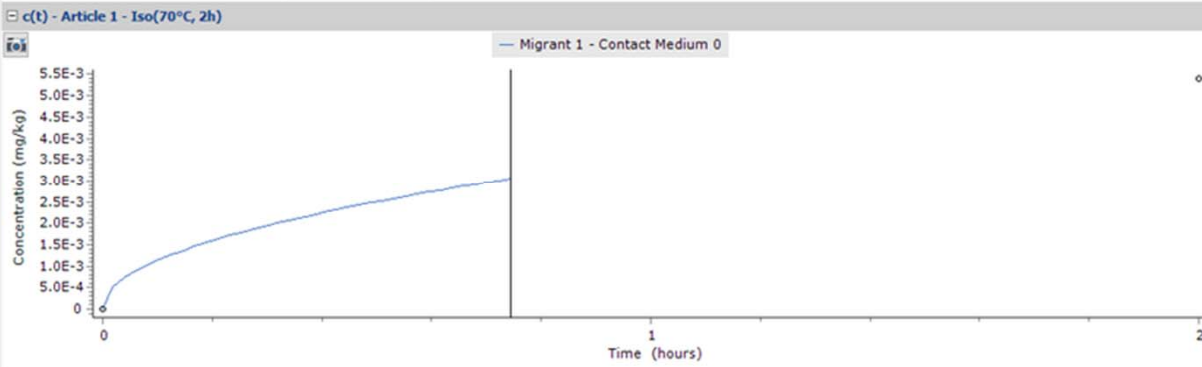
- Package SAN 24h at 40C optimized
 - Article 1
 - Iso(40°C, 1d)
- Package SAN 2h at 70C
 - Article 1
 - Iso(70°C, 2h)

Temperature: 70 (°C) | Display unit: mg/kg | c(t) : draw mean concentration c(t) : draw concentration at 0 % of thickness from surface

Grid

Article	Layer 1	Contact Med...
	ACRYLONIT...	Acetic acid 3%
	Thickness (µm)	1.667E04
	300	
<input checked="" type="checkbox"/> Migrant 1	ACRYLONIT...	0.0001

Concentration | Diffusion Coefficient | Partition Coefficient | Solubility



Package SAN 2h at 70C

Geometry: Rectangular

Contact Surface (cm²): 600

Volume of Contact Medium (cm³): 1000

Width (cm): 10

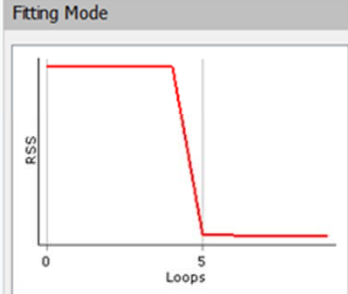
Height (cm): 10

Length (cm): 10

Surface and mass of contact medium by article

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

Total surface of all articles (cm²): 600



Loops per serie: 20 | Iterations: 9

mtau: 1

mtolg: 1E-6

mtolx: 1E-6 | mrealstep: 1E-3

Parameter Name	Value
Layer 1-Op-Known(cm ² /s)	2.822E-11

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Package Properties Output Calculation

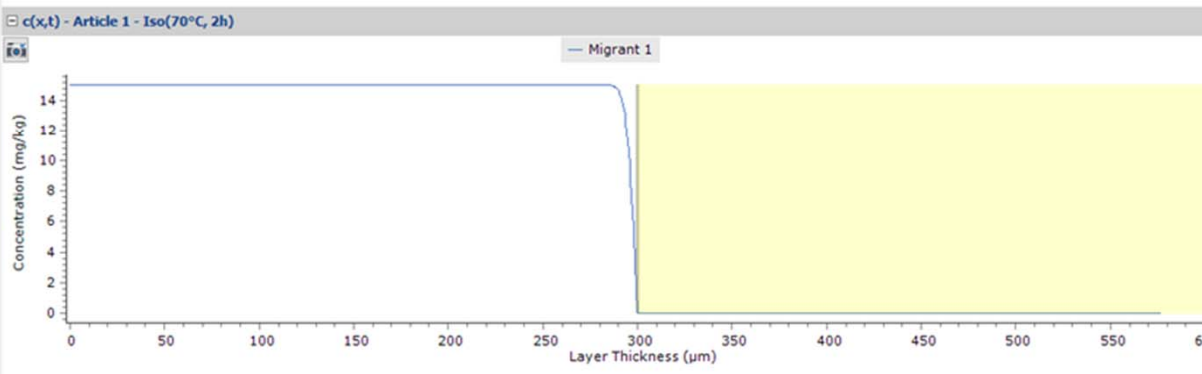
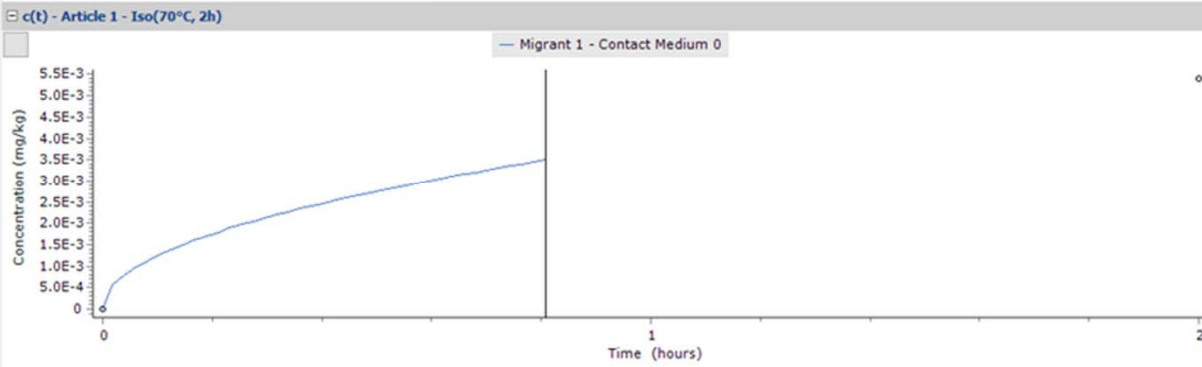
- Package SAN 24h at 40C optimized
 - Article 1
 - Iso(40°C, 1d)
- Package SAN 2h at 70C
 - Article 1
 - Iso(70°C, 2h)

Temperature: 70 (°C) Display unit: mg/kg c(t) : draw mean concentration c(t) : draw concentration at 0 % of thickness from surface

Grid

Article	Layer	Contact Med...
Migrant 1	Layer 1	ACRYLONIT... Acetic acid 3%
		Thickness (µm) 300 1.667E04
		0.0001

Concentration Diffusion Coefficient Partition Coefficient Solubility



Package SAN 2h at 70C

Geometry: Rectangular

Contact Surface (cm²): 600

Volume of Contact Medium (cm³): 1000

Width (cm): 10

Height (cm): 10

Length (cm): 10

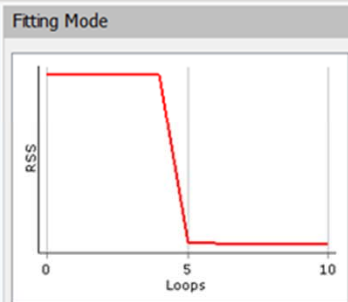
Add Article

Surface and mass of contact medium by article

Articles	Surfaces (cm ²)	Mass (g)
Article 1	600	1000

Total surface of all articles (cm²): 600

Switch Package in Fitting Mode



Loops per serie: 20 Iterations: 10

Optimize Refresh

Correlation

mtau: 1

mtolg: 1E-6

mtolx: 1E-6 mrealstep: 1E-3

Parameter Name	Value
Layer 1-Op-Known(cm ² /s)	3.408E-11

Close Fitting Mode for This Package

Create Global Package

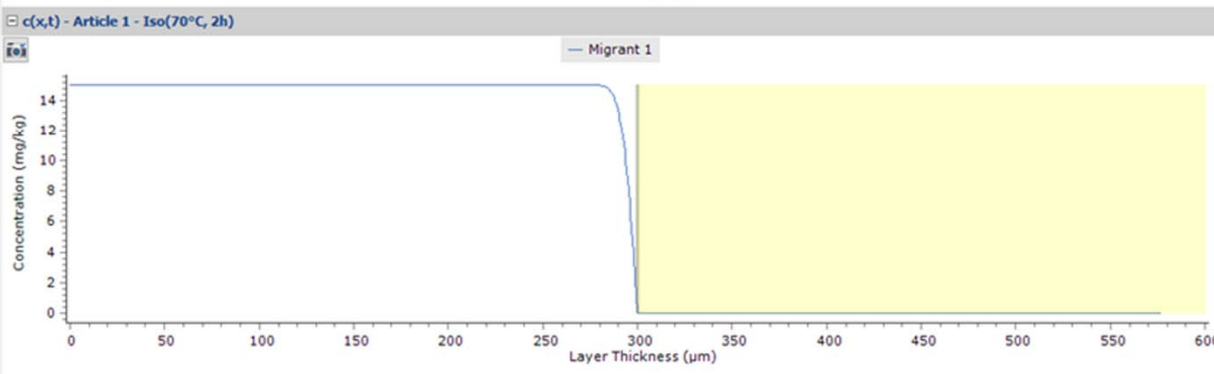
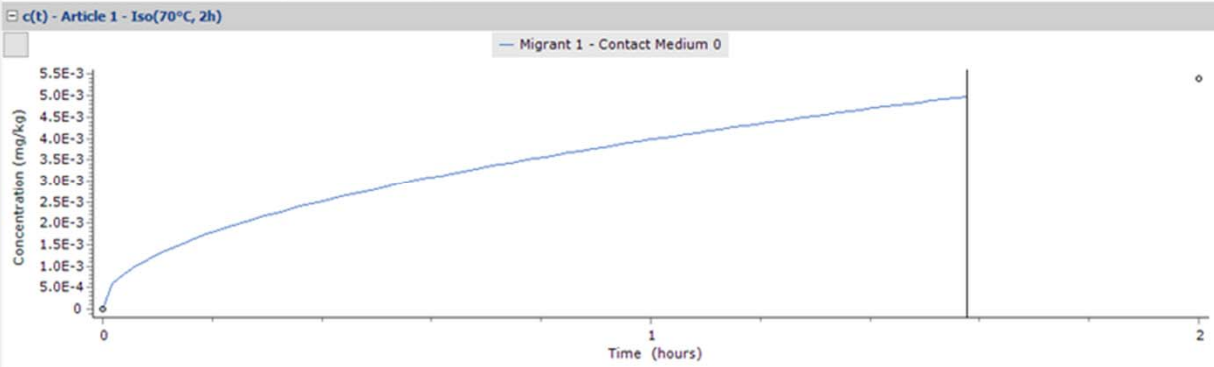
Package Properties | Output Calculation

- Package SAN 24h at 40C optimized
 - Article 1
 - Iso(40°C, 1d)
- Package SAN 2h at 70C
 - Article 1
 - Iso(70°C, 2h)

Temperature: 70 (°C) | Display unit: mg/kg | c(t) : draw mean concentration c(t) : draw concentration at 0 % of thickness from surface

Grid

Article	Layer	Contact Med...
	Layer 1	ACRYLONIT... Acetic acid 3%
	Thickness (µm)	300 1.667E04
<input checked="" type="checkbox"/>	Migrant 1	ACRYLONIT... 0.0001



Package SAN 2h at 70C

Geometry: Rectangular

Contact Surface (cm²): 600

Volume of Contact Medium (cm³): 1000

Width (cm): 10

Height (cm): 10

Length (cm): 10

Articles	Surfaces (cm ²)	Mass (g)
Article 1	600	1000

Total surface of all articles (cm²): 600

Fitting Mode

Loops per serie: 20 | Iterations: 11

mtau: 1

mtolg: 1E-6

mtolx: 1E-6 | mrealstep: 1E-3

Parameter Name	Value
Layer 1-Op-Known(cm ² /s)	3.563E-11

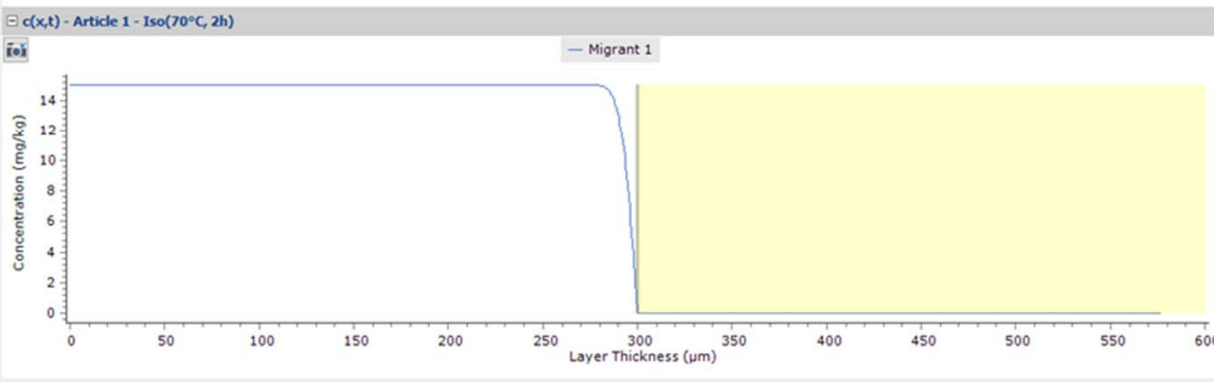
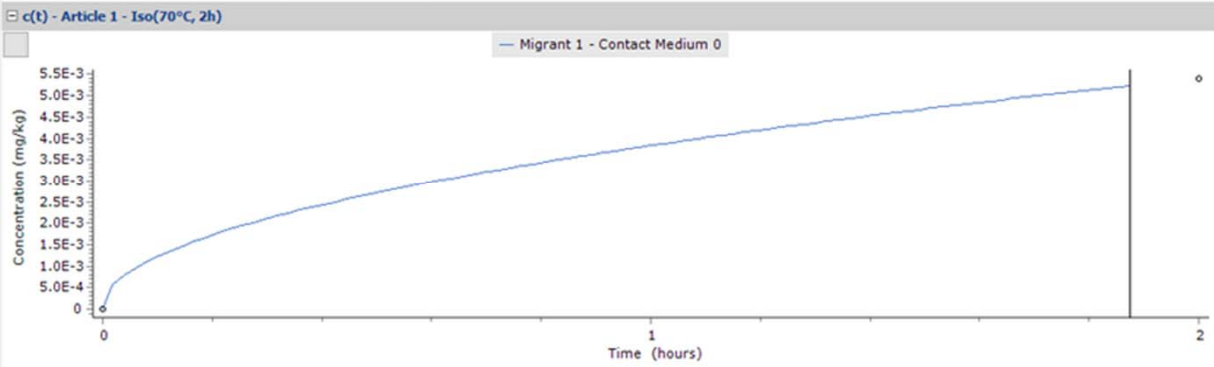
Package Properties Output Calculation

- Package SAN 24h at 40C optimized
 - Article 1
 - Iso(40°C, 1d)
- Package SAN 2h at 70C
 - Article 1
 - Iso(70°C, 2h)

Temperature: 70 (°C) Display unit: mg/kg c(t) : draw mean concentration c(t) : draw concentration at 0 % of thickness from surface

Grid	Article	Layer 1	Contact Med...
		ACRYLONIT...	Acetic acid 3%
		Thickness (µm)	1.667E04
		300	
<input checked="" type="checkbox"/>	Migrant 1	ACRYLONIT...	0.0001

Concentration Diffusion Coefficient Partition Coefficient Solubility



Package SAN 2h at 70C

Geometry: Rectangular

Contact Surface (cm²): 600

Volume of Contact Medium (cm³): 1000

Width (cm): 10

Height (cm): 10

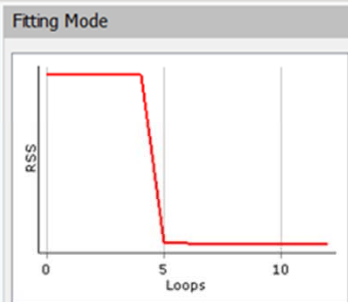
Length (cm): 10

Add Article

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

Total surface of all articles (cm²): 600

Switch Package in Fitting Mode



Loops per serie: 20 Iterations: 12

Optimize Refresh

Correlation

mtau: 1

mtolg: 1E-6

mtolx: 1E-6 mrealstep: 1E-3

Parameter Name	Value
Layer 1-Op-Known(cm ² /s)	3.316E-11

Close Fitting Mode for This Package

Create Global Package

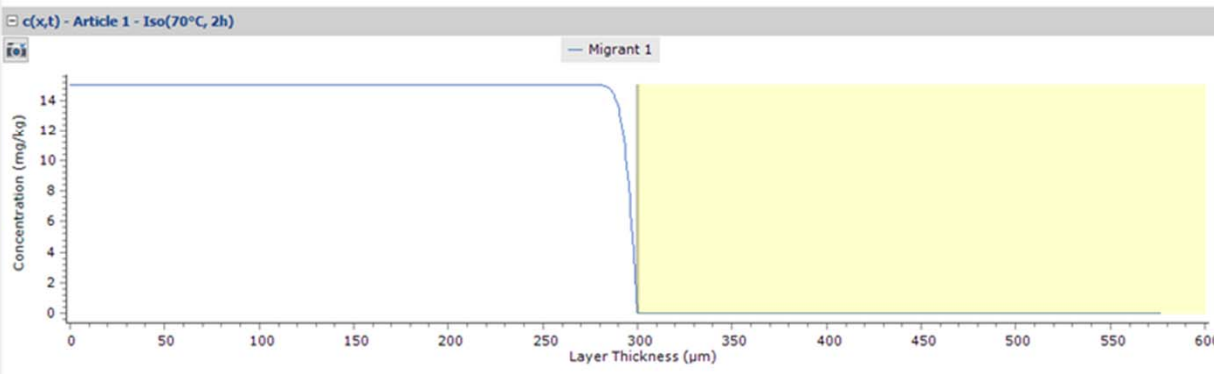
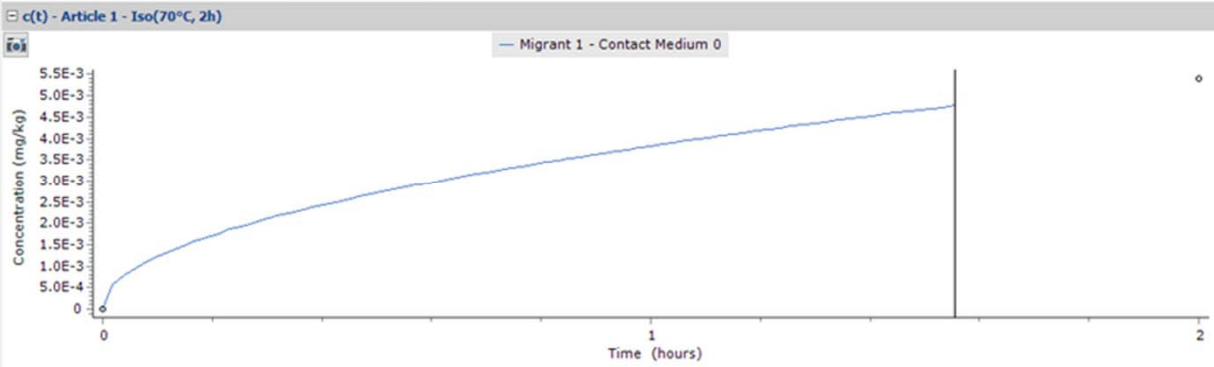
Package Properties Output Calculation

- Package SAN 24h at 40C optimized
 - Article 1
 - Iso(40°C, 1d)
- Package SAN 2h at 70C
 - Article 1
 - Iso(70°C, 2h)

Temperature: 70 (°C) Display unit: mg/kg c(t) : draw mean concentration c(t) : draw concentration at 0 % of thickness from surface

Grid

Article	Layer	Contact Med...
	Layer 1	Acetic acid 3%
	ACRYLONIT...	1.667E04
	Thickness (µm)	300
<input checked="" type="checkbox"/>	Migrant 1	ACRYLONIT... 0.0001



Package SAN 2h at 70C

Geometry: Rectangular

Contact Surface (cm²): 600

Volume of Contact Medium (cm³): 1000

Width (cm): 10

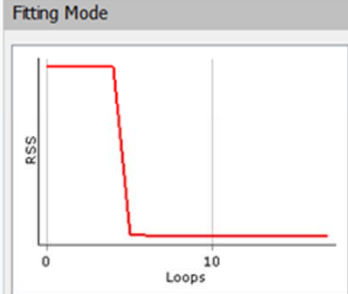
Height (cm): 10

Length (cm): 10

Surface and mass of contact medium by article

Articles	Surfaces (cm ²)	Mass (g)
Article 1	600	1000

Total surface of all articles (cm²): 600



Loops per serie: 20 Iterations: 17

mtau: 1

mtolg: 1E-6

mtolx: 1E-6 mrealstep: 1E-3

Parameter Name	Value
Layer 1-Op-Known(cm ² /s)	3.302E-11

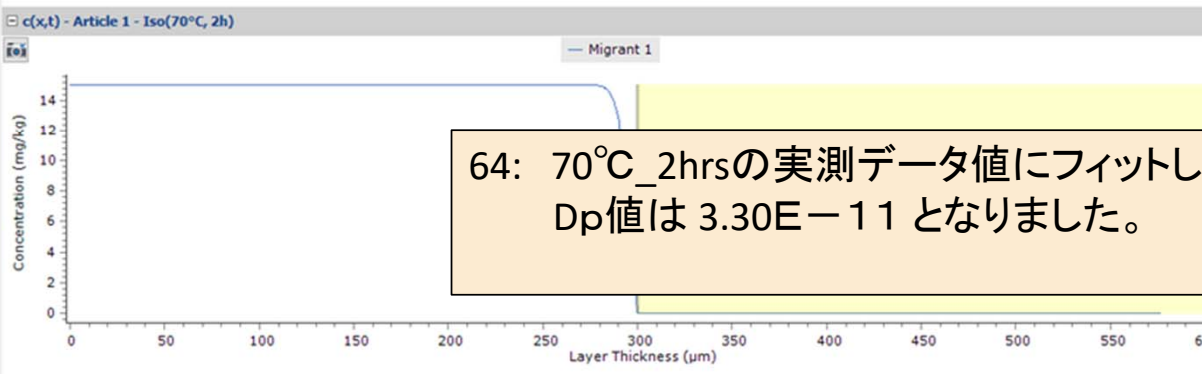
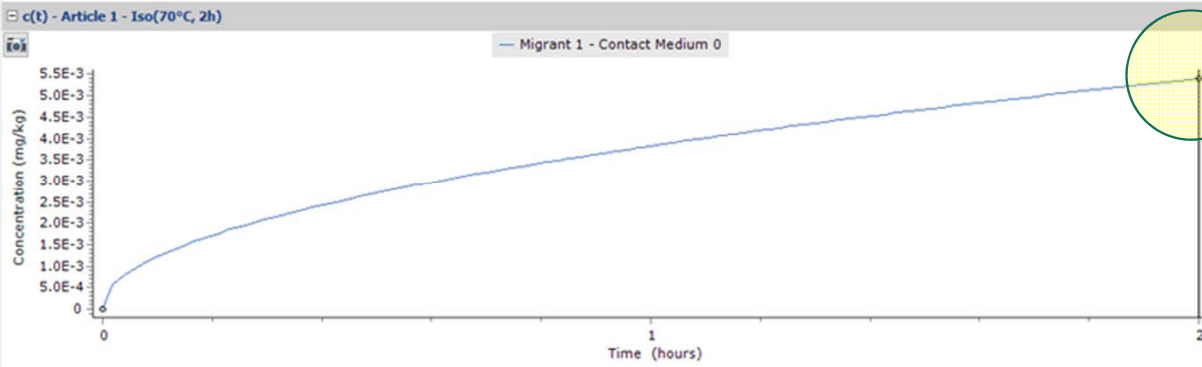
Package Properties Output Calculation

- Package SAN 24h at 40C optimized
 - Article 1
 - Iso(40°C, 1d)
- Package SAN 2h at 70C
 - Article 1
 - Iso(70°C, 2h)

Temperature : 70 (°C) Display unit mg/kg c(t) : draw mean concentration c(t) : draw concentration at 0 % of thickness from surface

Grid

Article	Layer 1	Contact Med...
	ACRYLONIT...	Acetic acid 3%
	Thickness (µm)	1.667E04
<input checked="" type="checkbox"/> Migrant 1	ACRYLONIT...	0.0001



Package SAN 2h at 70C

Geometry: Rectangular

Contact Surface (cm²): 600

Volume of Contact Medium (cm³): 1000

Width (cm): 10

Height (cm): 10

Length (cm): 10

Articles	Surfaces (cm ²)	Mass (g)
Article 1	600	1000

Total surface of all articles (cm²): 600

Fitting Mode

Loops per serie: 20 Iterations: 20

Correlation

mtau: 1

mtolg: 1E-6

mtolx: 1E-6 mrealstep: 1E-3

Parameter Name	Value
Layer 1-Dp-Known(cm ² /s)	3.302E-11

64: 70°C_2hrsの実測データ値にフィットした結果
Dp値は 3.30E-11 となりました。

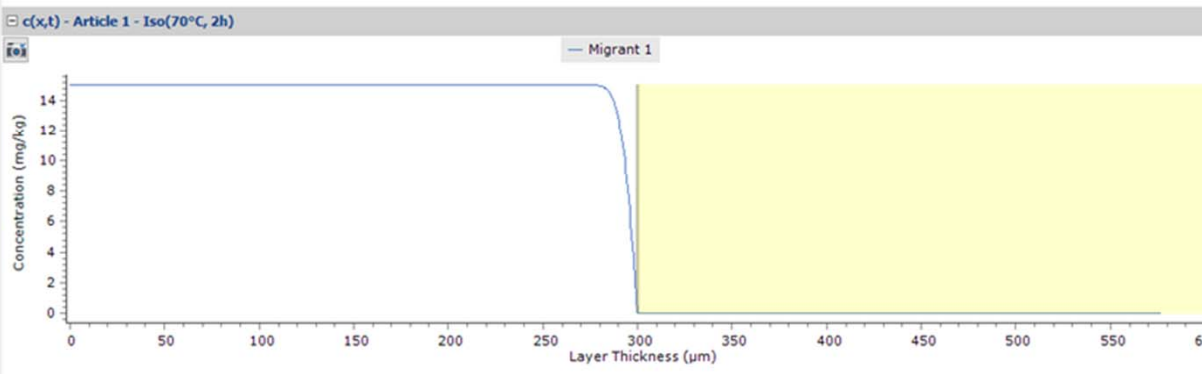
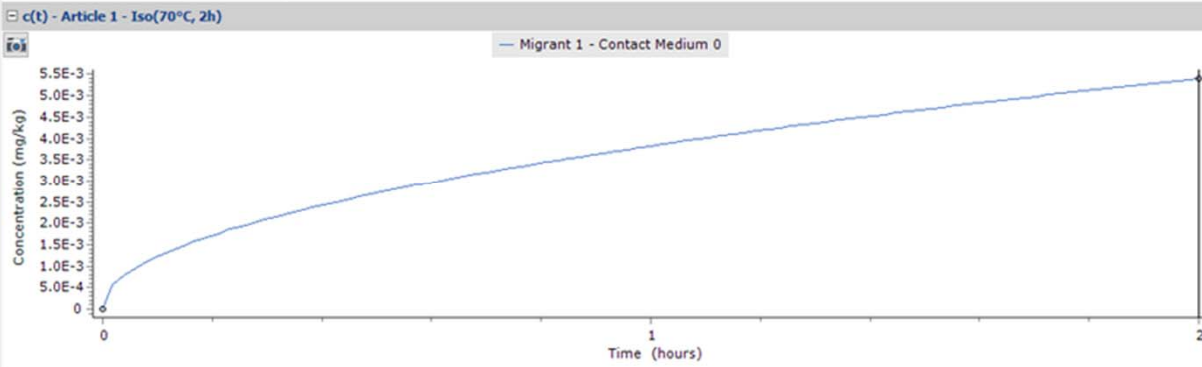
Package Properties Output Calculation

- Package SAN 24h at 40C optimized
 - Article 1
 - Iso(40°C, 1d)
- Package SAN 2h at 70C
 - Article 1
 - Iso(70°C, 2h)

Temperature : 70 (°C) Display unit : mg/kg c(t) : draw mean concentration c(t) : draw concentration at 0 % of thickness from surface

Grid

Article	Layer 1	Contact Med...
	ACRYLONIT...	Acetic acid 3%
	Thickness (µm)	1.667E04
<input checked="" type="checkbox"/>	Migrant 1	ACRYLONIT... 0.005379



Package SAN 2h at 70C

Geometry: Rectangular

Contact Surface (cm²): 600

Volume of Contact Medium (cm³): 1000

Width (cm): 10

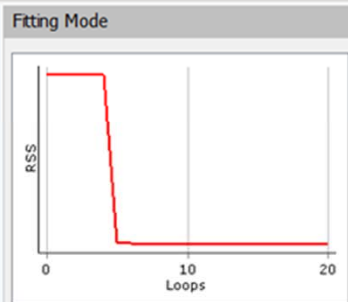
Height (cm): 10

Length (cm): 10

Surface and mass of contact medium by article

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

Total surface of all articles (cm²): 600



Loops per serie: 20 Iterations: 20

Correlation

mtau: 1

mtolg: 1E-6

mtolx: 1E-6 mrealstep: 1E-3

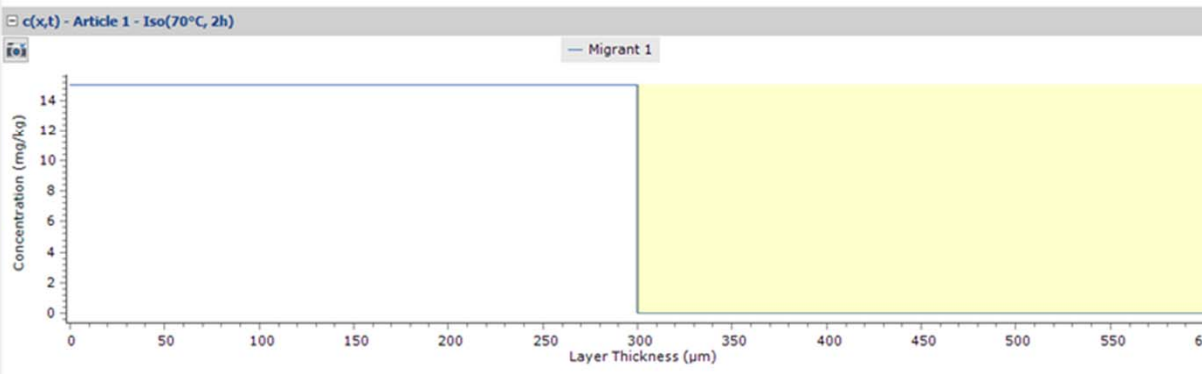
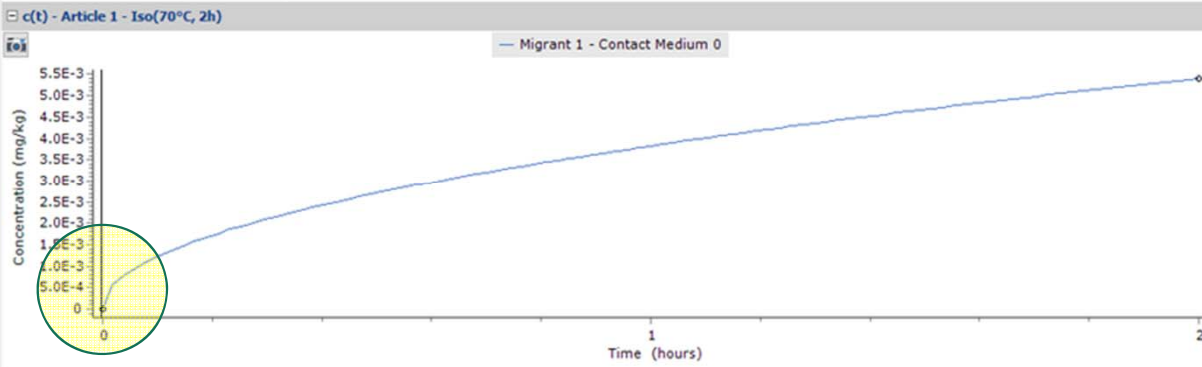
Parameter Name	Value
Layer 1-Op-Known(cm ² /s)	3.302E-11

Package Properties Output Calculation

- Package SAN 24h at 40C optimized
 - Article 1
 - Iso(40°C, 1d)
- Package SAN 2h at 70C
 - Article 1
 - Iso(70°C, 2h)

Temperature: 70 (°C) Display unit: mg/kg c(t) : draw mean concentration c(t) : draw concentration at 0 % of thickness from surface

Grid	Article	Layer 1	Contact Med...
		ACRYLONIT...	Acetic acid 3%
		Thickness (µm)	1.667E04
		300	
<input checked="" type="checkbox"/>	Migrant 1	ACRYLONIT...	3.62E-11



Package SAN 2h at 70C

Geometry: Rectangular

Contact Surface (cm²): 600

Volume of Contact Medium (cm³): 1000

Width (cm): 10

Height (cm): 10

Length (cm): 10

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

Total surface of all articles (cm²): 600

Fitting Mode

Loops per serie: 20 Iterations: 20

Correlation

mtau: 1

mtolg: 1E-6

mtolx: 1E-6 mrealstep: 1E-3

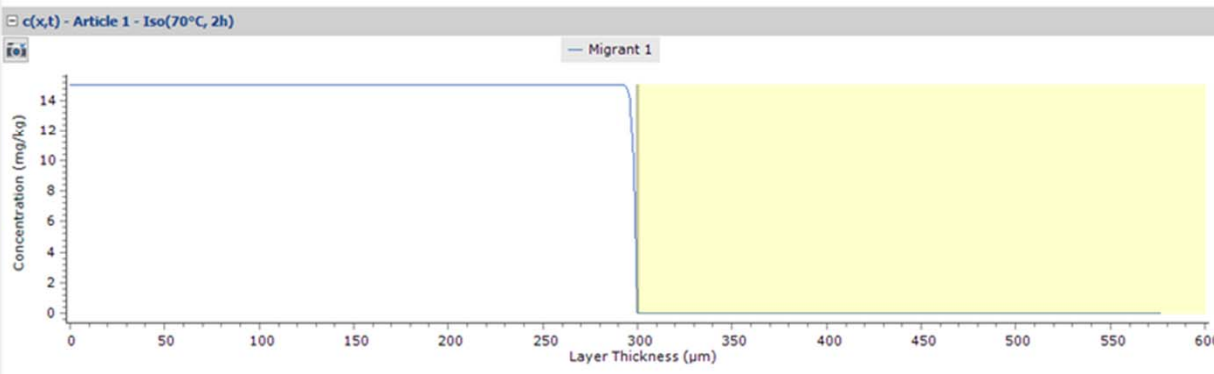
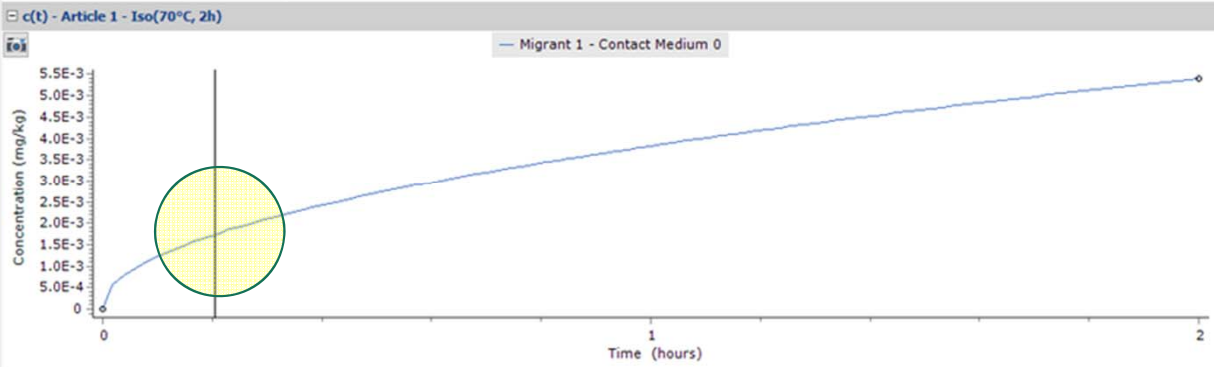
Parameter Name	Value
Layer 1-Op-Known(cm ² /s)	3.302E-11

Package Properties Output Calculation

- Package SAN 24h at 40C optimized
 - Article 1
 - Iso(40°C, 1d)
- Package SAN 2h at 70C
 - Article 1
 - Iso(70°C, 2h)

Temperature: 70 (°C) Display unit: mg/kg c(t) : draw mean concentration c(t) : draw concentration at 0 % of thickness from surface

Grid	Article	Layer 1	Contact Med...
		ACRYLONIT...	Acetic acid 3%
		Thickness (µm)	1.667E04
		300	
<input checked="" type="checkbox"/>	Migrant 1	ACRYLONIT...	0.001766



Package SAN 2h at 70C

Geometry: Rectangular

Contact Surface (cm²): 600

Volume of Contact Medium (cm³): 1000

Width (cm): 10

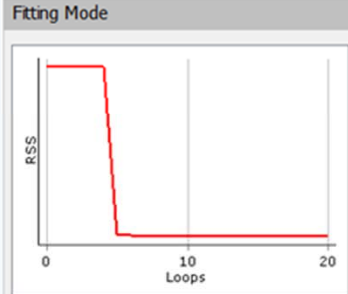
Height (cm): 10

Length (cm): 10

Surface and mass of contact medium by article

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

Total surface of all articles (cm²): 600



Loops per serie: 20 Iterations: 20

Correlation

mtau: 1

mtolg: 1E-6

mtolx: 1E-6 mrealstep: 1E-3

Parameter Name	Value
Layer 1-Op-Known(cm ² /s)	3.302E-11

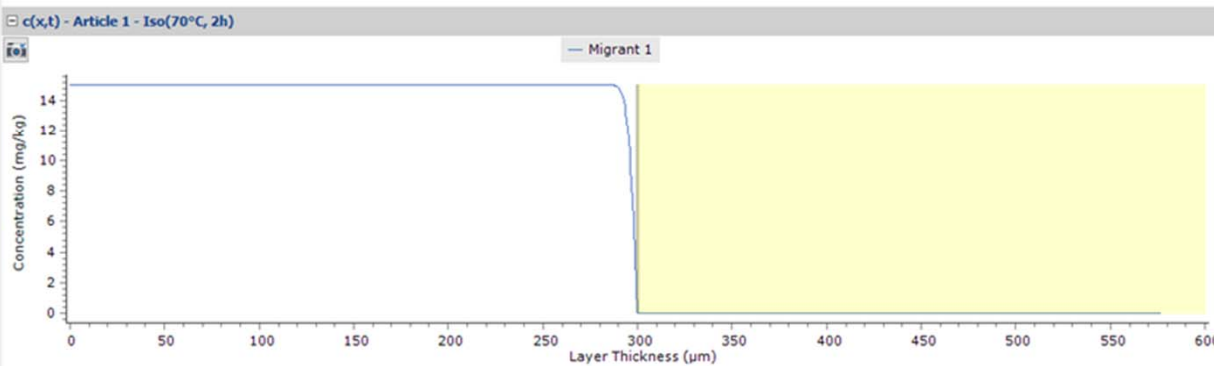
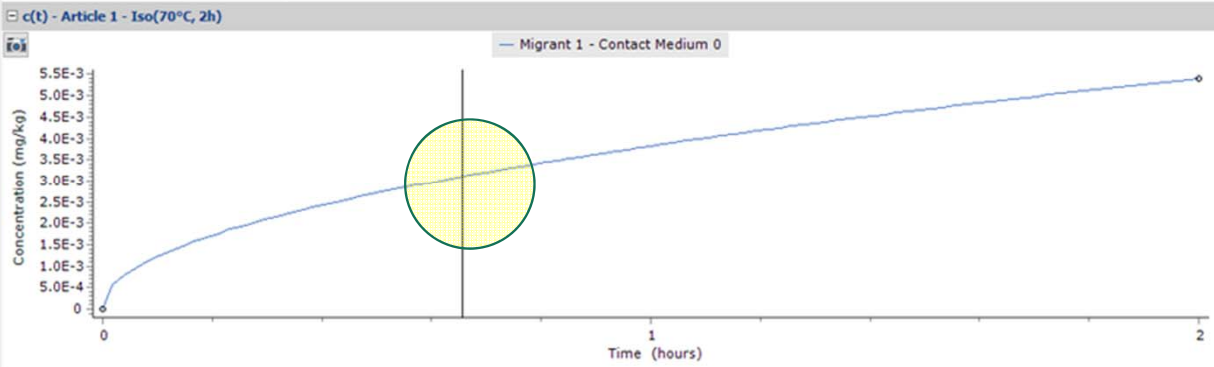
Package Properties Output Calculation

- Package SAN 24h at 40C optimized
 - Article 1
 - Iso(40°C, 1d)
- Package SAN 2h at 70C
 - Article 1
 - Iso(70°C, 2h)

Temperature: 70 (°C) Display unit: mg/kg c(t) : draw mean concentration c(t) : draw concentration at 0 % of thickness from surface

Grid

Article	Layer 1	Contact Med...
	ACRYLONIT...	Acetic acid 3%
	Thickness (µm)	1.667E04
	300	
<input checked="" type="checkbox"/>	Migrant 1	ACRYLONIT... 0.003108



Package SAN 2h at 70C

Geometry: Rectangular

Contact Surface (cm²): 600

Volume of Contact Medium (cm³): 1000

Width (cm): 10

Height (cm): 10

Length (cm): 10

Articles	Surfaces (cm ²)	Mass (g)
Article 1	600	1000

Total surface of all articles (cm²): 600

Fitting Mode

Loops per serie: 20 Iterations: 20

Correlation

mtau: 1

mtolg: 1E-6

mtolx: 1E-6 mrealstep: 1E-3

Parameter Name	Value
Layer 1-Op-Known(cm ² /s)	3.302E-11

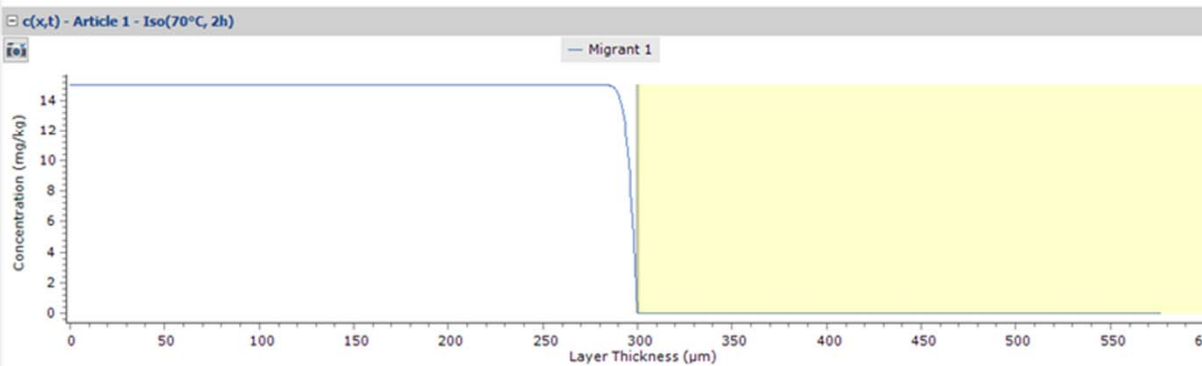
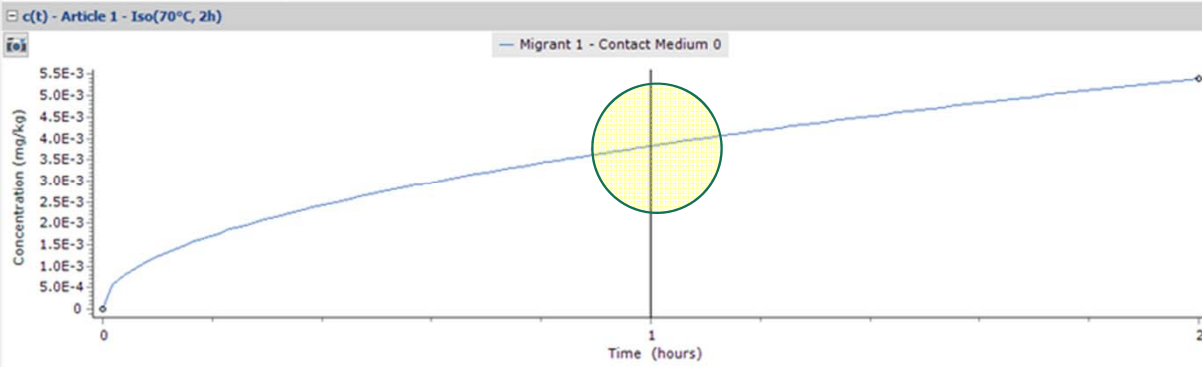
Package Properties Output Calculation

- Package SAN 24h at 40C optimized
 - Article 1
 - Iso(40°C, 1d)
- Package SAN 2h at 70C
 - Article 1
 - Iso(70°C, 2h)

Temperature: 70 (°C) Display unit: mg/kg c(t) : draw mean concentration c(t) : draw concentration at 0 % of thickness from surface

Grid

Article	Layer 1	Contact Med...
	ACRYLONIT...	Acetic acid 3%
	Thickness (µm)	1.667E04
	300	
<input checked="" type="checkbox"/> Migrant 1	ACRYLONIT...	0.003825



Package SAN 2h at 70C

Geometry: Rectangular

Contact Surface (cm²): 600

Volume of Contact Medium (cm³): 1000

Width (cm): 10

Height (cm): 10

Length (cm): 10

Surface and mass of contact medium by article

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

Total surface of all articles (cm²): 600

Fitting Mode

Loops per serie: 20 Iterations: 20

Correlation

mtau: 1

mtolg: 1E-6

mtolx: 1E-6 mrealstep: 1E-3

Parameter Name	Value
Layer 1-Op-Known(cm ² /s)	3.302E-11

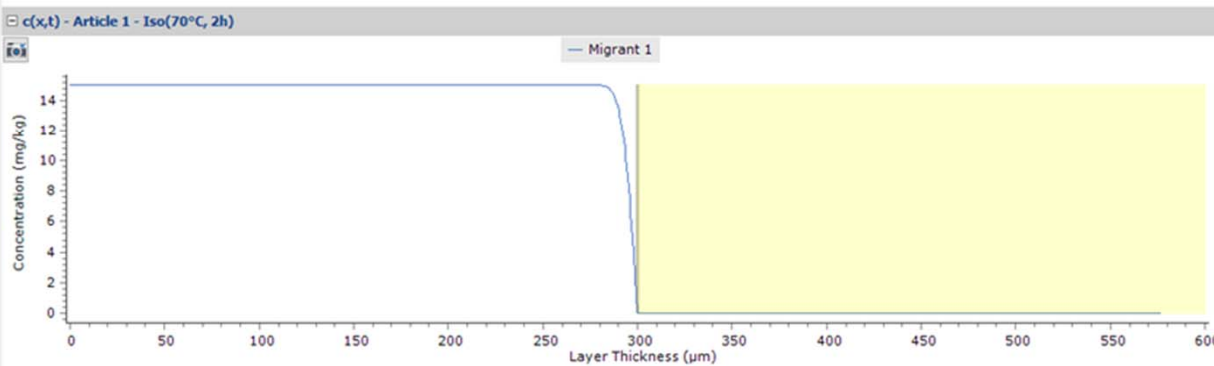
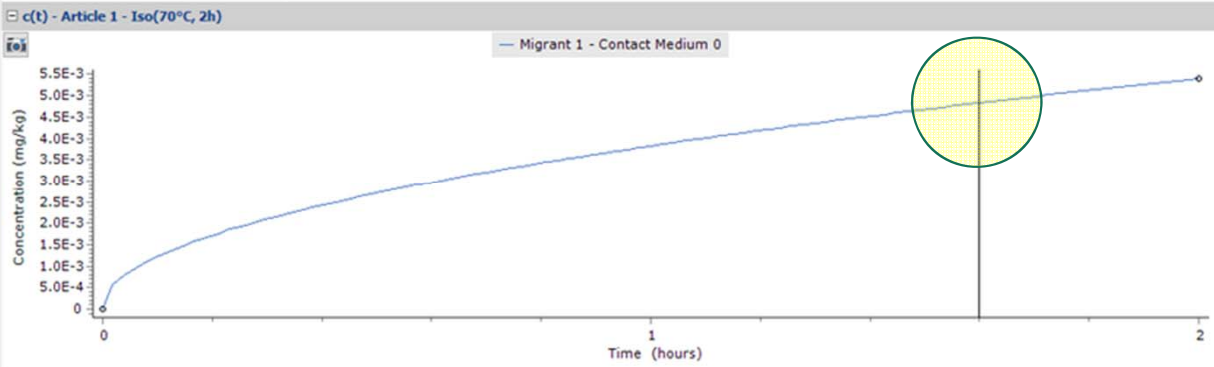
Package Properties Output Calculation

- Package SAN 24h at 40C optimized
 - Article 1
 - Iso(40°C, 1d)
- Package SAN 2h at 70C
 - Article 1
 - Iso(70°C, 2h)

Temperature: 70 (°C) Display unit: mg/kg c(t) : draw mean concentration c(t) : draw concentration at 0 % of thickness from surface

Grid

Article	Layer	Contact Med...
	Layer 1	ACRYLONIT... Acetic acid 3%
	Thickness (µm)	300 1.667E04
<input checked="" type="checkbox"/>	Migrant 1	ACRYLONIT... 0.004831



Package SAN 2h at 70C

Geometry: Rectangular

Contact Surface (cm²): 600

Volume of Contact Medium (cm³): 1000

Width (cm): 10

Height (cm): 10

Length (cm): 10

Articles	Surfaces (cm ²)	Mass (g)
Article 1	600	1000

Total surface of all articles (cm²): 600

Fitting Mode

Loops per serie: 20 Iterations: 20

Correlation

mtau: 1

mtolg: 1E-6

mtolx: 1E-6 mrealstep: 1E-3

Parameter Name	Value
Layer 1-Op-Known(cm ² /s)	3.302E-11

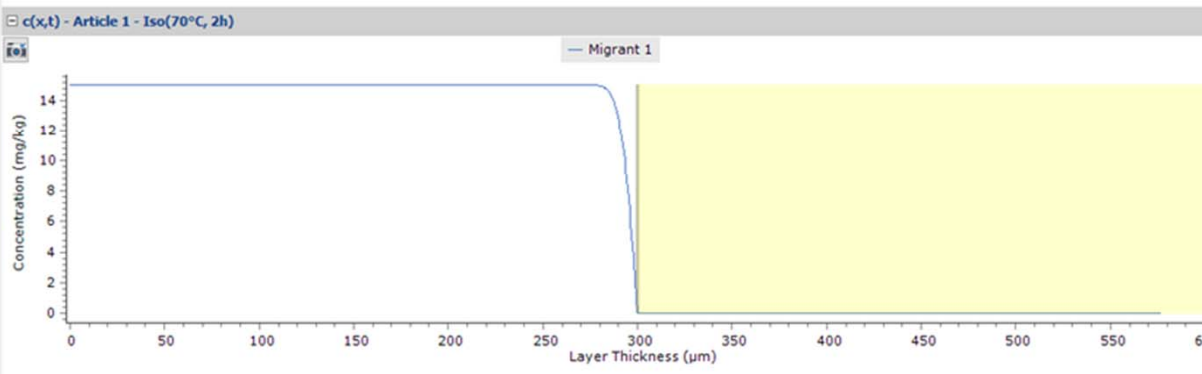
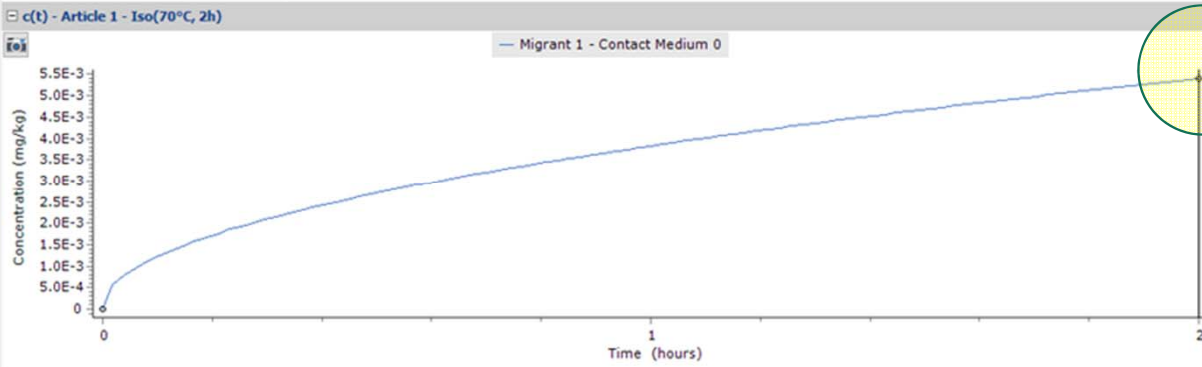
2023/7/2

Package Properties Output Calculation

- Package SAN 24h at 40C optimized
 - Article 1
 - Iso(40°C, 1d)
- Package SAN 2h at 70C
 - Article 1
 - Iso(70°C, 2h)

Temperature: 70 (°C) Display unit: mg/kg c(t) : draw mean concentration c(t) : draw concentration at 0 % of thickness from surface

Grid	Article	Layer 1	Contact Med...
		ACRYLONIT...	Acetic acid 3%
		Thickness (µm)	1.667E04
		300	
<input checked="" type="checkbox"/>	Migrant 1	ACRYLONIT...	0.0054



Package SAN 2h at 70C

Geometry: Rectangular

Contact Surface (cm²): 600

Volume of Contact Medium (cm³): 1000

Width (cm): 10

Height (cm): 10

Length (cm): 10

Fitting Mode

Loops per serie: 20 Iterations: 20

Correlation

mtau: 1

mtolg: 1E-6

mtolx: 1E-6 mrealstep: 1E-3

Parameter Name	Value
Layer 1-Op-Known(cm ² /s)	3.302E-11

Package Properties

Output Calculation

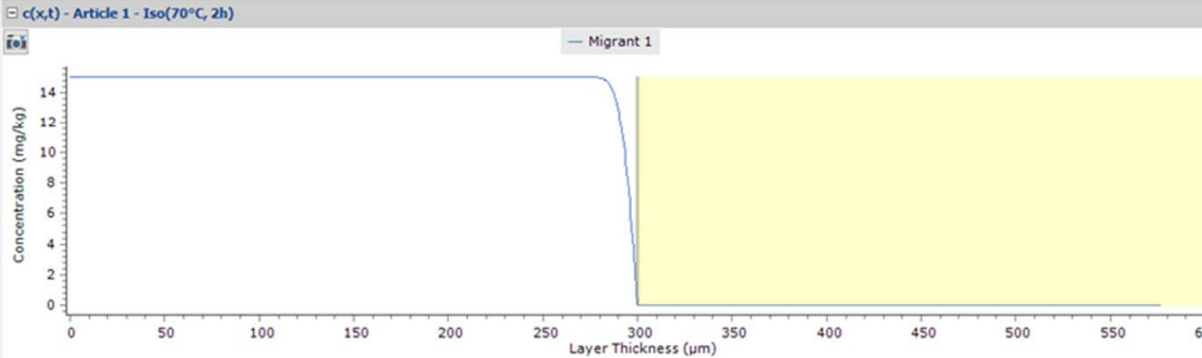
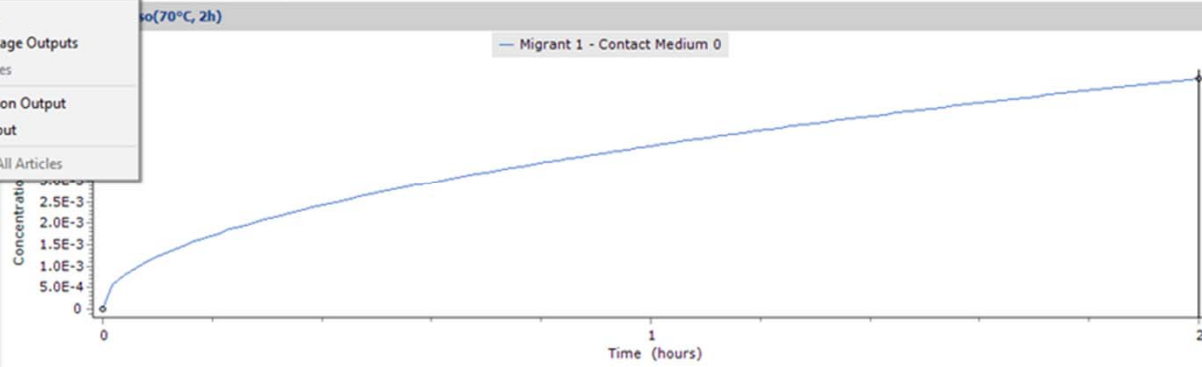
- New Package
- Open Package
- Save Package
- Duplicate Package
- Close Package
- Save Package As
- Save All Packages
- Package Details

- New Article
- Open Article
- Import Article
- Save Article
- Duplicate Article
- Close Article
- Import Initial Concentration
- Prediction on This Article
- Prediction on All Articles
- Close All Articles
- Delete All Article Outputs
- Close All

- Package SAN 24h at 40C optimized
 - Article 1
- Package SAN 2h at 70C
 - Article 1

Temperature: 70 (°C) Display unit: mg/kg $c(t)$: draw mean concentration $c(t)$: draw concentration at 0 % of thickness from surface

Layer	Material	Thickness (µm)	Contact Med...
Layer 1	ACRYLONIT...	300	Acetic acid 3%
	ACRYLONIT...		0.0054



Package SAN 2h at 70C

Geometry: Rectangular

Contact Surface (cm²): 600

Volume of Contact Medium (cm³): 1000

Width (cm): 10

Height (cm): 10

Length (cm): 10

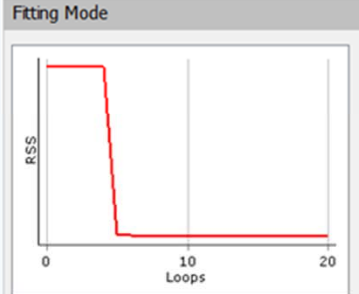
Add Article

Surface and mass of contact medium by article

Articles	Surfaces (cm ²)	Mass (g)
Article 1	600	1000

Total surface of all articles (cm²): 600

Switch Package in Fitting Mode



Loops per serie: 20 Iterations: 20

Optimize Refresh

Correlation

mtau: 1

mtolg: 1E-6

mtolx: 1E-6 mrealstep: 1E-3

Parameter Name	Value
Layer 1-Op-Known(cm ² /s)	3.302E-11

Close Fitting Mode for This Package

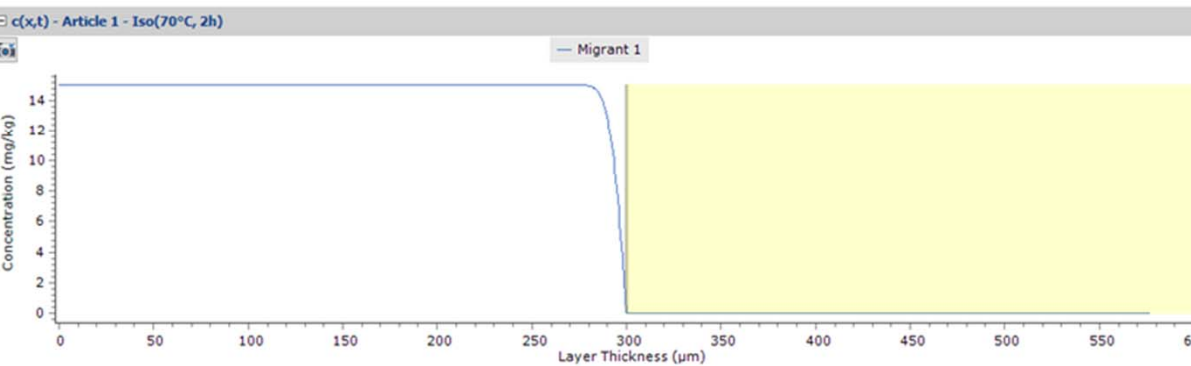
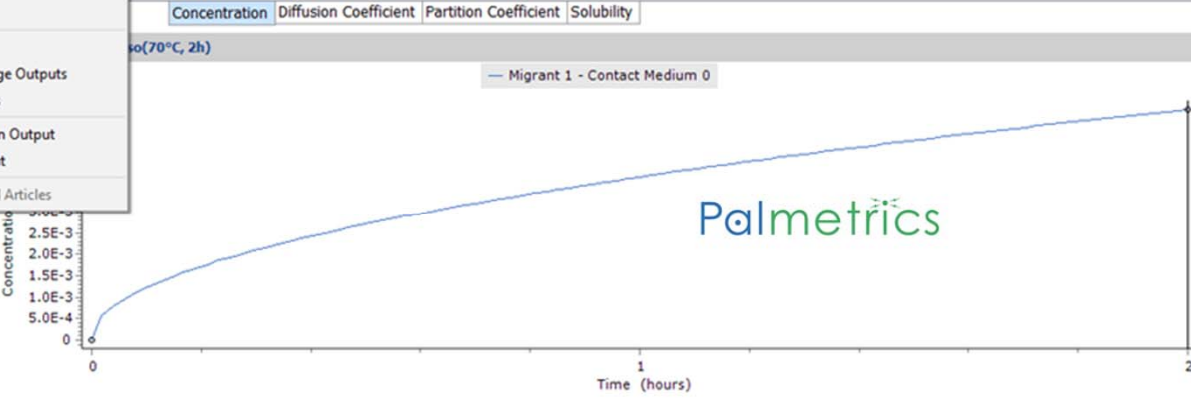
Create Global Package

Package Properties Output Calculation

- Package SAN 24h at 40C optimized
 - Article 1
 - Iso(40°C, 1d)
- Package SAN 2h at 70C
 - Article 1
 - Iso(70°C)

c(t) : draw mean concentration
 c(t) : draw concentration at 0 % of thickness from surface

Layer	Material	Thickness (µm)	Contact Med...
Layer 1	ACRYLONIT...	300	Acetic acid 3%
	ACRYLONIT...		1.667E04
			0.0054



Package SAN 2h at 70C

Geometry: Rectangular

Contact Surface (cm²): 600

Volume of Contact Medium (cm³): 1000

Width (cm): 10

Height (cm): 10

Length (cm): 10

Surface and mass of contact medium by article

Articles	Surfaces (cm ²)	Mass (g)
Article 1	600	1000

Total surface of all articles (cm²): 600

Fitting Mode

Loops per serie: 20

Iterations: 20

Optimize Refresh

Correlation

mtau: 1

mtolg: 1E-6

mtolx: 1E-6 mrealstep: 1E-3

Parameter Name	Value
Layer 1-Op-Known(cm ² /s)	3.302E-11

Close Fitting Mode for This Package

Create Global Package

2023/7/2

Save As

This PC > Desktop > example fitting

Organise New folder

Name	Date modified	Type	Size
Package SAN 24h at 40C.sml	02.09.2022 14:37	SML File	2 KB
Package SAN 24h at 40C optimized.sml	02.09.2022 15:01	SML File	106 KB

File name: Package SAN 2h at 70C.sml

Save as type: SML v5 (*.sml)

Save Cancel



Palmetrics

AN 2h at 70C

Surface (cm²): 600

Contact Medium (cm³): 1000

Loops per serie: 20

Iterations: 20

Optimize Refresh

Correlation

mtau: 1

mtolg: 1E-6

mtolx: 1E-6 mrealstep: 1E-3

Parameter Name	Value
Layer 1-Op-Known(cm ² /s)	3.302E-11

Close Fitting Mode for This Package

Create Global Package

115

2023/7/2

Save As

This PC > Desktop > example fitting

Organise New folder

Name	Date modified	Type	Size
Package SAN 24h at 40C.sml	02.09.2022 14:37	SML File	2 KB
Package SAN 24h at 40C optimized.sml	02.09.2022 15:01	SML File	106 KB

File name: Package SAN 2h at 70C Optimized.sml

Save as type: SML v5 (*.sml)

Save Cancel

Palmetrics

AN 2h at 70C

Surface (cm²): 600

Contact Medium (cm³): 1000

Loops per serie: 20 Iterations: 20

Optimize Refresh

Correlation

mtau: 1

mtolg: 1E-6

mtolx: 1E-6 mrealstep: 1E-3

Parameter Name	Value
Layer 1-Op-Known(cm ² /s)	3.302E-11

Close Fitting Mode for This Package

Create Global Package

116



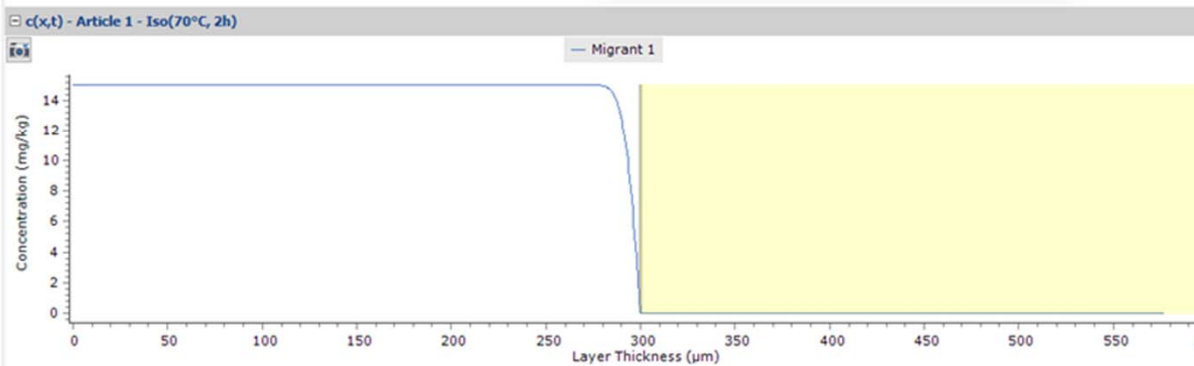
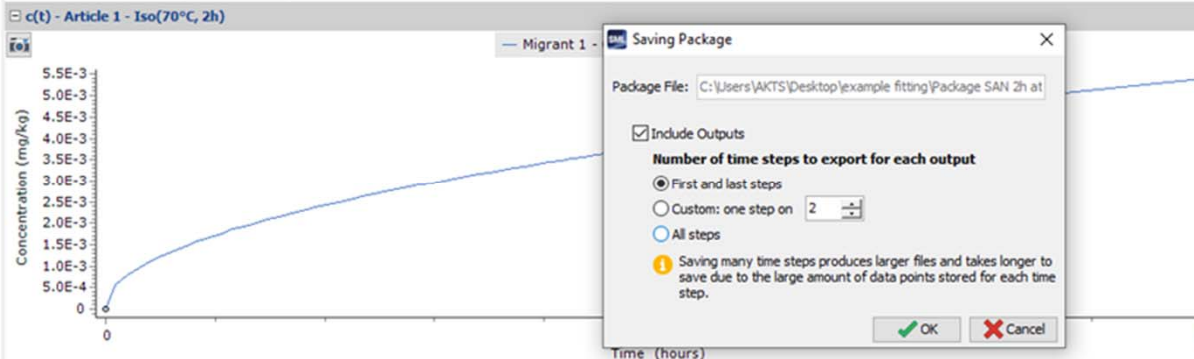
2023/7/2

Package Properties Output Calculation

- Package SAN 24h at 40C optimized
 - Article 1
 - Iso(40°C, 1d)
- Package SAN 2h at 70C Optimized
 - Article 1
 - Iso(70°C, 2h)

Temperature: 70 (°C) Display unit: mg/kg c(t) : draw mean concentration c(t) : draw concentration at 0 % of thickness from surface

Grid	Article	Layer 1	Contact Med...
		ACRYLONIT...	Acetic acid 3%
		Thickness (µm)	1.667E04
		300	
<input checked="" type="checkbox"/>	Migrant 1	ACRYLONIT...	0.0054



Package SAN 2h at 70C

Geometry: Rectangular

Contact Surface (cm²): 600

Volume of Contact Medium (cm³): 1000

Width (cm): 10

Height (cm): 10

Length (cm): 10

Surface and mass of contact medium by article

Articles	Surfaces (cm ²)	Mass (g)
Article 1	600	1000

Total surface of all articles (cm²): 600

Fitting Mode

Loops per serie: 20 Iterations: 20

Correlation

mtau: 1

mtolg: 1E-6

mtolx: 1E-6 mrealstep: 1E-3

Parameter Name	Value
Layer 1-Op-Known(cm ² /s)	3.302E-11

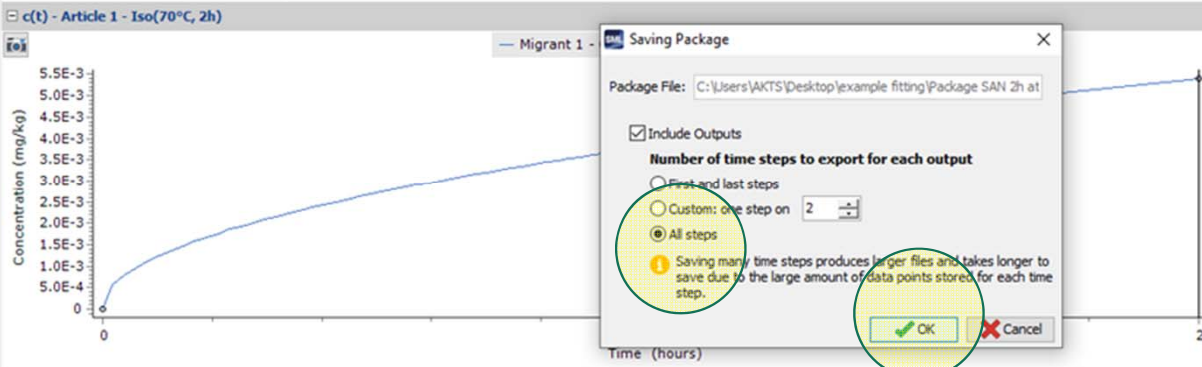
Package Properties Output Calculation

- Package SAN 2h at 40C optimized
 - Article 1
 - Iso(40°C, 1d)
- Package SAN 2h at 70C Optimized
 - Article 1
 - Iso(70°C, 2h)

Temperature: 70 (°C) Display unit: mg/kg c(t) : draw mean concentration c(t) : draw concentration at 0 % of thickness from surface

Grid	Article	Layer 1	Contact Med...
		ACRYLONIT...	Acetic acid 3%
		Thickness (µm)	1.667E04
		300	
<input checked="" type="checkbox"/>	Migrant 1	ACRYLONIT...	0.0054

Concentration Diffusion Coefficient Partition Coefficient Solubility



Saving Package

Package File: C:\Users\AKTS\Desktop\example fitting\Package SAN 2h at

Include Outputs

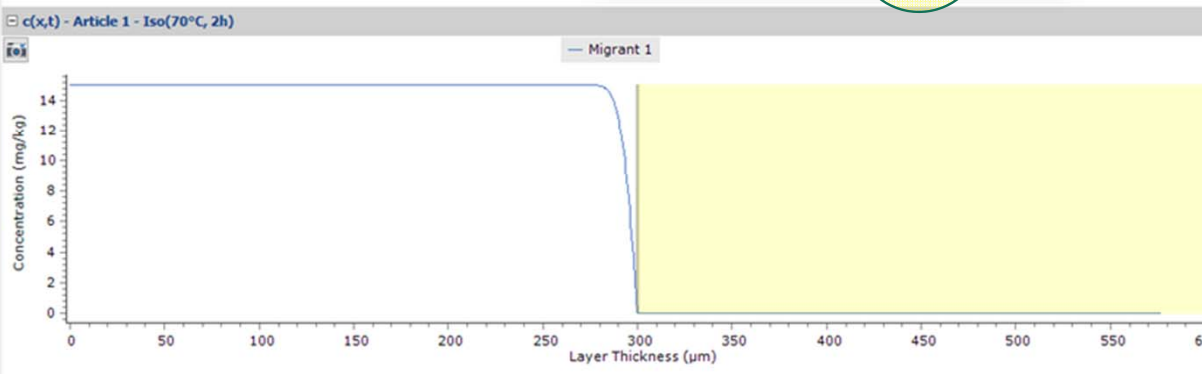
Number of time steps to export for each output

First and last steps

Custom: one step on 2

All steps

Saving many time steps produces larger files and takes longer to save due to the large amount of data points stored for each time step.



Package SAN 2h at 70C

Geometry: Rectangular

Contact Surface (cm²): 600

Volume of Contact Medium (cm³): 1000

Width (cm): 10

Height (cm): 10

Length (cm): 10

Surface and mass of contact medium by article

Articles	Surfaces (cm ²)	Mass (g)
Article 1	600	1000

Total surface of all articles (cm²): 600

Fitting Mode

Loops per serie: 20 Iterations: 20

Correlation

mtau: 1

mtolg: 1E-6

mtolx: 1E-6 mrealstep: 1E-3

Parameter Name	Value
Layer 1-Op-Known(cm ² /s)	3.302E-11

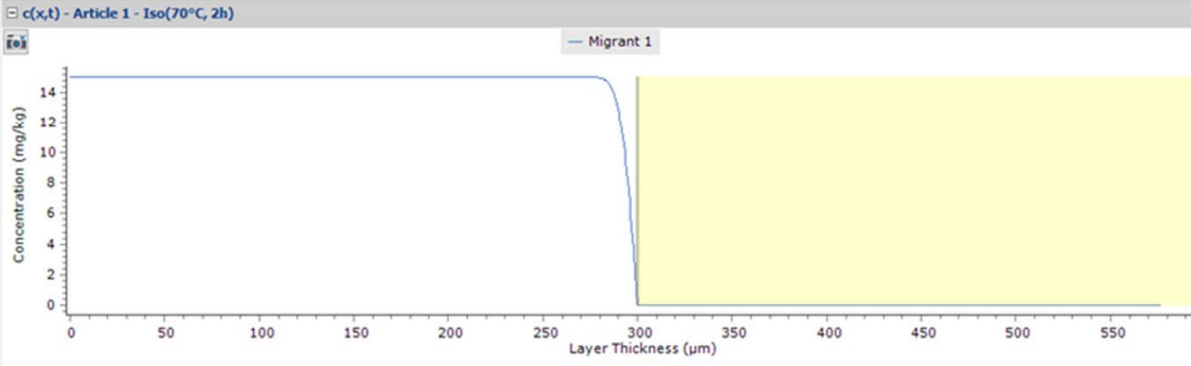
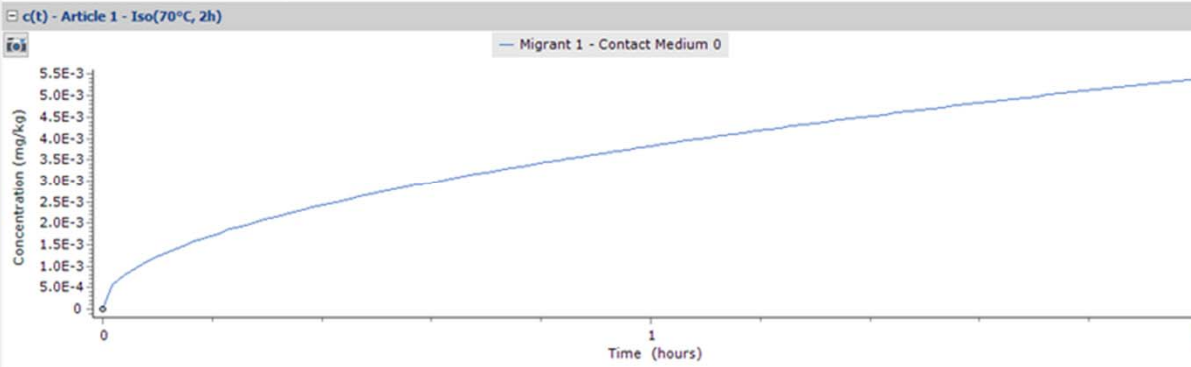
Package Properties Output Calculation

- Package SAN 24h at 40C optimized
 - Article 1
 - Iso(40°C, 1d)
- Package SAN 2h at 70C Optimized
 - Article 1
 - Iso(70°C, 2h)

c(t) : draw mean concentration
 c(t) : draw concentration at 0 % of thickness from surface

Grid

Article	Layer 1	Contact Med...
	ACRYLONIT...	Acetic acid 3%
	Thickness (µm)	1.667E04
<input checked="" type="checkbox"/>	Migrant 1	ACRYLONIT... 0.0054



Package SAN 2h at 70C Optimized

Geometry: Rectangular

Contact Surface (cm²): 600

Volume of Contact Medium (cm³): 1000

Width (cm): 10

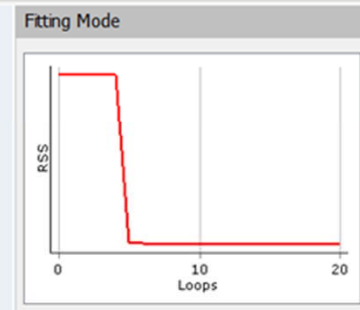
Height (cm): 10

Length (cm): 10

Surface and mass of contact medium by article

Articles	Surfaces (cm ²)	Mass (g)
Article 1	600	1000

Total surface of all articles (cm²): 600



Loops per serie: 20 Iterations: 20

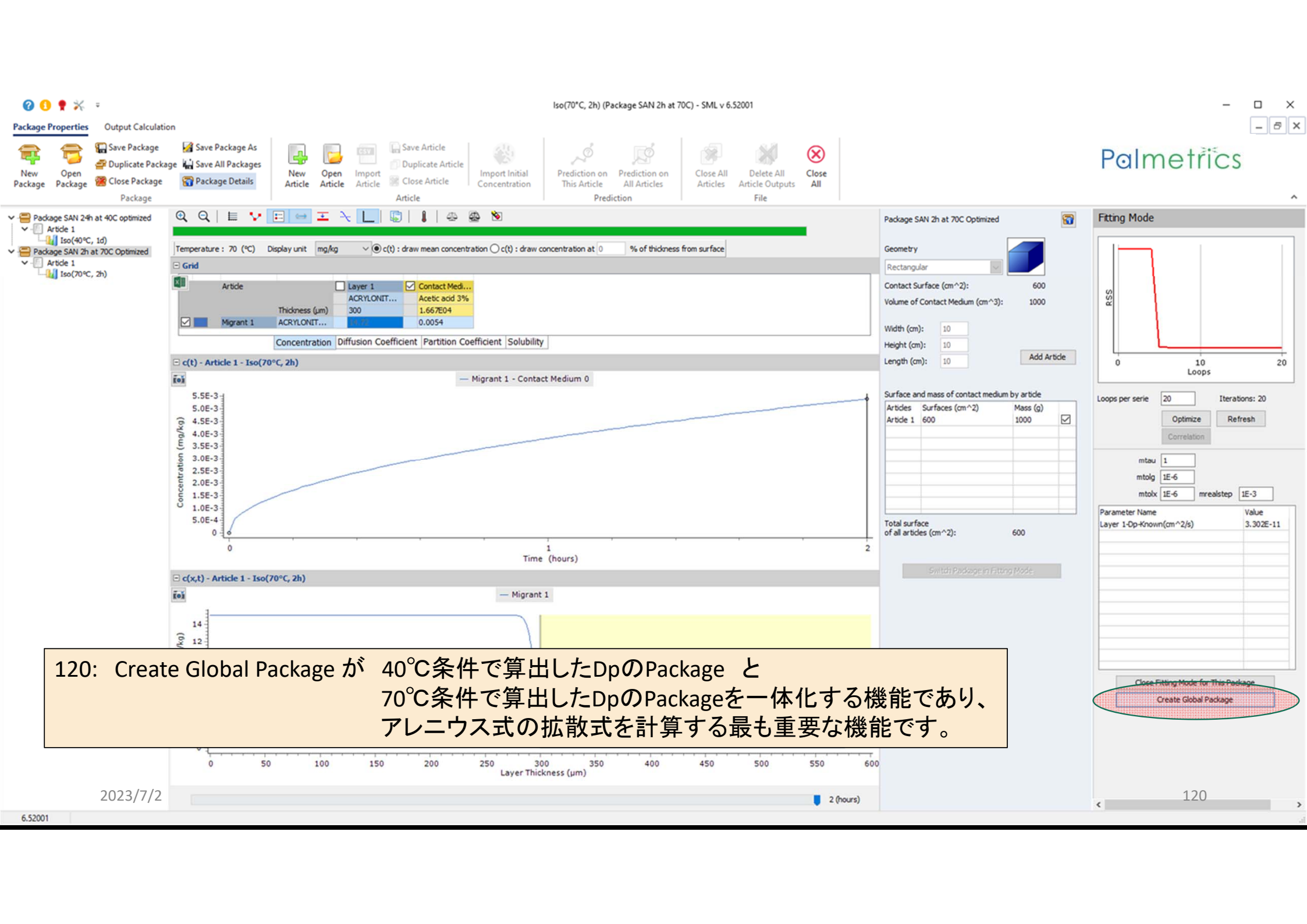
Correlation

mtau: 1

mtolg: 1E-6

mtolx: 1E-6 mrealstep: 1E-3

Parameter Name	Value
Layer 1-Op-Known(cm ² /s)	3.302E-11



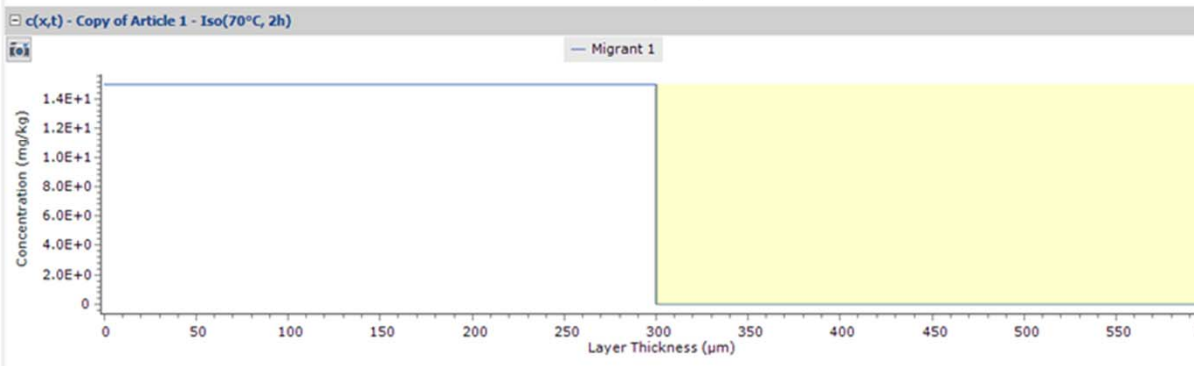
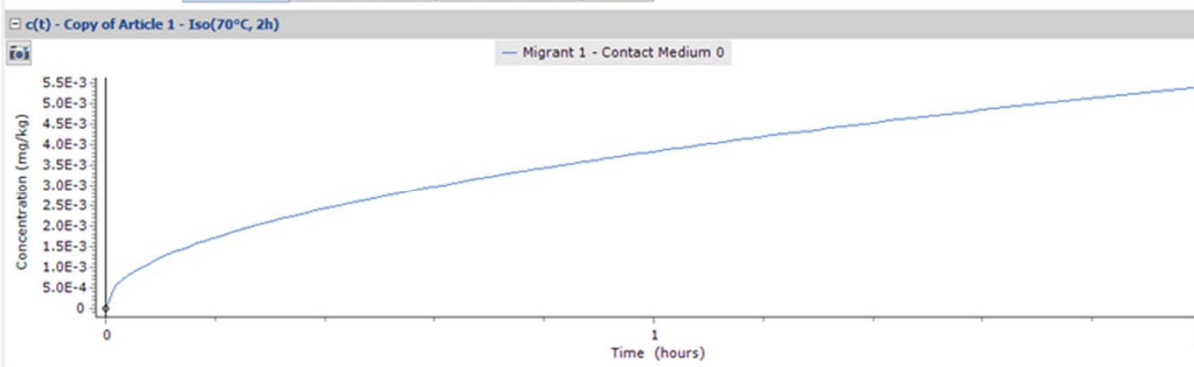
120: Create Global Package が 40°C条件で算出したDpのPackage と 70°C条件で算出したDpのPackageを一体化する機能であり、アレニウス式の拡散式を計算する最も重要な機能です。

Package Properties Output Calculation

- Package SAN 24h at 40C optimized
 - Article 1
 - Iso(40°C, 1d)
- Package SAN 2h at 70C Optimized
 - Article 1
 - Iso(70°C, 2h)
- Copy of Package SAN 24h at 40C optir
 - Copy of Article 1
 - Iso(40°C, 1d)
 - Iso(70°C, 2h)

Temperature: 70 (°C) Display unit: mg/kg c(t) : draw mean concentration c(t) : draw concentration at 0 % of thickness from surface

Article	Layer 1	Contact Med...
1. Migrant 1	ACRYLONIT...	Acetic acid 3%
	Thickness (µm)	1.667E04
		0



Copy of Package SAN 24h at 40C optimized

Geometry: Rectangular

Contact Surface (cm²): 600
Volume of Contact Medium (cm³): 1000

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

Surface and mass of contact medium by article

Articles	Surfaces (cm ²)	Mass (g)
Copy o...	600	1000

Total surface of all articles (cm²): 600

Fitting Mode

Loops per serie: 20 Iterations: 20

Optimize Refresh

Correlation

mtau: 1
mtolg: 1E-6
mtolx: 1E-6 mrealstep: 1E-3

Parameter Name	Value
Layer 1-Dp-Arrhenius-E(kJ/mol)	69.767
Layer 1-Dp-Arrhenius-A(cm ² /s)	1.378

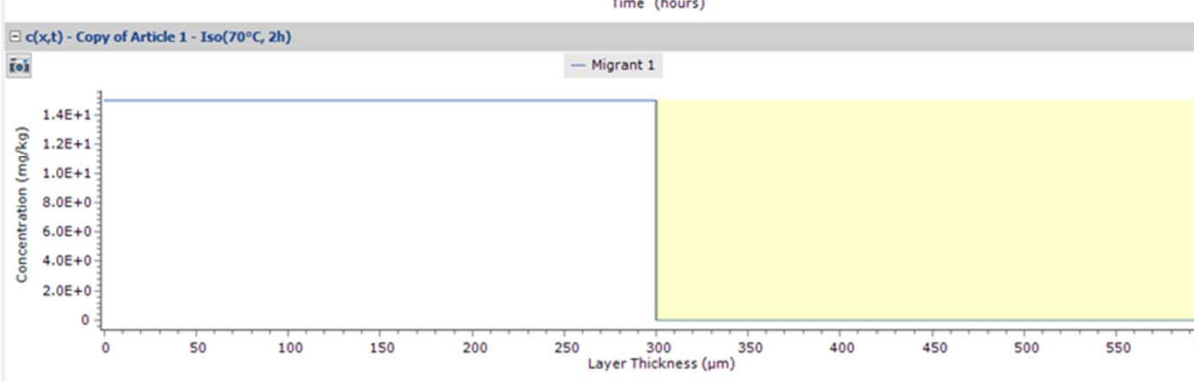
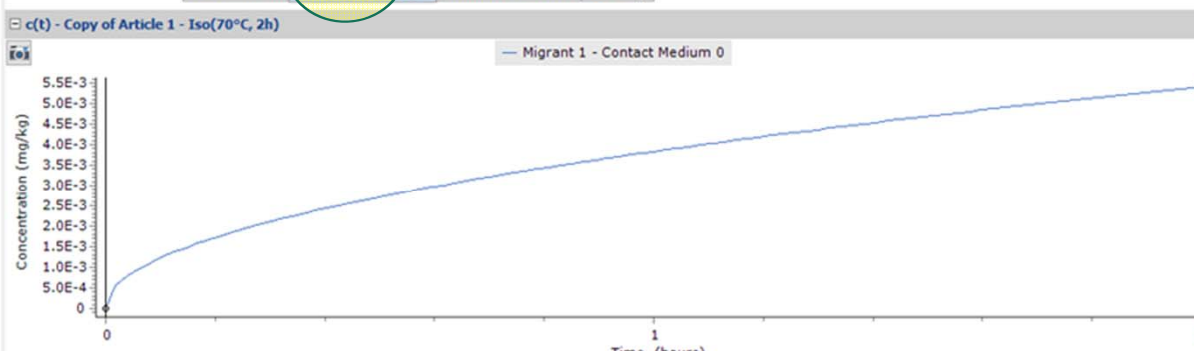
Close Fitting Mode for This Package
Create Global Package

Package Properties Output Calculation

- Package SAN 24h at 40C optimized
 - Article 1
 - Iso(40°C, 1d)
- Package SAN 2h at 70C Optimized
 - Article 1
 - Iso(70°C, 2h)
- Copy of Package SAN 24h at 40C optir
 - Copy of Article 1
 - Iso(40°C, 1d)
 - Iso(70°C, 2h)

c(t) : draw mean concentration
 c(t) : draw concentration at 0 % of thickness from surface

Article	Layer 1	Contact Med...
1. Migrant 1	ACRYLONIT... Thickness (µm) 300	Acetic acid 3% 1.667E04
	ACRYLONIT... A(3.302E-11)	0.0001



Copy of Package SAN 24h at 40C optimized

Geometry: Rectangular

Contact Surface (cm²): 600

Volume of Contact Medium (cm³): 1000

Width (cm): 10

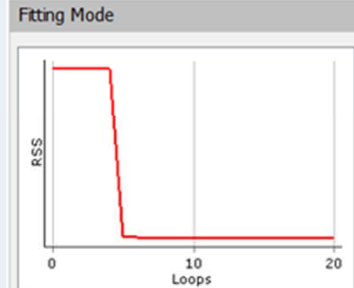
Height (cm): 10

Length (cm): 10

Surface and mass of contact medium by article

Articles	Surfaces (cm ²)	Mass (g)
Copy o...	600	1000

Total surface of all articles (cm²): 600



Loops per serie: 20

Iterations: 20

Correlation

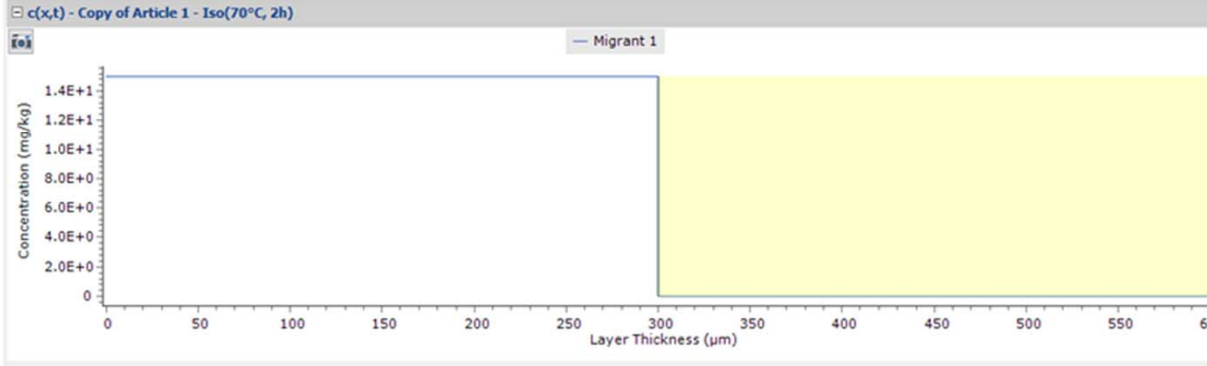
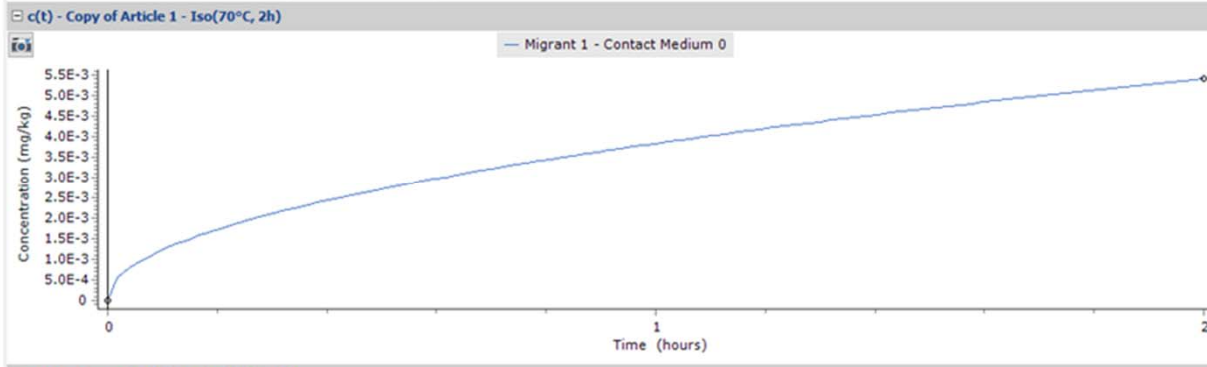
Parameter Name	Value
Layer 1-Dp-Arrhenius-E(kJ/mol)	69.767
Layer 1-Dp-Arrhenius-A(cm ² /s)	1.378

Package Properties Output Calculation

- Package SAN 24h at 40C optimized
 - Article 1
 - Iso(40°C, 1d)
- Package SAN 2h at 70C Optimized
 - Article 1
 - Iso(70°C, 2h)
- Copy of Package SAN 24h at 40C optir
 - Copy of Article 1
 - Iso(40°C, 1d)
 - Iso(70°C, 2h)

Temperature: 70 (°C) Display unit: mg/kg c(t): draw mean concentration c(t): draw concentration at 0 % of thickness from surface

Article	Layer 1	Contact Med...
	ACRYLONIT...	Acetic acid 3%
	Thickness (µm)	1.667E04
	300	
<input checked="" type="checkbox"/> 1. Migrant 1	ACRYLONIT...	0.0001
	A(3.302E-11)	



Copy of Package SAN 24h at 40C optimized

Geometry: Rectangular

Contact Surface (cm²): 600

Volume of Contact Medium (cm³): 1000

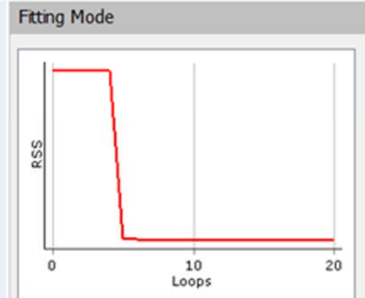
Width (cm): 10

Height (cm): 10

Length (cm): 10

Articles	Surfaces (cm ²)	Mass (g)
Copy o...	600	1000

Total surface of all articles (cm²): 600



Loops per serie: 20 Iterations: 20

Correlation

mtau: 1

mtolg: 1E-6

mtolx: 1E-6 mrealstep: 1E-3

Parameter Name	Value
Layer 1-Dp-Arrhenius-E(kJ/mol)	69.767
Layer 1-Dp-Arrhenius-A(cm ² /s)	1.378

Package Properties Output Calculation

- Package SAN 24h at 40C optimized
 - Article 1
 - Iso(40°C, 1d)
- Package SAN 2h at 70C Optimized
 - Article 1
 - Iso(70°C, 2h)
- Copy of Package SAN 24h at 40C optir
 - Copy of Article 1
 - Iso(40°C, 1d)
 - Iso(70°C, 2h)

Surface (cm²) 600

Article	Layer 1	Contact Medi...
	ACRYLONIT...	Acetic acid 3%
	Thickness (µm) 300	1.667E04
Migrant 1	ACRYLONIT...	A(3.30E-11) 0.0001

Layer (Layer 1) Migrant Data

Type: Polymer Contact Medium

Thickness (µm): 300

Density (g/cm³): 1.09

Layer Abbreviation: Layer 1

Material: ACRYLONITRILE-STYRENE, COPOLYMER (AS)

Layer Details

Molecular Weight (g/mol): 471.64 Glass Transition Temperature (°C): 97

Log Pow: N/A

Material specific constants for estimation of diffusion coefficients according to Pringer

Upper Limit: A^{*p}: N/A Tau: N/A A^{*p}: N/A
 Realistic Case: A^p: N/A Tau: N/A A^p: N/A

Coefficients for estimation of diffusion coefficients according to Welle

a (K⁻¹): N/A c (A⁻³): N/A
 b (cm⁻²s⁻¹): N/A d (K⁻¹): N/A

Copy of Package SAN 24h at 40C optimized

Geometry: Rectangular

Contact Surface (cm²): 600

Volume of Contact Medium (cm³): 1000

Width (cm): 10

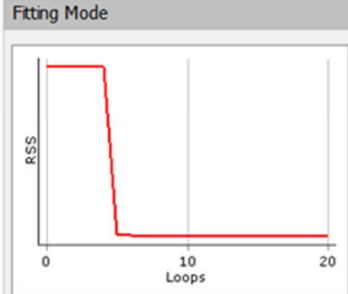
Height (cm): 10

Length (cm): 10

Surface and mass of contact medium by article

Articles	Surfaces (cm ²)	Mass (g)	
Copy o...	600	1000	<input checked="" type="checkbox"/>

Total surface of all articles (cm²): 600



mtau: 1

mtolg: 1E-6

mtolx: 1E-6 mrealstep: 1E-3

Parameter Name	Value
Layer 1-Dp-Arrhenius-E(kJ/mol)	69.767
Layer 1-Dp-Arrhenius-A(cm ² /s)	1.378

Package Properties Output Calculation

- Package SAN 24h at 40C optimized
 - Article 1
 - Iso(40°C, 1d)
- Package SAN 2h at 70C Optimized
 - Article 1
 - Iso(70°C, 2h)
- Copy of Package SAN 24h at 40C optir
 - Copy of Article 1
 - Iso(40°C, 1d)
 - Iso(70°C, 2h)

Surface (cm²) 600

Article	Layer 1	Contact Medi...
	ACRYLONIT...	Acetic acid 3%
	Thickness (µm)	1.667E04
Migrant 1	ACRYLONIT...	A(3.30E-11) 0.0001

Diffusion Coefficient Example Temperature (°C): 70

- Known
- Interpolation based on Tg
- Pringer
- Arrhenius
- Customized Equation
- Brandsch Equation
- Welle Equation
- In-Silico

Arrhenius Calculation Parameters

Activation Energy (kJ/mol): 69.767 Optimize
 Pre-exponential Factor (cm²/s): 1.3776 Optimize

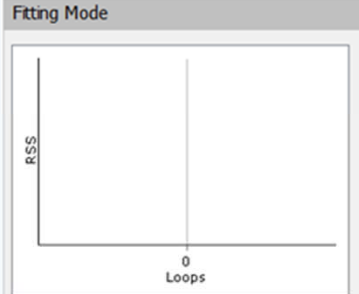
Copy of Package SAN 24h at 40C optimized

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

Surface and mass of contact medium by article

Articles	Surfaces (cm ²)	Mass (g)
Copy o...	600	1000

Total surface of all articles (cm²): 600



Loops per serie: 20

Correlation

mtau: 1
 mtol: 1E-6
 mtolx: 1E-6 mrealstep: 1E-5

Parameter Name	Value
Layer 1-Op-Arrhenius-E(kJ/mol)	69.767
Layer 1-Op-Arrhenius-A(cm ² /s)	1.378

Package Properties Output Calculation

- Package SAN 24h at 40C optimized
 - Article 1
- Package SAN 2h at 70C Optimized
 - Article 1
- Copy of Package SAN 24h at 40C optir
 - Copy of Article 1

Surface (cm²) 600

Article	Layer 1	Contact Medi...
	ACRYLONIT...	Acetic acid 3%
	Thickness (µm)	1.667E04
Migrant 1	ACRYLONIT...	A(3.30E-11) 0.0001

Diffusion Coefficient

Example Temperature (°C): 70

Known
 Interpolation based on Tg
 Pringer
 Arrhenius
 Customized Equation
 Brandsch Equation
 Welle Equation
 In-Silico

Arrhenius Calculation Parameters

Activation Energy (kJ/mol): 69.767 Optimize
 Pre-exponential Factor (cm²/s): 1.3776 Optimize

Copy of Package SAN 24h at 40C optimized

Geometry: Rectangular

Contact Surface (cm²): 600

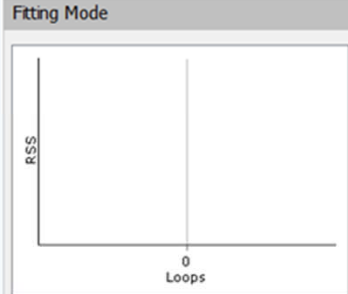
Volume of Contact Medium (cm³): 1000

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

Surface and mass of contact medium by article

Articles	Surfaces (cm ²)	Mass (g)
Copy o...	600	1000

Total surface of all articles (cm²): 600



Loops per serie: 20

Correlation

mtau: 1
 mtol: 1E-6
 mtolx: 1E-6 mrealstep: 1E-3

Parameter Name	Value
Layer 1-Op-Arrhenius-E(kJ/mol)	69.767
Layer 1-Op-Arrhenius-A(cm ² /s)	1.378

Package Properties Output Calculation

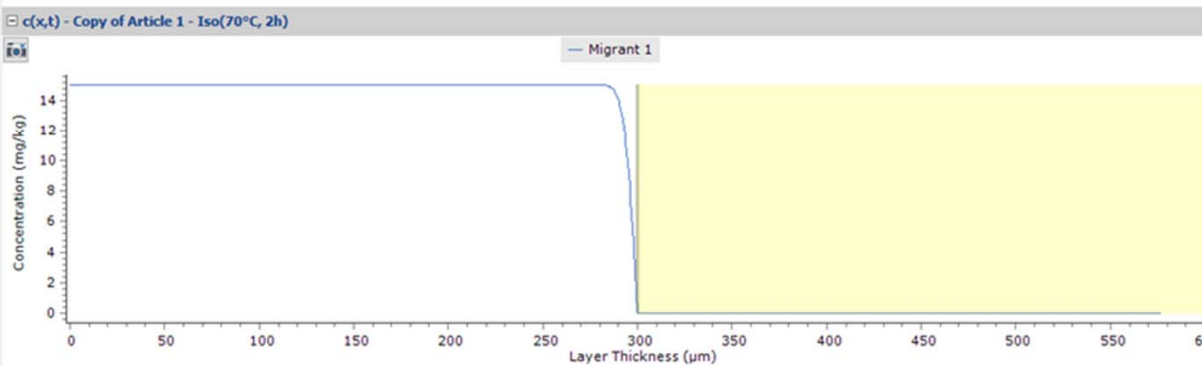
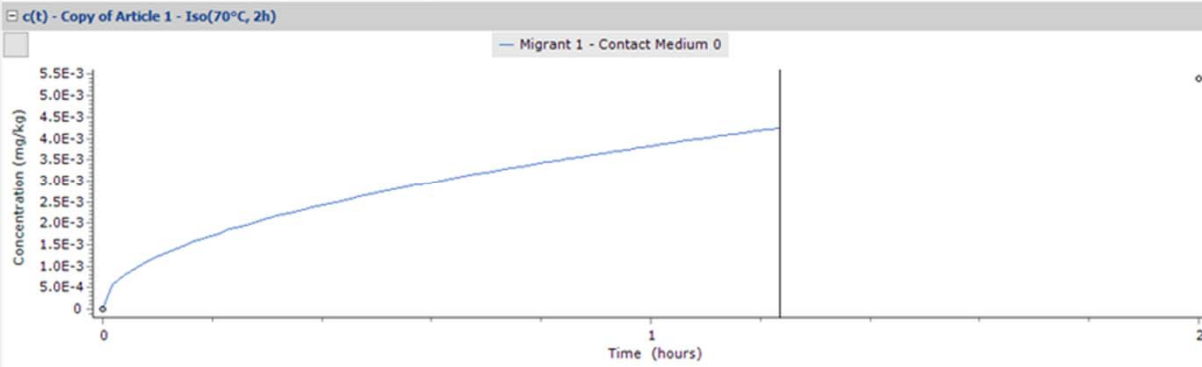
- Package SAN 24h at 40C optimized
 - Article 1
 - Iso(40°C, 1d)
- Package SAN 2h at 70C Optimized
 - Article 1
 - Iso(70°C, 2h)
- Copy of Package SAN 24h at 40C optir
 - Copy of Article 1
 - Iso(40°C, 1d)
 - Iso(70°C, 2h)

Temperature : 70 (°C) Display unit : mg/kg c(t) : draw mean concentration c(t) : draw concentration at 0 % of thickness from surface

Grid

Article	Layer 1	Contact Med...
	ACRYLONIT...	Acetic acid 3%
	Thickness (µm)	1.667E04
	300	
<input checked="" type="checkbox"/>	1. Migrant 1	ACRYLONIT...
		4(3.302E-11)
		0.0001

Concentration Diffusion Coefficient Partition Coefficient Solubility



Copy of Package SAN 24h at 40C optimized

Geometry: Rectangular

Contact Surface (cm²): 600

Volume of Contact Medium (cm³): 1000

Width (cm): 10

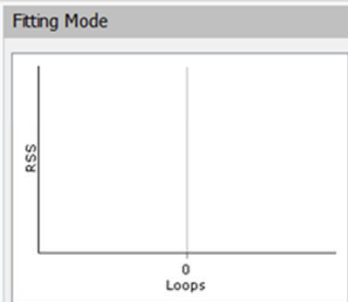
Height (cm): 10

Length (cm): 10

Surface and mass of contact medium by article

Articles	Surfaces (cm ²)	Mass (g)
Copy o...	600	1000

Total surface of all articles (cm²): 600



Loops per serie: 20

Correlation

mtau: 1

mtolg: 1E-6

mtolx: 1E-6 mrealstep: 1E-3

Parameter Name	Value
Layer 1-Dp-Arrhenius-E(kJ/mol)	69.767
Layer 1-Dp-Arrhenius-A(cm ² /s)	1.378

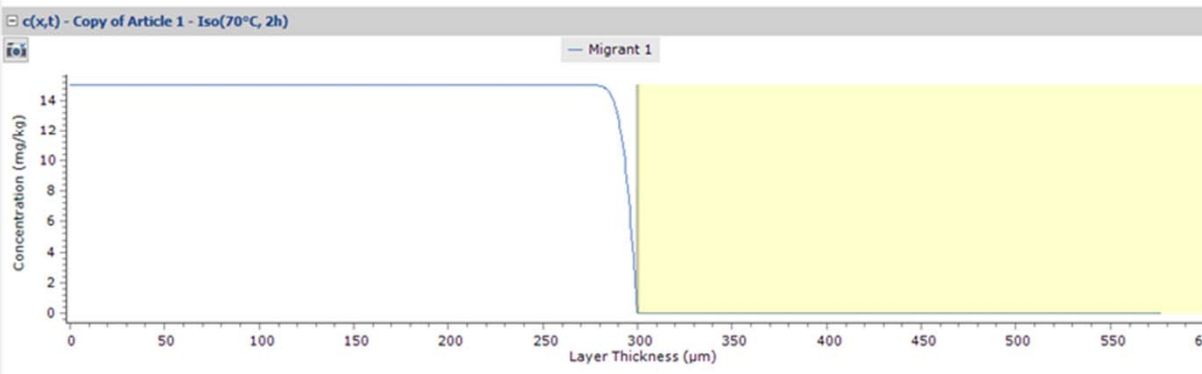
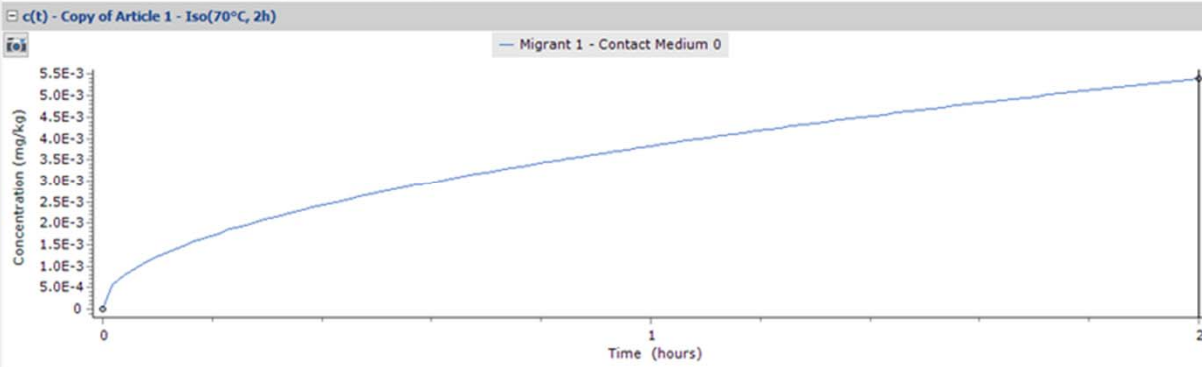
Package Properties | Output Calculation

- Package SAN 24h at 40C optimized
 - Article 1
 - Iso(40°C, 1d)
- Package SAN 2h at 70C Optimized
 - Article 1
 - Iso(70°C, 2h)
- Copy of Package SAN 24h at 40C optir
 - Copy of Article 1
 - Iso(40°C, 1d)
 - Iso(70°C, 2h)

Temperature : 70 (°C) Display unit mg/kg c(t) : draw mean concentration c(t) : draw concentration at 0 % of thickness from surface

Article	Layer 1	Contact Med...
	ACRYLONIT...	Acetic acid 3%
	Thickness (µm)	1.667E04
	300	
<input checked="" type="checkbox"/> 1. Migrant 1	ACRYLONIT...	0.0001
	4(3.302E-11)	

Concentration | Diffusion Coefficient | Partition Coefficient | Solubility



Copy of Package SAN 24h at 40C optimized

Geometry: Rectangular

Contact Surface (cm²): 600

Volume of Contact Medium (cm³): 1000

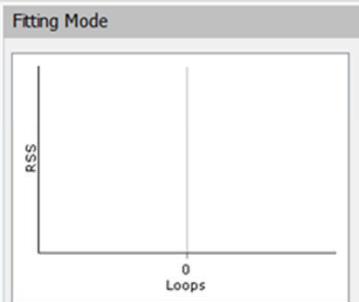
Width (cm): 10

Height (cm): 10

Length (cm): 10

Articles	Surfaces (cm ²)	Mass (g)
Copy o...	600	1000

Total surface of all articles (cm²): 600



Loops per serie: 20

Correlation

Run optimization

mtau: 1

mtolg: 1E-6

mtolx: 1E-6 mrealstep: 1E-3

Parameter Name	Value
Layer 1-Dp-Arrhenius-E(kJ/mol)	69.767
Layer 1-Dp-Arrhenius-A(cm ² /s)	1.378

Package Properties | Output Calculation

Temperature: 70 (°C) | Display unit: mg/kg | c(t) : draw mean concentration | c(t) : draw concentration at 0 | % of thickness from surface

Grid

Layer	Material	Thickness (µm)	Diffusion Coefficient	Partition Coefficient	Solubility
Layer 1	ACRYLONIT...	300			
	Contact Med...				
	Acetic acid 3%		1.667E04		
	...		3.302E-11	0.0001	

Migration: Diffusion Coefficient | Partition Coefficient | Solubility

Time (hours)

Concentration (mg/kg)

Layer Thickness (µm)

Layer 1 - Iso(70°C, 2h)

Copy of Package SAN 24h at 40C optimized

Geometry: Rectangular

Contact Surface (cm²): 600

Volume of Contact Medium (cm³): 1000

Width (cm): 10

Height (cm): 10

Length (cm): 10

Surface and mass of contact medium by article

Articles	Surfaces (cm ²)	Mass (g)	
Copy o...	600	1000	<input checked="" type="checkbox"/>

Total surface of all articles (cm²): 600

Switch Package in Fitting Mode

Fitting Mode

Loops per serie: 20

Optimize | Refresh

Correlation

mtau: 1

mtolg: 1E-6

mtolx: 1E-6 | mrealstep: 1E-3

Parameter Name	Value
Layer 1-Dp-Arrhenius-E(kJ/mol)	69.767
Layer 1-Dp-Arrhenius-A(cm ² /s)	1.378

Close Fitting Mode for This Package

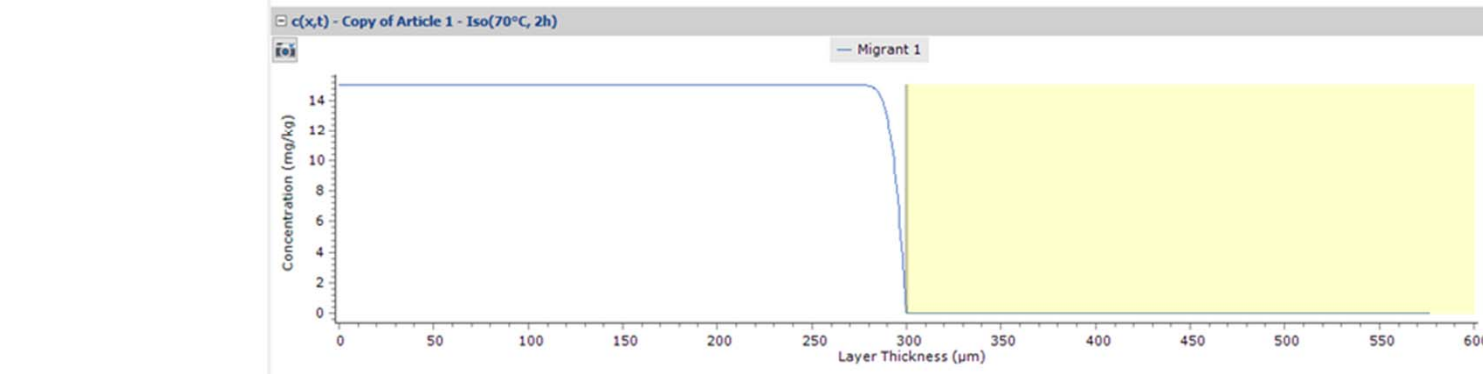
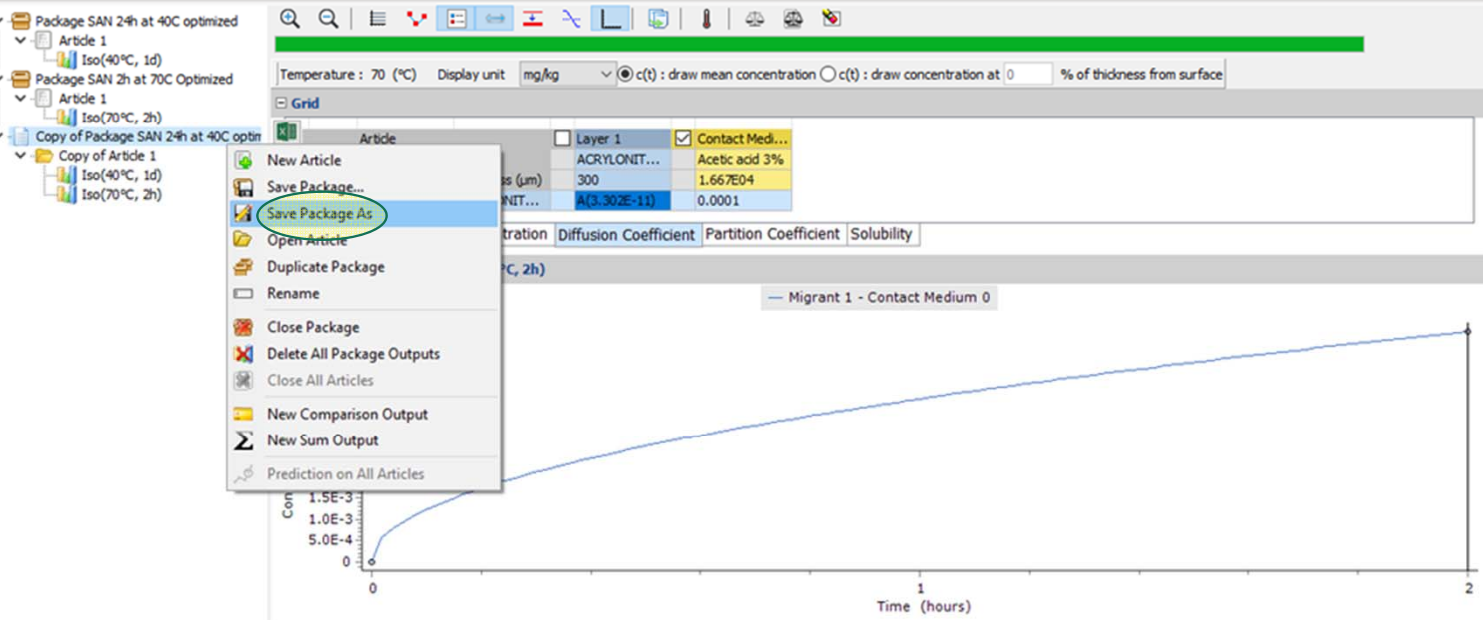
Create Global Package

Package Properties Output Calculation

New Package Open Package Save Package Save Package As Duplicate Package Save All Packages Package Details

New Article Open Article Import Article Save Article Duplicate Article Close Article

Import Initial Concentration Prediction on This Article Prediction on All Articles Close All Articles Delete All Article Outputs Close All



Copy of Package SAN 24h at 40C optimized

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)
Copy o...	600	1000

Total surface of all articles (cm²): 600

Switch Package in Fitting Mode

Fitting Mode

Loops per serie: 20

Optimize Refresh

Correlation

mtau: 1

mtolg: 1E-6

mtolx: 1E-6 mrealstep: 1E-3

Parameter Name	Value
Layer 1-Dp-Arrhenius-E(kJ/mol)	69.767
Layer 1-Dp-Arrhenius-A(cm ² /s)	1.378

Close Fitting Mode for This Package

Create Global Package

2023/7/2

Save As

This PC > Desktop > example fitting

Organise New folder

Name	Date modified	Type	Size
Package SAN 24h at 40C.sml	02.09.2022 14:37	SML File	2 KB
Package SAN 24h at 40C optimized.sml	02.09.2022 15:01	SML File	106 KB
Package SAN 2h at 70C Optimized.sml	02.09.2022 15:06	SML File	178 KB

File name: Package SAN 24h at 40C and 2h at 70C optimized.sml

Save as type: SML v5 (*.sml)

Save Cancel



Package SAN 24h at 40C optimized

Surface (cm²): 600

Contact Medium (cm³): 1000

Surfaces (cm²) Mass (g)

Surfaces (cm ²)	Mass (g)
600	1000

Total surface of all articles (cm²): 600

Switch Package in Fitting Mode

Fitting Mode

RSS

Loops

Loops per serie: 20

Optimize Refresh

Correlation

mtau: 1

mtolg: 1E-6

mtolx: 1E-6 mrealstep: 1E-3

Parameter Name	Value
Layer 1-Dp-Arrhenius-E(kJ/mol)	69.767
Layer 1-Dp-Arrhenius-A(cm ² /s)	1.378

Close Fitting Mode for This Package

Create Global Package

2023/7/2

6.52001

2 (hours)

132

Package Properties Output Calculation

- Package SAN 24h at 40C optimized
 - Article 1
 - Iso(40°C, 1d)
- Package SAN 2h at 70C Optimized
 - Article 1
 - Iso(70°C, 2h)
- Package SAN 24h at 40C and 2h at 70C
 - Copy of Article 1
 - Iso(40°C, 1d)
 - Iso(70°C, 2h)

Temperature: 70 (°C) Display unit: mg/kg c(t) : draw mean concentration c(t) : draw concentration at 0 % of thickness from surface

Grid

Article	Layer	Contact Med...
1. Migrant 1	Layer 1	ACRYLONIT... Acetic acid 3%
		Thickness (µm) 300 1.667E04
		ACRYLONIT... 0.0001

Concentration Diffusion Coefficient Partition Coefficient Solubility

c(t) - Copy of Article 1 - Iso(70°C, 2h)

Concentration (mg/kg) vs Time (hours)

Saving Package

Package File: C:\Users\AKTS\Desktop\example fitting\Package SAN 24h

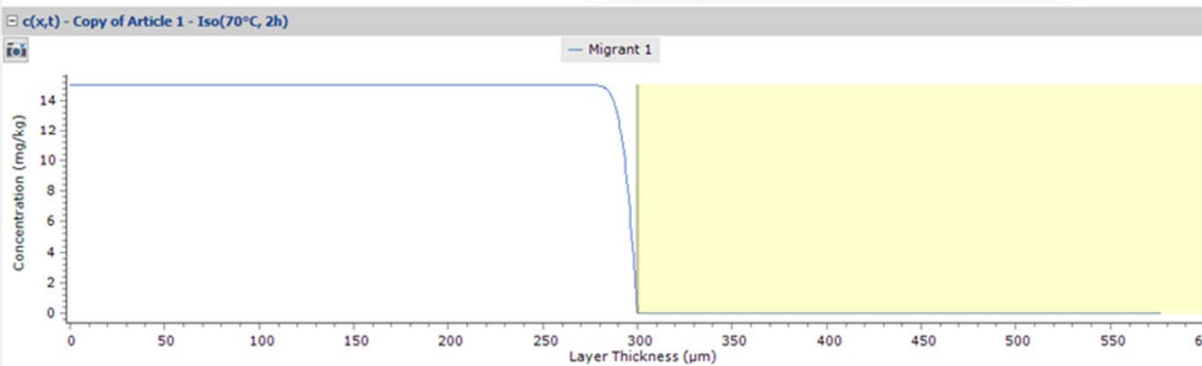
Include Outputs

Number of time steps to export for each output

First and last steps
 Custom: one step on 2
 All steps

Saving many time steps produces larger files and takes longer to save due to the large amount of data points stored for each time step.

OK Cancel



Copy of Package SAN 24h at 40C optimized

Geometry: Rectangular

Contact Surface (cm²): 600

Volume of Contact Medium (cm³): 1000

Width (cm): 10

Height (cm): 10

Length (cm): 10

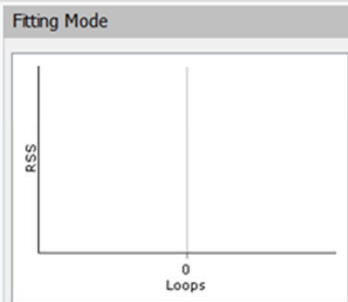
Add Article

Surface and mass of contact medium by article

Articles	Surfaces (cm ²)	Mass (g)
Copy o...	600	1000

Total surface of all articles (cm²): 600

Switch Package in Fitting Mode



Loops per serie: 20

Optimize Refresh

Correlation

mtau: 1

mtolg: 1E-6

mtolx: 1E-6 mrealstep: 1E-3

Parameter Name	Value
Layer 1-Op-Arrhenius-E(kJ/mol)	69.767
Layer 1-Op-Arrhenius-A(cm ² /s)	1.378

Close Fitting Mode for This Package

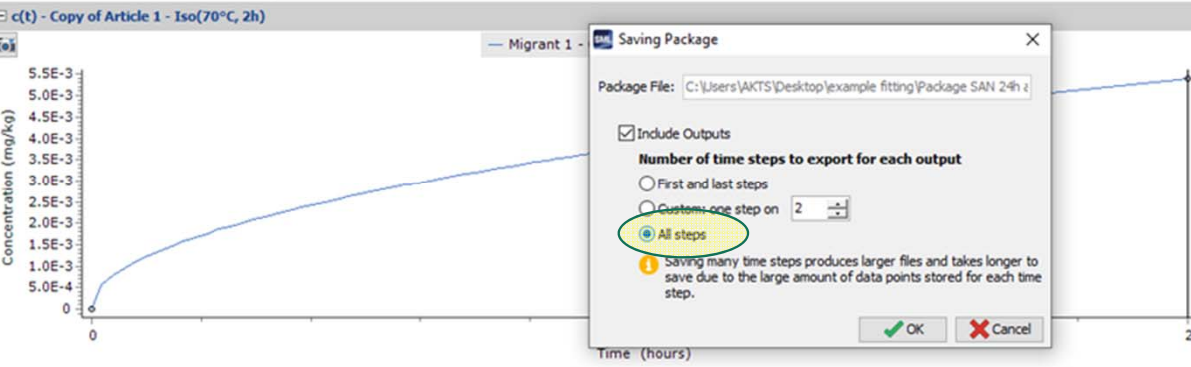
Create Global Package

Package Properties Output Calculation

- Package SAN 24h at 40C optimized
 - Article 1
 - Iso(40°C, 1d)
 - Package SAN 2h at 70C Optimized
 - Article 1
 - Iso(70°C, 2h)
 - Package SAN 24h at 40C and 2h at 70C
 - Copy of Article 1
 - Iso(40°C, 1d)
 - Iso(70°C, 2h)

Temperature: 70 (°C) Display unit: mg/kg c(t) : draw mean concentration c(t) : draw concentration at 0 % of thickness from surface

Article	Layer	Contact Med...
1. Migrant 1	ACRYLONIT...	Acetic acid 3%
	Thickness (µm)	1.667E04
		0.0001



Saving Package

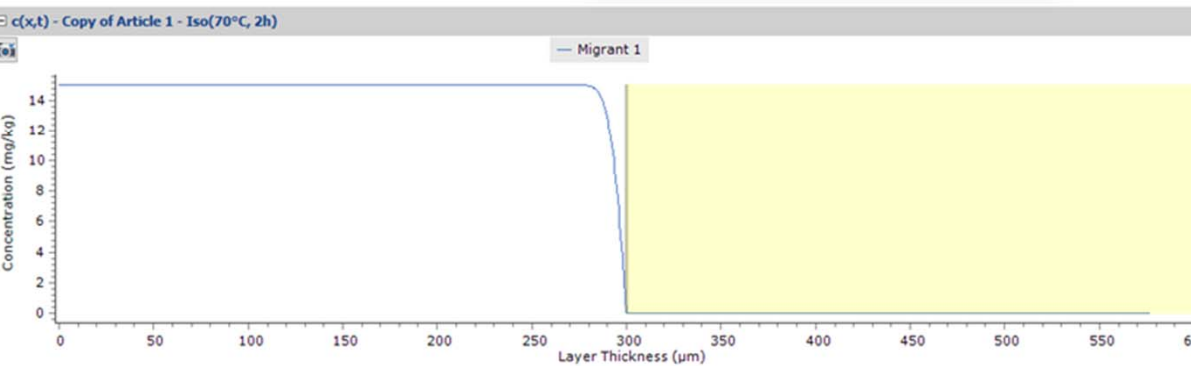
Package File: C:\Users\AKTS\Desktop\example fitting\Package SAN 24h

Include Outputs

Number of time steps to export for each output

First and last steps
 Custom: one step on 2
 All steps

1 Saving many time steps produces larger files and takes longer to save due to the large amount of data points stored for each time step.



Copy of Package SAN 24h at 40C optimized

Geometry: Rectangular

Contact Surface (cm²): 600

Volume of Contact Medium (cm³): 1000

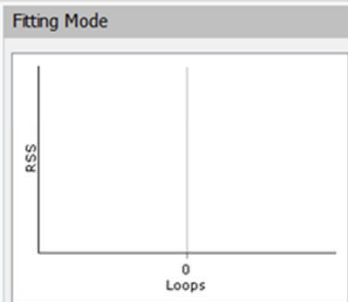
Width (cm): 10

Height (cm): 10

Length (cm): 10

Articles	Surfaces (cm ²)	Mass (g)
Copy o...	600	1000

Total surface of all articles (cm²): 600



Loops per serie: 20

Correlation

mtau: 1

mtolg: 1E-6

mtolx: 1E-6 mrealstep: 1E-3

Parameter Name	Value
Layer 1-Op-Arrhenius-E(kJ/mol)	69.767
Layer 1-Op-Arrhenius-A(cm ² /s)	1.378

Package Properties Output Calculation

- Package SAN 24h at 40C optimized
 - Article 1
 - Iso(40°C, 1d)
- Package SAN 2h at 70C Optimized
 - Article 1
 - Iso(70°C, 2h)
- Package SAN 24h at 40C and 2h at 70C
 - Copy of Article 1
 - Iso(40°C, 1d)
 - Iso(70°C, 2h)

Temperature : 70 (°C) Display unit : mg/kg c(t) : draw mean concentration c(t) : draw concentration at 0 % of thickness from surface

Grid

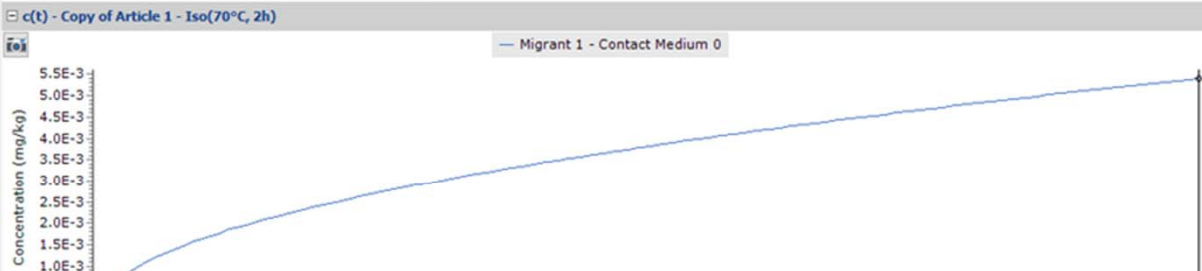
Article	Layer 1	Contact Med...
	ACRYLONIT...	Acetic acid 3%
	Thickness (µm)	1.667E04
		0.0001
<input checked="" type="checkbox"/> 1. Migrant 1	ACRYLONIT...	A(3.302E-11)

Concentration Diffusion Coefficient Partition Coefficient Solubility

c(t) - Copy of Article 1 - Iso(70°C, 2h)

Migrant 1 - Contact Medium 0

Time (hours)	Concentration (mg/kg)
0	0
0.5	~1.5E-3
1	~3.5E-3
2	~5.5E-3



Package SAN 24h at 40C and 2h at 70C optimized

Geometry: Rectangular

Contact Surface (cm²): 600

Volume of Contact Medium (cm³): 1000

Width (cm): 10

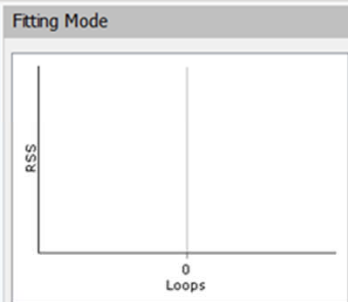
Height (cm): 10

Length (cm): 10

Surface and mass of contact medium by article

Articles	Surfaces (cm ²)	Mass (g)
Copy o...	600	1000

Total surface of all articles (cm²): 600



Loops per serie: 20

Correlation

mtau: 1

mtolg: 1E-6

mtolx: 1E-6 mrealstep: 1E-3

Parameter Name	Value
Layer 1-Dp-Arrhenius-E(k)/mol	69.767
Layer 1-Dp-Arrhenius-A(cm ² /s)	1.378

Package Properties Output Calculation

- Package SAN 24h at 40C optimized
 - Article 1
 - Iso(40°C, 1d)
- Package SAN 2h at 70C Optimized
 - Article 1
 - Iso(70°C, 2h)
- Package SAN 24h at 40C and 2h at 70C
 - Copy of Article 1
 - Iso(40°C, 1d)
 - Iso(70°C, 2h)

Surface (cm²) 600

Article	Layer 1	Contact Medi...
	ACRYLONIT...	Acetic acid 3%
	Thickness (µm)	1.667E04
Migrant 1	ACRYLONIT...	A(3.30E-11) 0.0001

Layer (Layer 1) Migrant (Migrant 1) **Data (Diffusion Coefficient)**

Example Temperature (°C): 70

Diffusion Coefficient

Known
 Interpolation based on Tg
 Pringer
 Arrhenius
 Customized Equation
 Brandsch Equation
 Welle Equation
 In-Silico

Arrhenius Calculation Parameters

Activation Energy (kJ/mol): 69.767 Optimize
 Pre-exponential Factor (cm²/s): 1.3776 Optimize

Package SAN 24h at 40C and 2h at 70C optimized

Geometry: Rectangular

Contact Surface (cm²): 600

Volume of Contact Medium (cm³): 1000

Width (cm): 10

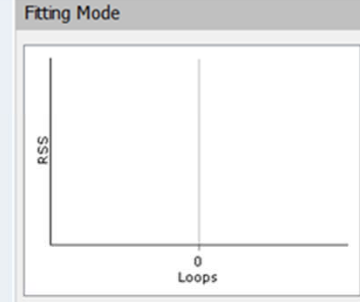
Height (cm): 10

Length (cm): 10

Surface and mass of contact medium by article

Articles	Surfaces (cm ²)	Mass (g)
Copy o...	600	1000

Total surface of all articles (cm²): 600



Loops per serie: 20

Correlation

mtau: 1

mtolg: 1E-6

mtolx: 1E-6 mrealstep: 1E-3

Parameter Name	Value
Layer 1-Op-Arrhenius-E(kJ/mol)	69.767
Layer 1-Op-Arrhenius-A(cm ² /s)	1.378

Package Properties Output Calculation

- Package SAN 24h at 40C optimized
 - Article 1
 - Iso(40°C, 1d)
- Package SAN 2h at 70C Optimized
 - Article 1
 - Iso(70°C, 2h)
- Package SAN 24h at 40C and 2h at 70C
 - Copy of Article 1
 - Iso(40°C, 1d)
 - Iso(70°C, 2h)

Surface (cm²) 600

Article	Layer 1	Contact Medi...
	ACRYLONIT...	Acetic acid 3%
	Thickness (µm)	1.667E04
Migrant 1	ACRYLONIT...	A(3.30E-11) 0.0001

Layer (Layer 1) Migrant

Diffusion Coefficient

Known
 Interpolation based on Tg
 Pringer
 Arrhenius
 Customized Equation
 Brandsch Equation
 Welle Equation
 In-Silico

Predictions

Temperature Profiles

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

Isothermal Conditions

Temperature = 20 °C
 ΔT = 20 °C
 Number of Isotherms = 1
 Final Temperature = 20 °C

Time Max 10 day
 Without Statistics
 Monte Carlo Runs
 Number of Runs 10
 Include Sobol Runs
 Fast Distribution

Number of steps for this output: 100

Package SAN 24h at 40C and 2h at 70C optimized

Geometry: Rectangular

Contact Surface (cm²): 600

Volume of Contact Medium (cm³): 1000

Article	Mass (g)	<input type="checkbox"/>
2)	1000	<input checked="" type="checkbox"/>

600

Fitting Mode

RSS

0 Loops

Loops per serie 20

Correlation

mtau 1
 mtolg 1E-6
 mtolx 1E-6 mrealstep 1E-3

Parameter Name	Value
Layer 1-Op-Arrhenius-E(kJ/mol)	69.767
Layer 1-Op-Arrhenius-A(cm ² /s)	1.378

Package Properties Output Calculation

- Package SAN 24h at 40C optimized
 - Article 1
 - Iso(40°C, 1d)
- Package SAN 2h at 70C Optimized
 - Article 1
 - Iso(70°C, 2h)
- Package SAN 24h at 40C and 2h at 70C
 - Copy of Article 1
 - Iso(40°C, 1d)
 - Iso(70°C, 2h)

Surface (cm²) 600

Article	Layer 1	Contact Medi...
	ACRYLONIT...	Acetic acid 3%
	Thickness (µm)	1.667E04
Migrant 1	ACRYLONIT...	A(3.30E-11) 0.0001

Layer (Layer 1) Migrant

Diffusion Coefficient

Known
 Interpolation based on Tg
 Pringer
 Arrhenius
 Customized Equation
 Brandsch Equation
 Welle Equation
 In-Silico

Predictions

Temperature Profiles: Iso, Non-Iso, **Step**, Modulated, Shock, Worldwide, STANAG, Customized, Repeated Use

Stepwise Conditions

Time Unit: min Time Max: 0 min Number of Cycles: 1

From Temp (°C) To Temp (°C) Heating Rate (K/min) Time (min)

°C °C K/min min

Without Statistics
 Monte Carlo Runs
 Fast Distribution

Number of Runs: 10

Include Sobol Runs

Number of steps for this output: 100

Package SAN 24h at 40C and 2h at 70C optimized

Geometry: Rectangular

Contact Surface (cm²): 600

Volume of Contact Medium (cm³): 1000

Article	Mass (g)
2)	1000

600

Fitting Mode

RSS

0 Loops

Loops per serie: 20

Correlation

mtau: 1
 mtol: 1E-6
 mtolx: 1E-6 mrealstep: 1E-3

Parameter Name	Value
Layer 1-Dp-Arrhenius-E(kJ/mol)	69.767
Layer 1-Dp-Arrhenius-A(cm ² /s)	1.378

Package Properties Output Calculation

- Package SAN 24h at 40C optimized
 - Article 1
 - Iso(40°C, 1d)
- Package SAN 2h at 70C Optimized
 - Article 1
 - Iso(70°C, 2h)
- Package SAN 24h at 40C and 2h at 70C
 - Copy of Article 1
 - Iso(40°C, 1d)
 - Iso(70°C, 2h)

Surface (cm²) 600

Article	Layer 1	Contact Medi...
	ACRYLONIT...	Acetic acid 3%
	Thickness (µm)	300
		1.667E04
Migrant 1	ACRYLONIT...	A(3.30E-11)
		0.0001

Layer (Layer 1) Migrant

Diffusion Coefficient

Known
 Interpolation based on Tg
 Pringer
 Arrhenius
 Customized Equation
 Brandsch Equation
 Welle Equation
 In-Silico

Predictions

Temperature Profiles

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

Stepwise Conditions

Time Unit: min Time Max: 0 min Number of Cycles: 1

From Temp (°C) To Temp (°C) Heating Rate (K/min) Time (min)

°C
 °C
 K/min
 min

Without Statistics
 Monte Carlo Runs
 Number of Runs: 10
 Include Sobol Runs
 Fast Distribution

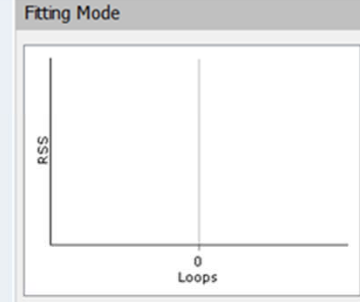
Number of steps for this output: 100

Package SAN 24h at 40C and 2h at 70C optimized

Geometry: Rectangular

Contact Surface (cm²): 600

Volume of Contact Medium (cm³): 1000



Loops per serie: 20

Correlation

mtau: 1
 mtolg: 1E-6
 mtolx: 1E-6 mrealstep: 1E-3

Parameter Name	Value
Layer 1-Dp-Arrhenius-E(kJ/mol)	69.767
Layer 1-Dp-Arrhenius-A(cm ² /s)	1.378

Package Properties Output Calculation

- Package SAN 24h at 40C optimized
 - Article 1
 - Iso(40°C, 1d)
- Package SAN 2h at 70C Optimized
 - Article 1
 - Iso(70°C, 2h)
- Package SAN 24h at 40C and 2h at 70C
 - Copy of Article 1
 - Iso(40°C, 1d)
 - Iso(70°C, 2h)

Surface (cm²) 600

Article	Layer 1	Contact Medi...
	ACRYLONIT...	Acetic acid 3%
	Thickness (µm)	300
		1.667E04
Migrant 1	ACRYLONIT...	A(3.30E-11)
		0.0001

Layer (Layer 1) Migrant

Diffusion Coefficient

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

Predictions

Temperature Profiles

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

Stepwise Conditions

Time Unit: min Time Max: 0 min Number of Cycles: 1

From Temp (°C)	To Temp (°C)	Heating Rate (K/min)	Time (min)
40			

Without Statistics
 Monte Carlo Runs
 Number of Runs: 10
 Include Sobol Runs
 Fast Distribution

Number of steps for this output: 100

Package SAN 24h at 40C and 2h at 70C optimized

Geometry: Rectangular

Contact Surface (cm²): 600

Volume of Contact Medium (cm³): 1000

Article	Mass (g)
2)	1000

Fitting Mode

RSS

0 Loops

Loops per serie: 20

mtau: 1
 mtolg: 1E-6
 mtolx: 1E-6 mrealstep: 1E-3

Parameter Name	Value
Layer 1-Dp-Arrhenius-E(kJ/mol)	69.767
Layer 1-Dp-Arrhenius-A(cm ² /s)	1.378

Package Properties Output Calculation

- Package SAN 24h at 40C optimized
 - Article 1
 - Iso(40°C, 1d)
- Package SAN 2h at 70C Optimized
 - Article 1
 - Iso(70°C, 2h)
- Package SAN 24h at 40C and 2h at 70C
 - Copy of Article 1
 - Iso(40°C, 1d)
 - Iso(70°C, 2h)

Surface (cm²) 600

Article	Layer 1	Contact Medi...
	ACRYLONIT...	Acetic acid 3%
	Thickness (µm)	300
		1.667E04
Migrant 1	ACRYLONIT...	A(3.30E-11)
		0.0001

Layer (Layer 1) Migrant

Diffusion Coefficient

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

Predictions

Temperature Profiles: Iso, Non-Iso, **Step**, Modulated, Shock, Worldwide, STANAG, Customized, Repeated Use

Stepwise Conditions

Time Unit: min Time Max: 60 min Number of Cycles: 1

From Temp (°C)	To Temp (°C)	Heating Rate (K/min)	Time (min)
40	40	0	60
40			

Without Statistics
 Monte Carlo Runs
 Number of Runs: 10
 Include Sobol Runs
 Fast Distribution

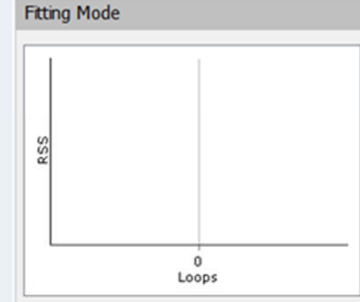
Number of steps for this output: 100

Package SAN 24h at 40C and 2h at 70C optimized

Geometry: Rectangular

Contact Surface (cm²): 600

Volume of Contact Medium (cm³): 1000



Loops per serie: 20

Correlation

mtau: 1
 mtolg: 1E-6
 mtolx: 1E-6 mrealstep: 1E-3

Parameter Name	Value
Layer 1-Dp-Arrhenius-E(kJ/mol)	69.767
Layer 1-Dp-Arrhenius-A(cm ² /s)	1.378

Package Properties Output Calculation

- Package SAN 24h at 40C optimized
 - Article 1
 - Iso(40°C, 1d)
- Package SAN 2h at 70C Optimized
 - Article 1
 - Iso(70°C, 2h)
- Package SAN 24h at 40C and 2h at 70C
 - Copy of Article 1
 - Iso(40°C, 1d)
 - Iso(70°C, 2h)

Surface (cm²) 600

Article	Layer 1	Contact Medi...
	ACRYLONIT...	Acetic acid 3%
	Thickness (µm)	300
		1.667E04
Migrant 1	ACRYLONIT...	A(3.30E-11)
		0.0001

Layer (Layer 1) Migrant

Diffusion Coefficient

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

Predictions

Temperature Profiles

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

Stepwise Conditions

Time Unit: min Time Max: 60 min Number of Cycles: 1

From Temp (°C)	To Temp (°C)	Heating Rate (K/min)	Time (min)
40	40	0	60
40			

Without Statistics
 Monte Carlo Runs
 Number of Runs: 10
 Include Sobol Runs
 Fast Distribution

Number of steps for this output: 100

Package SAN 24h at 40C and 2h at 70C optimized

Geometry: Rectangular

Contact Surface (cm²): 600

Volume of Contact Medium (cm³): 1000

Article	Mass (g)
2)	1000

600

Fitting Mode

RSS

0 Loops

Loops per serie: 20

mtau: 1
 mtolg: 1E-6
 mtolx: 1E-6 mrealstep: 1E-3

Parameter Name	Value
Layer 1-Dp-Arrhenius-E(kJ/mol)	69.767
Layer 1-Dp-Arrhenius-A(cm ² /s)	1.378

Package Properties Output Calculation

- Package SAN 24h at 40C optimized
 - Article 1
 - Iso(40°C, 1d)
- Package SAN 2h at 70C Optimized
 - Article 1
 - Iso(70°C, 2h)
- Package SAN 24h at 40C and 2h at 70C
 - Copy of Article 1
 - Iso(40°C, 1d)
 - Iso(70°C, 2h)

Surface (cm²) 600

Article	Layer 1	Contact Medi...
	ACRYLONIT...	Acetic acid 3%
	Thickness (µm)	300
		1.667E04
Migrant 1	ACRYLONIT...	A(3.30E-11)
		0.0001

Layer (Layer 1) Migrant

Diffusion Coefficient

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

Predictions

Temperature Profiles: Iso, Non-Iso, **Step**, Modulated, Shock, Worldwide, STANAG, Customized, Repeated Use

Stepwise Conditions

Time Unit: min Time Max: 60 min Number of Cycles: 1

From Temp (°C)	To Temp (°C)	Heating Rate (K/min)	Time (min)
40	40	0	60
40	70		

Without Statistics
 Monte Carlo Runs
 Number of Runs: 10
 Include Sobol Runs
 Fast Distribution

Number of steps for this output: 100

Package SAN 24h at 40C and 2h at 70C optimized

Geometry: Rectangular

Contact Surface (cm²): 600

Volume of Contact Medium (cm³): 1000

Article	Mass (g)
2)	1000

Fitting Mode

RSS

0 Loops

Loops per serie: 20

mtau: 1
 mtolg: 1E-6
 mtolx: 1E-6 mrealstep: 1E-3

Parameter Name	Value
Layer 1-Dp-Arrhenius-E(kJ/mol)	69.767
Layer 1-Dp-Arrhenius-A(cm ² /s)	1.378

Package Properties Output Calculation

- Package SAN 24h at 40C optimized
 - Article 1
 - Iso(40°C, 1d)
- Package SAN 2h at 70C Optimized
 - Article 1
 - Iso(70°C, 2h)
- Package SAN 24h at 40C and 2h at 70C
 - Copy of Article 1
 - Iso(40°C, 1d)
 - Iso(70°C, 2h)

Surface (cm²) 600

Article	Layer 1	Contact Medi...
	ACRYLONIT...	Acetic acid 3%
	Thickness (µm)	1.667E04
Migrant 1	ACRYLONIT...	A(3.30E-11) 0.0001

Layer (Layer 1) Migrant

Diffusion Coefficient

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

Predictions

Temperature Profiles

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

Stepwise Conditions

Time Unit: min Time Max: 60.3 min Number of Cycles: 1

From Temp (°C)	To Temp (°C)	Heating Rate (K/min)	Time (min)
40	40	0	60
40	70	100	0.3
70			

Without Statistics
 Monte Carlo Runs
 Fast Distribution

Number of Runs: 10

Number of steps for this output: 100

Package SAN 24h at 40C and 2h at 70C optimized

Geometry: Rectangular

Contact Surface (cm²): 600

Volume of Contact Medium (cm³): 1000

Article	Mass (g)
2)	1000

Fitting Mode

RSS

0 Loops

Loops per serie: 20

mtau: 1
 mtolg: 1E-6
 mtolx: 1E-6 mrealstep: 1E-3

Parameter Name	Value
Layer 1-Op-Arrhenius-E(kJ/mol)	69.767
Layer 1-Op-Arrhenius-A(cm ² /s)	1.378

Package Properties Output Calculation

- Package SAN 24h at 40C optimized
 - Article 1
 - Iso(40°C, 1d)
- Package SAN 2h at 70C Optimized
 - Article 1
 - Iso(70°C, 2h)
- Package SAN 24h at 40C and 2h at 70C
 - Copy of Article 1
 - Iso(40°C, 1d)
 - Iso(70°C, 2h)

Surface (cm²) 600

Article	Layer 1	Contact Medi...
	ACRYLONIT...	Acetic acid 3%
	Thickness (µm)	1.667E04
Migrant 1	ACRYLONIT...	A(3.30E-11) 0.0001

Layer (Layer 1) Migrant

Diffusion Coefficient

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 Welle Equation
 In-Silico

Predictions

Temperature Profiles

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

Stepwise Conditions

Time Unit: min Time Max: 60.3 min Number of Cycles: 1

From Temp (°C)	To Temp (°C)	Heating Rate (K/min)	Time (min)
40	40	0	60
40	70	100	0.3
70			

Without Statistics
 Monte Carlo Runs
 Fast Distribution

Number of Runs: 10

Number of steps for this output: 100

Package SAN 24h at 40C and 2h at 70C optimized

Geometry: Rectangular

Contact Surface (cm²): 600

Volume of Contact Medium (cm³): 1000

Article	Mass (g)
2)	1000

Fitting Mode

RSS

0 Loops

Loops per serie: 20

mtau: 1
 mtolg: 1E-6
 mtolx: 1E-6 mrealstep: 1E-3

Parameter Name	Value
Layer 1-Op-Arrhenius-E(kJ/mol)	69.767
Layer 1-Op-Arrhenius-A(cm ² /s)	1.378

Package Properties Output Calculation

- Package SAN 24h at 40C optimized
 - Article 1
 - Iso(40°C, 1d)
- Package SAN 2h at 70C Optimized
 - Article 1
 - Iso(70°C, 2h)
- Package SAN 24h at 40C and 2h at 70C
 - Copy of Article 1
 - Iso(40°C, 1d)
 - Iso(70°C, 2h)

Surface (cm²) 600

Article	Layer 1	Contact Medi...
	ACRYLONIT...	Acetic acid 3%
	Thickness (µm)	1.667E04
Migrant 1	ACRYLONIT...	A(3.30E-11) 0.0001

Layer (Layer 1) Migrant

Diffusion Coefficient

Known
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 Pringer
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 Customized Equation
 Bransch Equation
 Welle Equation
 In-Silico

Predictions

Temperature Profiles

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

Stepwise Conditions

Time Unit: min Time Max: 240.3 min Number of Cycles: 1

From Temp (°C)	To Temp (°C)	Heating Rate (K/min)	Time (min)
40	40	0	60
40	70	100	0.3
70	70	0	180
70			

Without Statistics
 Monte Carlo Runs
 Number of Runs: 10
 Include Sobol Runs
 Fast Distribution

Number of steps for this output: 100

Package SAN 24h at 40C and 2h at 70C optimized

Geometry: Rectangular

Contact Surface (cm²): 600

Volume of Contact Medium (cm³): 1000

Article	Mass (g)
2)	1000

Fitting Mode

RSS

0 Loops

Loops per serie: 20

mtau: 1
 mtolg: 1E-6
 mtolx: 1E-6 mrealstep: 1E-3

Parameter Name	Value
Layer 1-Dp-Arrhenius-E(kJ/mol)	69.767
Layer 1-Dp-Arrhenius-A(cm ² /s)	1.378

Package Properties Output Calculation

- Package SAN 24h at 40C optimized
 - Article 1
 - Iso(40°C, 1d)
- Package SAN 2h at 70C Optimized
 - Article 1
 - Iso(70°C, 2h)
- Package SAN 24h at 40C and 2h at 70C
 - Copy of Article 1
 - Iso(40°C, 1d)
 - Iso(70°C, 2h)

Surface (cm²) 600

Article	Layer 1	Contact Medi...
	ACRYLONIT...	Acetic acid 3%
	Thickness (µm)	1.667E04
Migrant 1	ACRYLONIT...	A(3.30E-11) 0.0001

Layer (Layer 1) Migrant

Diffusion Coefficient

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

Predictions

Temperature Profiles

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

Stepwise Conditions

Time Unit: min Time Max: 240.3 min Number of Cycles: 1

From Temp (°C)	To Temp (°C)	Heating Rate (K/min)	Time (min)
40	40	0	60
40	70	100	0.3
70	70	0	180
70			

Without Statistics
 Monte Carlo Runs
 Number of Runs: 10
 Include Sobol Runs
 Fast Distribution

Number of steps for this output: 100

Package SAN 24h at 40C and 2h at 70C optimized

Geometry: Rectangular

Contact Surface (cm²): 600

Volume of Contact Medium (cm³): 1000

Article	Mass (g)
2)	1000

Fitting Mode

RSS

0 Loops

Loops per serie: 20

mtau: 1
 mtolg: 1E-6
 mtolx: 1E-6 mrealstep: 1E-3

Parameter Name	Value
Layer 1-Dp-Arrhenius-E(kJ/mol)	69.767
Layer 1-Dp-Arrhenius-A(cm ² /s)	1.378

Package Properties Output Calculation

- Package SAN 24h at 40C optimized
 - Article 1
 - Iso(40°C, 1d)
- Package SAN 2h at 70C Optimized
 - Article 1
 - Iso(70°C, 2h)
- Package SAN 24h at 40C and 2h at 70C
 - Copy of Article 1
 - Iso(40°C, 1d)
 - Iso(70°C, 2h)

Surface (cm²) 600

Article	Layer 1	Contact Medi...
	ACRYLONIT...	Acetic acid 3%
	Thickness (µm)	1.667E04
Migrant 1	ACRYLONIT...	A(3.30E-11) 0.0001

Layer (Layer 1) Migrant

Diffusion Coefficient

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

Predictions

Temperature Profiles: Iso, Non-Iso, **Step**, Modulated, Shock, Worldwide, STANAG, Customized, Repeated Use

Stepwise Conditions

Time Unit: min Time Max: 240.3 min Number of Cycles: 1

From Temp (°C)	To Temp (°C)	Heating Rate (K/min)	Time (min)
40	40	0	60
40	70	100	0.3
70	70	0	180
70	20		

Without Statistics
 Monte Carlo Runs
 Number of Runs: 10
 Include Sobol Runs
 Fast Distribution

Number of steps for this output: 100

Package SAN 24h at 40C and 2h at 70C optimized

Geometry: Rectangular

Contact Surface (cm²): 600

Volume of Contact Medium (cm³): 1000

Article	Mass (g)
2)	1000

Fitting Mode

RSS

0 Loops

Loops per serie: 20

mtau: 1
 mtolg: 1E-6
 mtolx: 1E-6 mrealstep: 1E-3

Parameter Name	Value
Layer 1-Dp-Arrhenius-E(kJ/mol)	69.767
Layer 1-Dp-Arrhenius-A(cm ² /s)	1.378

Package Properties Output Calculation

- Package SAN 24h at 40C optimized
 - Article 1
 - Iso(40°C, 1d)
- Package SAN 2h at 70C Optimized
 - Article 1
 - Iso(70°C, 2h)
- Package SAN 24h at 40C and 2h at 70C
 - Copy of Article 1
 - Iso(40°C, 1d)
 - Iso(70°C, 2h)

Surface (cm²) 600

Article	Layer 1	Contact Medi...
	ACRYLONIT...	Acetic acid 3%
	Thickness (µm)	1.667E04
Migrant 1	ACRYLONIT...	A(3.30E-11) 0.0001

Layer (Layer 1) Migrant

Diffusion Coefficient

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

Predictions

Temperature Profiles: Iso, Non-Iso, **Step**, Modulated, Shock, Worldwide, STANAG, Customized, Repeated Use

Stepwise Conditions

Time Unit: min Time Max: 240.3 min Number of Cycles: 1

From Temp (°C)	To Temp (°C)	Heating Rate (K/min)	Time (min)
40	40	0	60
40	70	100	0.3
70	70	0	180
70	20		

Without Statistics
 Monte Carlo Runs
 Number of Runs: 10
 Include Sobol Runs
 Fast Distribution

Number of steps for this output: 100

Package SAN 24h at 40C and 2h at 70C optimized

Geometry: Rectangular

Contact Surface (cm²): 600

Volume of Contact Medium (cm³): 1000

Article	Mass (g)
2)	1000

Fitting Mode

RSS

0 Loops

Loops per serie: 20

mtau: 1
 mtolg: 1E-6
 mtolx: 1E-6 mrealstep: 1E-3

Parameter Name	Value
Layer 1-Op-Arrhenius-E(kJ/mol)	69.767
Layer 1-Op-Arrhenius-A(cm ² /s)	1.378

Package Properties Output Calculation

- Package SAN 24h at 40C optimized
 - Article 1
 - Iso(40°C, 1d)
- Package SAN 2h at 70C Optimized
 - Article 1
 - Iso(70°C, 2h)
- Package SAN 24h at 40C and 2h at 70C
 - Copy of Article 1
 - Iso(40°C, 1d)
 - Iso(70°C, 2h)

Surface (cm²) 600

Article	Layer 1	Contact Medi...
	ACRYLONIT...	Acetic acid 3%
	Thickness (µm)	1.667E04
Migrant 1	ACRYLONIT...	A(3.30E-11) 0.0001

Layer (Layer 1) Migrant

Diffusion Coefficient

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

Predictions

Temperature Profiles

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

Stepwise Conditions

Time Unit: min Time Max: 245.3 min Number of Cycles: 1

From Temp (°C)	To Temp (°C)	Heating Rate (K/min)	Time (min)
40	40	0	60
40	70	100	0.3
70	70	0	180
70	20	-10	5
20			

Without Statistics
 Monte Carlo Runs
 Number of Runs: 10
 Include Sobol Runs
 Fast Distribution

Number of steps for this output: 100

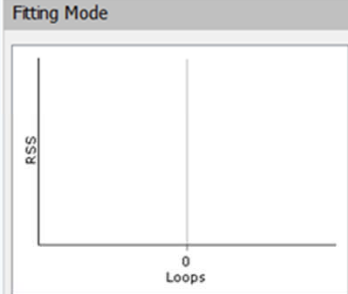
Package SAN 24h at 40C and 2h at 70C optimized

Geometry: Rectangular

Contact Surface (cm²): 600

Volume of Contact Medium (cm³): 1000

Article	Mass (g)
2)	1000



Loops per serie: 20

mtau: 1
 mtol: 1E-6
 mtolx: 1E-6 mrealstep: 1E-3

Parameter Name	Value
Layer 1-Dp-Arrhenius-E(kJ/mol)	69.767
Layer 1-Dp-Arrhenius-A(cm ² /s)	1.378

Package Properties Output Calculation

- Package SAN 24h at 40C optimized
 - Article 1
- Package SAN 2h at 70C Optimized
 - Article 1
- Package SAN 24h at 40C and 2h at 70C
 - Copy of Article 1

Surface (cm²) 600

Article	Layer 1	Contact Medi...
	ACRYLONIT...	Acetic acid 3%
	Thickness (µm)	1.667E04
Migrant 1	ACRYLONIT...	A(3.30E-11) 0.0001

Layer (Layer 1) Migrant

Diffusion Coefficient

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

Predictions

Temperature Profiles

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

Stepwise Conditions

Time Unit: min Time Max: 245.3 min Number of Cycles: 1

From Temp (°C)	To Temp (°C)	Heating Rate (K/min)	Time (min)
40	40	0	60
40	70	100	0.3
70	70	0	180
70	20	-10	5
20			

Without Statistics
 Monte Carlo Runs
 Fast Distribution

Number of Runs: 10

Number of steps for this output: 100

Package SAN 24h at 40C and 2h at 70C optimized

Geometry: Rectangular

Contact Surface (cm²): 600

Volume of Contact Medium (cm³): 1000

Article	Mass (g)
2)	1000

Fitting Mode

RSS

0 Loops

Loops per serie: 20

mtau: 1
 mtolg: 1E-6
 mtolx: 1E-6 mrealstep: 1E-3

Parameter Name	Value
Layer 1-Op-Arrhenius-E(kJ/mol)	69.767
Layer 1-Op-Arrhenius-A(cm ² /s)	1.378

Package Properties Output Calculation

- Package SAN 24h at 40C optimized
 - Article 1
- Package SAN 2h at 70C Optimized
 - Article 1
- Package SAN 24h at 40C and 2h at 70C
 - Copy of Article 1
 - Iso(40°C, 1d)
 - Iso(70°C, 2h)

Surface (cm²) 600

Article	Layer 1	Contact Medi...
	ACRYLONIT...	Acetic acid 3%
	Thickness (µm)	1.667E04
Migrant 1	ACRYLONIT...	A(3.30E-11) 0.0001

Layer (Layer 1) Migrant

Diffusion Coefficient

Known
 Interpolation based on Tg
 Pringer
 Arrhenius
 Customized Equation
 Brandsch Equation
 Welle Equation
 In-Silico

Predictions

Temperature Profiles

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

Stepwise Conditions

Time Unit: min Time Max: 305.3 min Number of Cycles: 1

From Temp (°C)	To Temp (°C)	Heating Rate (K/min)	Time (min)
40	70	100	0.3
70	70	0	180
70	20	-10	5
20	20	0	60
20			

Without Statistics
 Monte Carlo Runs
 Fast Distribution

Number of Runs: 10

Package SAN 24h at 40C and 2h at 70C optimized

Geometry: Rectangular

Contact Surface (cm²): 600

Volume of Contact Medium (cm³): 1000

Article	Mass (g)
2)	1000

Fitting Mode

RSS

0 Loops

Loops per serie: 20

mtau: 1
 mtolg: 1E-6
 mtolx: 1E-6 mrealstep: 1E-3

Parameter Name	Value
Layer 1-Op-Arrhenius-E(kJ/mol)	69.767
Layer 1-Op-Arrhenius-A(cm ² /s)	1.378

Package Properties Output Calculation

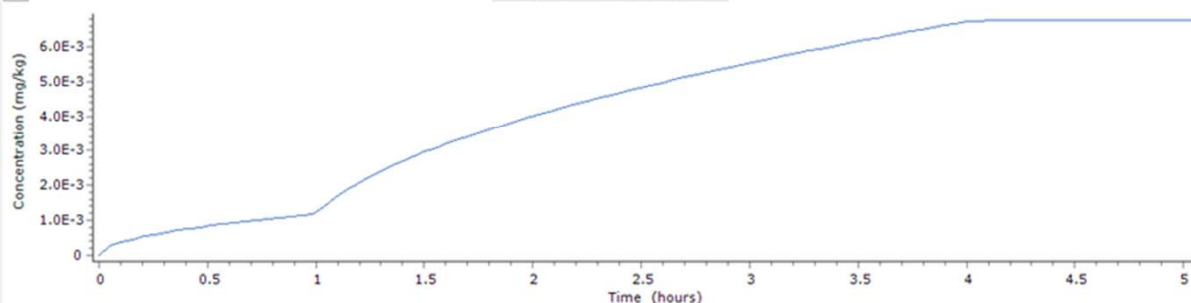
- Package SAN 24h at 40C optimized
 - Article 1
 - Iso(40°C, 1d)
- Package SAN 2h at 70C Optimized
 - Article 1
 - Iso(70°C, 2h)
- Package SAN 24h at 40C and 2h at 70C
 - Copy of Article 1
 - Iso(40°C, 1d)
 - Iso(70°C, 2h)
 - Step(40-70-70-20-20°C, 5 step)

Temperature: 20 (°C) Display unit: mg/kg c(t): draw mean concentration c(t): draw concentration at 0 % of thickness from surface

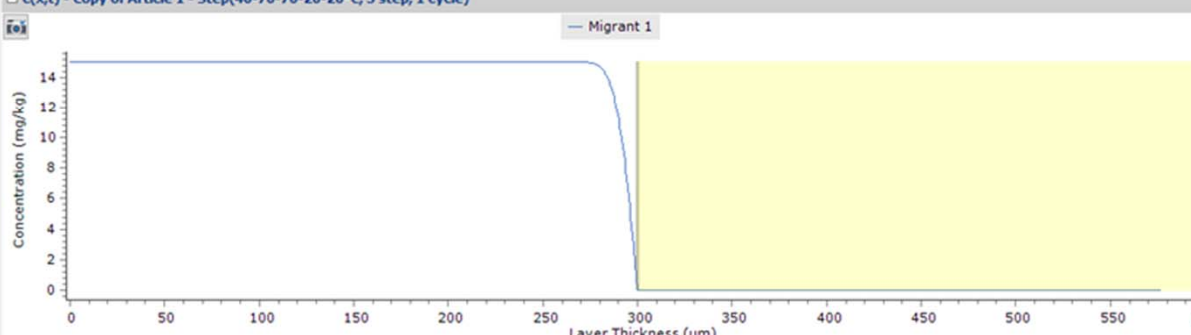
Article	Layer 1	Contact Med...
	ACRYLONIT...	Acetic acid 3%
	Thickness (µm)	1.667E04
	300	
<input checked="" type="checkbox"/> Migrant 1	ACRYLONIT...	0.00676
	14.66	

Concentration Diffusion Coefficient Partition Coefficient Solubility

c(t) - Copy of Article 1 - Step(40-70-70-20-20°C, 5 step, 1 cycle)



c(x,t) - Copy of Article 1 - Step(40-70-70-20-20°C, 5 step, 1 cycle)



Package SAN 24h at 40C and 2h at 70C optimized

Geometry: Rectangular

Contact Surface (cm²): 600

Volume of Contact Medium (cm³): 1000

Width (cm): 10

Height (cm): 10

Length (cm): 10

Add Article

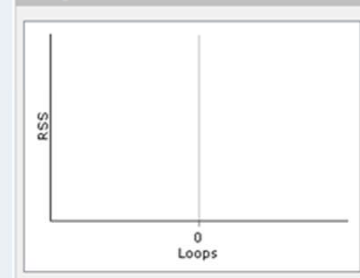
Surface and mass of contact medium by article

Articles	Surfaces (cm ²)	Mass (g)
Copy o...	600	1000

Total surface of all articles (cm²): 600

Switch Package in Fitting Mode

Fitting Mode



Loops per serie: 20

Optimize Refresh

Correlation

mtau: 1

mtolg: 1E-6

mtolx: 1E-6 mrealstep: 1E-3

Parameter Name	Value
Layer 1-Op-Arrhenius-E(kJ/mol)	69.767
Layer 1-Op-Arrhenius-A(cm ² /s)	1.378

Close Fitting Mode for This Package

Create Global Package

2023/7/2

Package Properties Output Calculation

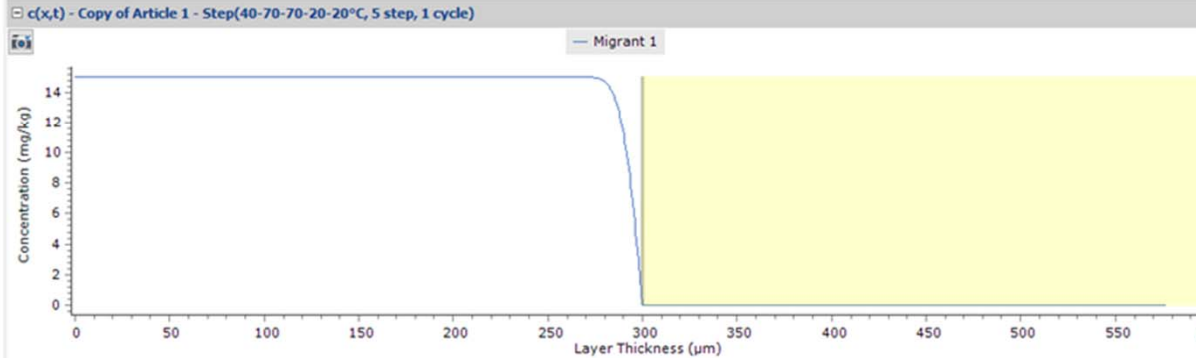
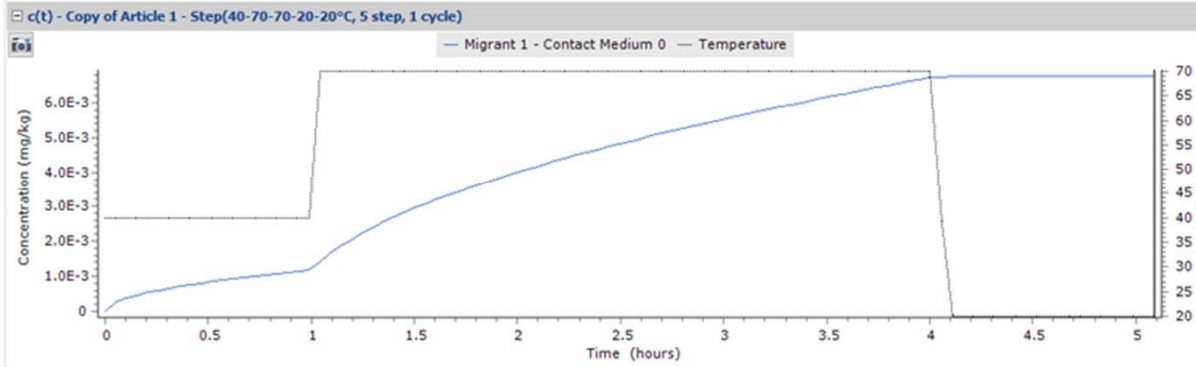
- Package SAN 24h at 40C optimized
 - Article 1
 - Iso(40°C, 1d)
- Package SAN 2h at 70C Optimized
 - Article 1
 - Iso(70°C, 2h)
- Package SAN 24h at 40C and 2h at 70C
 - Copy of Article 1
 - Iso(40°C, 1d)
 - Iso(70°C, 2h)
 - Step(40-70-70-20-20°C, 5 step, 1 cycle)

Temperature: 20 (°C) Display unit mg/kg c(t) : draw mean concentration c(t) : draw concentration at 0 % of thickness from surface

Grid

Article	Layer 1	Contact Med...
	ACRYLONIT...	Acetic acid 3%
	Thickness (µm)	1.667E04
	Migrant 1	ACRYLONIT... 14.66 0.00676

Concentration Diffusion Coefficient Partition Coefficient Solubility



Package SAN 24h at 40C and 2h at 70C optimized

Geometry: Rectangular

Contact Surface (cm²): 600
Volume of Contact Medium (cm³): 1000

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

Surface and mass of contact medium by article

Articles	Surfaces (cm ²)	Mass (g)
Copy o...	600	1000

Total surface of all articles (cm²): 600

Fitting Mode

Loops per serie: 20

Optimize Refresh

Correlation











mtau: 1
mtolg: 1E-6
mtolx: 1E-6 mrealstep: 1E-3

Parameter Name	Value
Layer 1-Dp-Arrhenius-E(kJ/mol)	69.767
Layer 1-Dp-Arrhenius-A(cm ² /s)	1.378

Close Fitting Mode for This Package
Create Global Package

2023/7/2

5.09 (hours)

	220902_To_0_2h at 70C	2022/09/17 7:54	テキスト ドキュメント	1 KB
	220902_To_0_24h at 40C	2022/09/17 7:54	テキスト ドキュメント	1 KB
	220902_To_1a_Package SAN 24h at 40C	2022/09/17 7:54	SML ファイル	2 KB
	220902_To_1b_Package SAN 24h at 40C optimi...	2022/09/17 7:54	SML ファイル	106 KB
	220902_To_2_Package SAN 2h at 70C Optimized	2022/09/17 7:54	SML ファイル	178 KB
	220902_To_3_Package SAN 24h at 40C and 2h ...	2022/09/19 12:28	SML ファイル	283 KB
	220919_To_3_Package SAN 24h at 40C and 2h ...	2022/09/18 16:59	SML ファイル	1 KB
	index	2018/08/20 19:08	Microsoft Edge HTM...	17 KB
	SML6_FM_001_ISO40C_1day	2022/09/19 12:39	JPG ファイル	131 KB
	SML6_FM_001_ISO70C_2hrs	2022/09/19 12:58	JPG ファイル	110 KB



2023/7/2

