

# SPECIFIC MIGRATION LIMITS Software (SML)

Prediction of Migration Rate of Species from Packaging Materials to Packed Goods

### CONTENT

**SML** 

**AKTS E-Learning** 

www.akts.com/sml/e-learning

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## **AKTS E-LEARNING**

The SPECIFIC MIGRATION LIMITS Software (SML) allows the specific migration assessment for complex materials with different geometries and any multi-layer structure. Simulation of the migration process is based on Fick's 2nd law of diffusion under consideration of partitioning between adjacent layers or contact media in closed systems. The software contains a database of more than 20'000 chemicals and offers comprehensive estimation procedures for diffusion and partitioning coefficients. In case of missing required parameters, the software marks the method in red and indicates which parameters are missing. The end-user can add these parameters manually (if known) or has to choose another method.



The use of SPECIFIC MIGRATION LIMITS Software (SML) can proceed in four steps:

The workflow has therefore four main steps:

- 1. Define the package by creating the different articles of the package and introduce their properties.
- 2. Predict the migration using different temperature profiles (iso, non-iso, worldwide climate, etc.).
- 3. Analyse the calculated outputs.
- 4. Check the conformity of the results with corresponding legislations.

#### PACKAGE STRUCTURE

A package is a group of different articles, each having different layers properties. For instance, a bottle can be treated as two articles: the bottle cap and the bottle body. An article is composed of one or more layers of different sizes and properties.



FIG. 1 - A package can be composed of multiple articles.



FIG. 2 - Click on 'Start SML' to start the work with the software.

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Package Properties Output Calculation				
Rew Package         Image: Duplicate Package         Image: Save All Package           Open Package         Image: Close Package         Image: Save Package           Save Package         Image: Save Package         Image: Save Package           Package         Image: Save Package         Image: Save Package           Package         Image: Save Package         Image: Save Package	Import Article     Import Article       Import Article     Close Article       Import Article     Close Article       Article     Article	ッダ Prediction on This Article 、ダ Prediction on All Articles Prediction	∭ M ⊗ File	^
Package	Article	Prediction	File	^



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Create a new empty package. A package is a group of different articles.					
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Packa	age	Article	concentration	Prediction	File	^
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				Geometry		
				Rectangular 🗸 🗸 🗸 🗸 🗸 🗸		]
		Concentration Diffusion Coefficient Part	tition Coefficient	Contact Surface (cm^2):	60	0
	Add Migrant(s)	📈 Run Predi	clion	Volume of Contact Medium (cm^3):	100	0
	Layer 👗 Mig	yrant 🥰 Data		Width (cm): 10 Height (cm): 10 Length (cm): 10 Surface and mass of contact mediu	Add m by article	Article
				Articles Surfaces (cm^2) Article 1 600	Mass (g)	
				Total surface of all articles (cm^2): Switch Package in Fitt	600 ng Mode	
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 $\ensuremath{\textbf{FIG. 5}}$  - Selection of the package geometry (e.g. rectangular).

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Package 1     Surface (cm^2) 6     Article     Add Micra	Concentration Diffusion Coefficient Partition Coefficient Solubility	Add Layer(s)

FIG. 6 – The package can contain one or more articles (e.g. bottle body and its lid).

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FIG. 7 - Construction of an article by adding layers.

Shirt V 6.20       Shirt V 6.20         Package Properties       Output Calculation         Open Package @ Duplicate Package       Prediction on This Article         Open Package @ Close Package       Open Article         Package @ Close Package       Prediction on This Article         Package @ Close Package       State (mr.2)         Package       Article         Package       Article         Package       State (mr.2)         State (mr.2)       State         Output Close       File         Package       Add Magnet(s)         State (mr.2)       State         Add Magnet(s)       State         State (mr.2)       State         Add Magnet(s)       State         State (mr.2)       State         State (mr.2)       State         State (mr.2)       State         State (mr.2)       State         State	■ <b>○ ○ ▲</b> ≥/ -		Ch.41 _ C 20				
Package Propertie:       Output Calculation	페 😢 🖳 🏋 🏹 🔻		SML v 6.20			_	
8 New Package © Duplicate Package 9 Gen Package © Sove Package A: Save All Package: © Open Article © Open Article © Duplicate Article © Duplicate Article © Article © Concentration Prediction on All Article © Energy Article © Open Article © Concentration Prediction on All Article © Energy Article © Open Article © Concentration Prediction on All Article © Energy Article © Open Article © Open Article © Concentration Prediction on All Article © Energy Article © Open Article ©	Package Properties Output	t Calculation					_ @ >
Save Package & Save Package As Package Details Import Article Concentration All Articles Package  Package I Prediction on All Articles Prediction on All A	😭 New Package 🛛 🚔 Duplicate I 🗁 Open Package 🏾 🎇 Close Pack	Package 🔚 Save All Packages kage	New Article         Save Article           Open Article         Duplicate Article	<b>**</b>	$\ensuremath{\swarrow}^{\ensuremath{\phi}}$ Prediction on This Article		
Package     Article     Prediction     File       Image: Surface (cm^2)     500     Image: Surface (cm^2)     Sourcentration       Image: Surface (cm^2)     Sourcentration     Diffusion Coefficient     Solubility       Image: Surface (cm^2)     Image: Surface (cm^2)     Image: Surface (cm^2)       Image: Surface (cm^2)     Image: Surface (cm^2)     Image: Surface (cm^2)       Image: Surface (cm^2)     Image: Surface (cm^2)     Image: Surface (cm^2)       Image: Surface (cm^2)     Image: Surface (cm^2)     Image: Surface (cm^2)       Image: Surface (cm^2)     Image: Surface (cm^2)     Image: Surface (cm^2)       Image: Surface (cm^2)     Image: Surface (cm^2)     Image: Surface (cm^2)       Image: Surface (cm^2)     Image: Surface (cm^2)     Image: Surface (cm^2)       Image: Surface (cm^2)     Image: Surface (cm^2)     Image: Surface (cm^2)       Image: Surface (cm^2)     Image: Surface (cm^2)     Image: Surface (cm^2)       Image: Surface (cm^2)     Image: Surface (cm^2)     Image: Surface (cm^2)       Image: Surface (cm^2)     Image: Surface (cm^2)     Image: Surface (cm^2)       Image: Surface (cm^2)     Image: Surface (cm^2)     Image: Surface (cm^2)       Image: Surface (cm^2)     Image: Surface (cm^2)     Image: Surface (cm^2)       Image: Surface (cm^2)     Image: Surface (cm^2)     Image: Surface (cm^2) <td>🔚 Save Package 🛛 📓 Save Packa</td> <td>age As Package Details</td> <td>📟 Import Article 🎉 Close Article</td> <td>Import Initial Concentration</td> <td>🔊 Prediction on All Articles</td> <td><math>\otimes</math></td> <td></td>	🔚 Save Package 🛛 📓 Save Packa	age As Package Details	📟 Import Article 🎉 Close Article	Import Initial Concentration	🔊 Prediction on All Articles	$\otimes$	
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**FIG. 9** - The properties of the polymer layer can be selected from the database.

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Package 1 LDPE-Ethanol 10%	Article	Brows Brows Reference N CAS Number	Selecting La e Database umber: [ :	ayer Mat	erial(s) ame: olecular Weight: ppe:	POLYMER Filt	×		Add Lay	er(s)
	Thickness (µm):	Namo			AC Number	Doforonco Numbor	Ef A			
	Density (g/cm^3)	CELLULOSE		00	009004-34-6	14500; 43280	5!			
	Layer Abbreviatio	CELLULOSE	ACETATE	00	009004-35-7	14505				
	Material:	CELLULOSE	ACETATE BUTYRATE ACETATE PROPIONATE	00	009004-36-8 009004-39-1	43300;14508; 43 14512	. 5!			
	Layer Details	ETHYLCELLU	JLOSE	00	009004-57-3	16925; 53280	5!			
	Malandaria	3-HYDROXY	BUTANOIC ACID-3-HYDR	ROXYPENTAN 00	080181-31-3	18888	7			
	molecular weigh	NITROCELL	ULOSÉ	00	09004-70-0	22450; 43330	50			
	Log Pow:	POLYBUTAD	JENE EDOVIDIZED	00	09003-17-2	23515				
		POLY(1 4-P		0/	25190-06-1	23530-76570				
	Material specifi	POLYDIMET	HYI STI OXANE (polymer)	00	009016-00-6	23330, 78370				
Uppe POLYHYDR			DXYBUTYRATE	00	29435-48-1	23615				
	🔘 Reali	20110		· ·			× I			
		<					>			
		Previo	ous Layer 🔰 📏 Nex	kt Layer	A	issign 🗙	Close			
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**FIG. 10** – For the search of polymer properties the several options can be applied (e.g. CAS number, name, etc...).

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Packa	ge			Article		Pre	diction	File		^
Package 1     LDPE-Ethanol 10%	Surface (cm^2)	Browse Da	lecting l	ayer Ma	aterial(s) Name:	- D	×		Add La	yer(s)
	C/	AS Number:			Molecular Weight:					
	📗 🛛 Layer (l				_					
	< >				Type:	POLYMER	~			
	Turner					Filte	er			
	Type:			· · · · ·						
	Thickness (µm):	Masterl	DB (1938)	UserDE	3 (1)					
	Density (g/cm^3)	Name			CAS Number	Reference Number	F( ^			
	C	CELLULOSE			0009004-34-6	14500; 43280	5!			
	Layer Abbreviatio	CELLULOSE ACE	TATE		0009004-35-7	14505	_			
	Material:	CELLULOSE ACE	TATE BUTYRATE		0009004-36-8	43300;14508; 43	5!			
	C	CELLULOSE ACE	TATE PROPIONAT	E	0009004-39-1	14512				
	Layer Details	THYLCELLULOS	E		0009004-57-3	16925; 53280	5!			
	Molecular Weich	3-HYDROXYBUT/	ANOIC ACID-3-HY	DROXYPENTAN	0080181-31-3	18888	7.			
	Notecular weigh	VI I ROCELLULOS	э <u>н</u>		0009004-70-0	22450; 43330	St			
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	O Realit		UCIC (DUA DUA	5-1A	0029433-40-1	23013	×			
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Package 1	Surface (cm^2)	Selecting Layer M e Database umber:	Aterial(s) Name: Molecular Weight: Type: P Clear Filt TOB (0) CAS Number 0009002-88-4 769 0009002-88-4 769 0009002-88-4 769			Add Layer(s) Set-Off

**FIG. 12 -** The results of the search: selection of the polymer.

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Package Properties Output	t Calculation			_ @ ×
Sew Package Puplicate Popen Package Close Pack Save Package Save Pack Package	Package kage age As Package Details	New Article     Save Article     Open Article     Duplicate Article     Import Article     Article     Article	Approximation     Approxi	ticle 🕅 cles ⊗
Packa No Contract 1	Surface (cm^2)	Alucie	Prediction	s rite
Package 1	Article Brows	Selecting Layer Mate	rial(s)	Add Layer(s)
	Add Mig Reference N	umber: Name	e: low density	Set-Off
	CAS Number	: Molec	cular Weight:	
				×
	Fill Missin	g Parameters		
	Log Pow not available in the	database	Required for	
	Please enter log Pow		Estimation of partition coefficients with Polarity	y scale
			[	✓ OK X Cancel
	Layer Details			
	Molecular Weigh			
	Log Pow:			
	Material specifie			
	Uppe			
	O Realit		>	
	Previ	ous Layer 📏 Next Layer	Assign 🔀 Close	
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FIG. 13 - Enter missing parameters (if known). In this example the log Pow is missing.

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Package Properties Output Calo	ulation					_ 8 ×
😨 New Package 💣 Duplicate Packa Den Package 🖀 Close Package E Save Package 🖌 Save Package A	age 🙀 Save All Packages <sub>Is</sub> 🛜 Package Details	New Article         Save Article           Open Article         Duplicate Article           Import Article         Close Article	Import Initial Concentration	$\mathcal{A}^{\phi}$ Prediction on This Article $\mathcal{A}^{\phi}$ Prediction on All Articles	<b>X</b>	
Package	6 ( ) 10 [100]	Article		Prediction	File	A
Package 1 Sur LDPE-Ethanol 10%	tide Thickness (µm)	Layer 1 Layer 2 POLYETHYLE Not Defined 100 100 Diffusion Coefficient Parti	tion Coefficient S	Solubility		Add Layer(s)
Add Migrant(s)						
Ty Th De La Ma L	Pe:      Polymer     idness (µm):     Imit (g/cm^3):     0.925     yer Abbreviation:     Layer 1     Pol.YETHYL Layer Details     tolecular Weight (g/mol):     15     og Pow:     N/ Material specific constants for     ① Upper Limit: A**p     ⑦ Realistic Case: A*p:	Copy From     Reset Layer     Set       O Contact Medium       Image: Set	re (°C): -125 > Piringer A*p: 11.5 Ap: 10	Database		
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FIG. 14 - Introducing thickness of the polymer layer.

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🎧 Save Package 🛛 🔏 Save Packa	age As	Import Article 🐹 Close Article	Concentration	> reaction on An Andrea	$\otimes$	
Packa	age	Article		Prediction	File	A
Package 1     DPE-Ethanol 10%	Surface (cm^2) 600					4
	Article	Layer 1 Layer 2				
	Thickness (um)	POLYETHYLE Not Defined				Add Layer(s)
		Letter Difference Confficient Darth	No. Configurate	Culturation .		0
		oncentration Diffusion Coefficient Part	uon coencient	Solubility		
	Add Migrant(s)			Run Prediction		Set-Off
	Layer (Layer 1)	🍝 Migrant 🦧 Data				
	< > X	Copy From Reset Layer	et to User Defined	😸 Database		
	Type:      OPolymer	O Contact Medium				
	Thickness (µm): 1000					
	Density (g/cm^3): 0.925					
	Laver Abbreviation: Laver 1					
	Material: POLYETHY	LENE, LOW DENSITY (PE)				
	Layer Details					
	Molecular Weight (g/mol): 1	Glass Transition Temperatu	re (°C): -125			
	Log Pow: N	/A				
	Material specific constants for	estimation of diffusion coefficients according to	Piringer			
	Upper Limit: A'*p	: 11.5 Tau: 0	A*p: 11.5			
	<ul> <li>Realistic Case: A'p:</li> </ul>	10 Tau: 0	Ap: 10			
6.20   32-bit						

FIG. 15 – The name of the layer can be changed (if requested).

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Package Properties Output	t Calculation					- 8	×
<ul> <li>New Package Puplicate</li> <li>Open Package Close Package</li> <li>Save Package</li> <li>Save Package</li> </ul>	Package 🕌 Save All Packages kage age As 🔐 Package Details	Image: New Article         Image: Save Article           Image: Open Article         Image: Duplicate Article           Image: Image: Article         Image: Close Article	Import Initial Concentration	ッダ Prediction on This Article ッダ Prediction on All Articles	<ul> <li>Image: Second sec</li></ul>		
Packa	surface (cm^2) 600	Article		Prediction	File	8	
LDPE-Ethanol 10%	Article Thickness (µm)	LDPE Layer 2 POLYETHYLE Not Defined 1000 100				Add Layer(	(s)
Concentration Diffusion Coefficient Partition Coefficient Solubility					Г		
	Add Migrant(s)			Run Prediction		Set-Off	
	Layer (LDPE)	Migrant 💰 Data					
Copy From Reset Layer 💄 Set to User Defined 📄 Database							
	Type: OPolymer	O Contact Medium					
	Thickness (µm): 1000						
	Density (g/cm^3): 0.925						
	Layer Abbreviation: LDPE						
	Material: POLYETHYL	ENE, LOW DENSITY (PE)					
	Layer Details						
	Molecular Weight (g/mol): 15	00 Glass Transition Temperature	e (°C): -125				
	Log Pow: N/	A					
	Material specific constants for	estimation of diffusion coefficients according to	Piringer				
	Upper Limit: A'*p	: 11.5 Tau: 0 /	A*p: 11.5				
	Realistic Case: A'p:	10 Tau: 0 /	Ap: 10				
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**FIG. 16 -** Introducing materials specific constants required for estimation of the diffusion coefficients by Piringer method with 'upper limit' or 'realistic case' calculation.

#### FOOD GROUP / SIMULANT -

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Package Properties Output	Calculation			– 🗗 🗙
😨 New Package 💣 Duplicate F 🏷 Open Package 🦉 Close Pack 🙀 Save Package 🚮 Save Packa	Package 🕌 Save All Packages kage age As 🖀 Package Details	Import Article         Import Initial Concentration	) )) (8)	
Packa	ge	Article Prediction	File	~
V Package 1	Surface (cm^2) 600 Article Thickness (µm)	LDPE         Layer 2           POLVETHYLE         Not Defined           1000         100		Add Layer(s)
	C	oncentration Diffusion Coefficient Partition Coefficient Solubility		
	Add Migrant(s)	Kun Prediction		Set-Off
	🚺 Layer (LDPE) 🧕	Migrant 🕰 Data		
	< > X	Copy From Reset Layer		
	Type:      OPolymer	O Contact Medium		
	Thickness (µm): 1000			
	Density (g/cm^3): 0.925			
	Layer Abbreviation: LDPE			
	Material: POLYETHY	LENE, LOW DENSITY (PE)		
	Layer Details			
	Molecular Weight (g/mol): 1	500 Glass Transition Temperature (°C): -125		
	Log Pow: N	A		
	Material specific constants for	estimation of diffusion coefficients according to Piringer		
	Upper Limit: A'*p	2: 11.5 Tau: 0 A*p: 11.5		
	<ul> <li>Realistic Case: A'p:</li> </ul>	10 Tau: 0 Ap: 10		
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FIG. 1 - Selection of the next layer, 'layer 2'.

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Package	Article		Prediction	File	^
Package 1     Surface (cm^2) 600     Article     Thickness (um)     C	LDPE Layer 2 POLYETHYLE Not Defined 1000 100 oncentration Diffusion Coefficient Part	ition Coefficient	Solubility		Add Layer(s)
Add Migrant(s)	A Migrant R Data		Run Prediction		Set-Off
Type:  Polymer Thickness (µm): 100 Density (g/cm^3): N/A Layer Abbreviation: Layer 2 Material: Not Define Layer Details Molecular Weight (g/mol): N Log Pow: N Material specific constants for @ Upper Limit: A'*;	Copy From Reset Layer	et to User Defined	Database		-
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FIG. 2 – For the layer 2 the change from 'polymer' into a 'contact medium' is required.

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Package Properties Output	t Calculation			-	a x
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Packa	inge AS	Article Prediction	File		~
Package 1	Surface (cm^2) 600		- The		~
LDPE-Ethanol 10%	Article Thickness (µm)	LDPE         Contact Med           POLYETHYLE         User Defined           1000         1.667E04		Add Lay	er(s)
	C	oncentration Diffusion Coefficient Partition Coefficient Solubility		-6	A
	Add Migrant(s)	ر Run Prediction		Set-O	<b>)</b> ff
	Layer (Contact Medi	ium 0) 🚺 Migrant 🕰 Data			
	< > X	Copy From Reset Layer			
	Type: OPolymer	Contact Medium			
	Thickness (um): 16667				
	Describe (c. (m. 6.2))				
	Density (g/cm <sup>-+</sup> 3): 0.98				
	Layer Abbreviation: Contact Me	edium 0			
	Contact Medium Details				
	Food group (according to Anne	x III of Regulation (EII) 10/2011 and some more)			
	Not Defined			~	-
	Simulant				- C
	User Defined			~	
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FIG. 4 - Selection of the requested food group (in English and Deutsch).

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Rew Package 💣 Duplicate F Dopen Package 🍘 Close Pack Save Package 📓 Save Packa Packa	Package 🕌 Save All Packages age ge As 😭 Package Details ge	Image: Save Article         Image: Save Article           Image: Open Article         Image: Duplicate Article           Image: Image: Save Article         Image: Close Article           Article         Article	Import Initial Concentration	of Prediction on This Article و مراجع Prediction on All Articles Prediction	∭ ∭ ⊗ File		~
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	Type: OPolymer Thickness (um): 16667 Density (g/cm^3): 0.98 Layer Abbreviation: Contact Me Contact Medium Details Food group (according to Anne Ethanol 10% - food simulant ( Simulant User Defined User Defined User Defined User Defined Contact Medium A: 0 Realistic Case A: 0	Copy From  Reset Layer  Copy From  Copy From  Reset Layer  Copy From  Reset Layer  Copy From  Reset Layer  Copy From  Reset Layer  Reset Layer Reset Layer  Reset Layer  Reset Layer  Reset Layer  Reset Layer  Reset Layer Reset Layer Reset Layer Res	ore) /Ethanol 10% - Leber	rsmittelsimulanz (nicht akoholische L	ebensr	nittel oc	5
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FIG. 5 - Selection of the 'Ethanol 10%' as a contact medium.

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Save Package Puplicate F Popen Package Puplicate F Save Package Puplicate F Save Package Puplicate Puplica	Package 🕌 Save All Packages age ige As 🖀 Package Details	Image: New Article         Save Article           Open Article         Duplicate Article           Import Article         Close Article	Import Initial Concentration	ッグ Prediction on This Article ッグ Prediction on All Articles	<ul> <li>(1)</li> <li>(2)</li> <li>(3)</li> <li>(3)</li> <li>(3)</li> <li>(4)</li> <li>(5)</li> <li>(5)</li> <li>(6)</li> <li>(6)</li> <li>(7)</li> <li>(7)</li></ul>		
Packa	ge Surface (cm 62)	Article		Prediction	File		
LDPE-Ethanol 10%	Article Thickness (µm)	LDPE         Contact Medi           POLYETHYLE         Ethanol 10%           1000         1.667E04				Add Lay	yer(s)
	C	oncentration Diffusion Coefficient Parti	ition Coefficient	Solubility		-6	à
	Add Migrant(s)	' '		Run Prediction		Set-C	9 Dff
	Layer (Contact Medi	um 0) 🧴 Migrant 🕰 Data					
	< > X	Copy From Reset Layer					
	Type: OPolymer	Contact Medium					
	Thickness (µm): 16667						
	Density (a/cm^3): 0.98						
	Laver Abbreviation: Contact Me	edium 0					
	Contact No						
	Contact Medium Details						
	Food group (according to Anne	x III of Regulation (EU) 10/2011 and some mor	e)				
	Ethanol 10% - food simulant (	non-alcoholic foods or alcoholic foods < 6%) / i	Ethanol 10% - Leber	nsmittelsimulanz (nicht alkoholische l	Lebensr	nittel oc	~
	Ethanol 10%						~
	Parameters required for estimation	tion of partition coefficient based on Powe					
	Upper Limit A: 1	B: -3					
	O Realistic Case A: 1.07	B: -1.82					
	Circumste case ini 1.07	D1 102					
6.20   32-bit							

**FIG. 6** - Introducing parameters required for estimation of the Octanol / Water partition coefficient by 'upper limit' or 'realistic case' method.

The migrant properties panel allows defining the properties of the currently selected migrant. When the migrant is set as user-defined, it is possible to enter its properties manually. Otherwise, if the migrant is loaded from the database, its properties are filled automatically.

The database allows browsing for known migrants (more than 20'000 chemicals: additives, monomers, photoinitiators, pigments, solvents, etc.).

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Package Properties Output	t Calculation					_ 8	×
🚭 New Package 🛛 Duplicate 🏠 Open Package 🎯 Close Pack 🔚 Save Package 📝 Save Pack	Package kage age As Package Details	Image: Sevential sevent	Import Initial Concentration	ッ <sup>d</sup> Prediction on This Article 、 <sup>d</sup> Prediction on All Articles	<b>X</b>		
Packa	ige	Article		Prediction	File		^
V Package 1	Surface (cm^2) (600 Article Thickness (um) Add Migrant(s)	LDPE Contact Medi POLVETHYLE Ethanol 10% 1000 1.667E04 oncentration Diffusion Coefficient Part	ition Coefficient	Solubility		Add Layer(	s)
	Type: Oplymer Thickness (um): 16667 Density (g/cm^3): 0.98 Layer Abbreviation: Contact Me Contact Medium Details Food group (according to Anne Ethanol 10% food simulant ( Simulant Ethanol 10% Parameters required for estima (© Upper Limit A: 1	Copy From Keset Layer  Copy From Keset Layer  Copy From Keset Layer  Copy From Keset Layer  Transmission (EU) 10/2011 and some mor  ron-alcoholic foods or alcoholic foods < 6%) /1  tion of partition coefficient based on Pow: B: -3	e) Ethanol 10% - Leber	nsmittelsimulanz (nicht alkoholische l	.ebensi	nittel oc 🗸	
6 20   32-1-i+	ORealistic Case A: 1.07	B: -1.82					

FIG. 1 - Adding migrants.

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Package Properties Output	t Calculation			_ 8 ×	
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Packa	ige	Article	Prediction	File ^	
V = Package 1	Surface (cm^2) 600			4	
LDPE-Ethanol 10%	Article Thickness (µm)	LDPE Contact Medi POLYETHYLE Ethanol 10% ) 1000 1.667E04		Add Layer(s)	
	C	Concentration Diffusion Coefficient Partiti	ion Coefficient Solubility		
Add Migrant(s)					
	Layer (Contact Med	dium 0) 🚺 💰 Migrant 🕰 Data	<u> </u>		
		Copy Fro	×		
	Thickness (µm): 16667		V OK Cancel		
	Density (g/cm^3): 0.98				
	Layer Abbreviation: Contact M	1edium 0			
	Contact Medium Details				
	Food group (according to Anne	ex III of Regulation (EU) 10/2011 and some more	)		
	Ethanol 10% - food simulant	(non-alcoholic foods or alcoholic foods $< 6\%)$ / Et	thanol 10% - Lebensmittelsimulanz (nicht alkoholisch	ie Lebensmittel oc $ \smallsetminus $	
	Simulant				
Ethanol 10%					
Parameters required for estimation of partition coefficient based on Pow:					
	Upper Limit A: 1	B: -3			
	O Realistic Case A: 1.07	B: -1.82			
6.20   32-bit					

FIG. 2 - Introducing number of migrants.

	SML v 6.20	_	Ц×
Package Properties Output Calculation			– 🗗 🗙
😨 New Package 🚽 Duplicate Package 🕌 Save All 🕑 Open Package 🎯 Close Package 🙀 Save Package 🛃 Save Package As 🗑 Package Package	ckages Rew Article Save Article Duplicate Article Import Initial Concentration Article & Close Article & Prediction on All Article & Prediction & Predict	) M S File	~
▼ Package 1 Surface (cm^2) 600			×
Package 1 LDPE-Ethanol 10% Article Migrant 1 Not Migrant Details Molecular Weight (g/ Density (g/cm^2) : Molecular Value (A	DPE Contact Med POLYETHYLE Ethanol 10% POLYETHYLE Ethanol 10% fined 0 0 0  Concentration Diffusion Coefficient Partition Coefficient Solubility  PHigrant (Higrant 1)  PHigrant (Higrant 1)  Phigrant 1  Not Defined  N(A Melting Point (°C): N/A  N/A Button 1  N/A Ing Prove: N/A		Add Layer(s)
6.20   32-bit			

**FIG. 3** - The properties of Migrants can be found in the database.

🔜 🕜 🚺 🌻 🔆 🔻		5	SML v 6.20					-		$\times$
Package Properties Output Calculation									-	a ×
<ul> <li>New Package Puplicate Package</li> <li>Open Package</li> <li>Close Package</li> <li>Save Package</li> <li>Save Package As</li> <li>Package</li> </ul>	e All Packages kage Details	New Article Open Article Import Article	Gave Article Duplicate Article Close Article Article	e Import Ini Concentrat	م می Prec itial مرف Prec tion	diction on Th diction on Al Prediction	is Article I Articles	💓 🔌 Rile		~
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620122 82	ACIDS, FAT ACIDS, FAT ACRYLAMID	IT, UNSATURATED(E: TY, UNSATURATED(C: E us Migrant > Ne	ext Migrant	068783-41-5	10599/92A; 11 10599/92A; 11 10630	05 7: 1. X Close				

FIG. 4 - Searching for the migrant in the database by using the 'reference number' option.

	SML v 6.20		- 🗆 ×
Package Properties Output Calculation     Package Properties Output Calculation     Package Duplicate Package     Save Package Close Package     Save Package Save Package As     Package     Package	s Rew Article Save Article Save Article Save Article Save Article Save Article Import Article Concentration Article	ッダ Prediction on This Article ッダ Prediction on All Articles Prediction	
Padage 1 Padage 1 DDPE-Ethanol 10% Artice Migrant 1 Migrant Abbreviat Migrant Abbreviat Migrant Detail Molecular Volume Molecular Volume	Selecting Migrant(s) wse Database Plumber: 68320 Name: Ser: Molecular Weight: Type: Z Clear Fil MasterDB (1) UserDB (1) CAS Number Ref CYL 3-(3,5-DI-tert-BUTYL-4HYDROXYPHE 0002082-79-3 683 vious Migrant Next Migrant Assi	- X	Add Layer(s) Set-Off
6.20   32-bit			

FIG. 5 - Selection of the required migrant by clicking the button "Assign".

🔜 🕜 1 🌻 💥 📼			SML v 6.20			-	
Package Properties Output	t Calculation						– @ ×
<ul> <li>New Package Puplicate</li> <li>Open Package Close Pack</li> <li>Save Package Save Packa</li> </ul>	Package 🕌 Save All Packages kage age As 😚 Package Details age	New Article	Gave Article	Import Initial Concentration	o Prediction on Thi مر Prediction on All Prediction	Articles	
V Package 1	Surface (cm^2)				-	1	4
LDPE-Ethanol 10%	Artide Migrant 1	Selecting	Migrant(s)				Add Layer(s)
	sml						×
	⑦ Fill Missin	g Parame	eters				
	Molecular volume not availa	ble in the databas	e	Required for			
	Please enter molecular volu	me		Estimation of diff	usion coefficients with W	elle	
						🖌 ОК	Cancel
	Migrant Detail						
	Molecular Weight						
	Density (g/cm^3)						
6 20 1 21 1-2	Molecular Volume	us Migrant	Next Migrant	Assig	n X Close		
6.20 32-bit							

FIG. 6 - Missing parameters, here the Molecular Volume, can be added (if known).

🔜 🕜 🜖 🌻 💥 📼		LDPE-Ethanol 10	0% (Package 1) - SML v	6.20		_	
Package Properties Output Calculation							_ 8 ×
중 New Package 중 Duplicate Package ⓒ Open Package 중 Close Package ⓒ Save Package 중 Save Package As Package	ave All Packages ackage Details	New Article	Gave Article	Import Initial Concentration	ッダ Prediction on This Article ッダ Prediction on All Articles Prediction	∭ ∭ ⊗ File	~
Package Package 1 LDPE-Ethanol 10% Mgrant 1 Mgrant 1 Mgrant 2 Migrant 2	2) 600 Thickness (um OCTADECYL (Migrant(s) viation: Mig viation: Mig ight (g/mol): 5 n^3): 0 ume (Å^3): N	LDPE Cor POLYETHYLE Eth ) 1000 1.6 0 0 Concentration Diffu Gopy From figrant 1 CTADECYL 3-(3,5-DI-b 30.88 .929 /A	Article	tion Coefficient	Solubility Solubility Database	File	Add Layer(s)
6.20   32-bit							

FIG. 7 - Layers of the article and migrant are defined.

#### - MIGRANTS PROPERTIES (CONCENTRATION, DIFFUSION -AND PARTITION COEFFICIENT

For the prediction of the migration process, it is necessary to introduce the key parameters of the migrant:

- ► The concentration
- ► The diffusion coefficient
- ► The partition coefficient

🔜 🕜 🜖 🌻 💥 🔻	LDPE-Ethanol 10% (Package 1) - SML v 6.20	- 🗆 X
Package Properties Output Calculation		_ @ ×
New Package      Duplicate Package     Save A     Open Package     Save Package      Save Package As     Package	I Packages e Details Packages e Details Prediction on This Article mport Article Close Article Minport Article Concentration Article Prediction on All Articles Prediction on All Articles Predict	Image: Second secon
Package 1 Surface (cm^2)	00	
E LDPE-Ethanol 10%	LDPE         Contact Medi           POLYETHYLE         Ethanol 10%           ideness (µm)         1000           1.667E04         TADECYL           0         0	Add Layer(s)
	Concentration Diffusion Coefficient Partition Coefficient Solubility	Set-Off
💧 Add Migr	nt(s)	
Layer (LD	PE) 👗 Migrant (Migrant 1) 🦧 Data (Concentration)	
Extended Pr Concentration (mg	operties kg) 0	

FIG. 1 - Defining the migrant concentration.



FIG. 2 - Introducing concentration of migrant in mg/kg (ppm).

🔜 🕜 🕦 🌻 💥 👳	LDPE-Ethanol 10% (Package 1) - SML v 6.20		_	
Package Properties Output Calculation				_ @ ×
<ul> <li>New Package Package Duplicate Package</li> <li>Open Package Close Package</li> <li>Save Package</li> <li>Save Package</li> <li>Save Package</li> <li>Package</li> </ul>	Image: New Article     Image: Save Article       Image: Open Article     Image: Duplicate Article       Image: Image: New Article     Image: Save Article       Image: Image: New Article     Image: Save Article       Image: Article     Article	ッダ Prediction on This Article ッダ Prediction on All Articles Prediction	) M (S) File	^
Package 1     Surface (cm^2) 600     Article     Thickness (um     Migrant 1 OCTADECYL.     Sufface (cm/2) 600     Article     Thickness (um     Migrant 1 OCTADECYL.     Sufface (cm/2) 600     Extended Properties     Concentration (mg/kg) 500		Solubility		Add Layer(s)
0.20 02-01				

FIG. 3 - Selection of diffusion coefficient.

🔜 🙆 🔒 🍨 😓		LDPE-Ethanol 10% (Package 1) - SML v 6.20		_	
Package Properties Output	Calculation				_ 🖻 X
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Packa	ge	Article	Prediction	File	~
<ul> <li>EDPE-Ethanol 10%</li> </ul>	Artide Thickness (µm) Migrant 1 OCTADECYL	LDPE Contact Medi POLYETHYLE Ethanol 10% 1000 1.667E04 1E-11 0.0001			Add Layer(s)
	C	ncentration Diffusion Coefficient Partition Coefficient	Solubility		CO Sat Off
	Add Migrant(s)		Run Prediction		Set-Off
	Layer (LDPE)	Migrant (Migrant 1)	ent)		
	Diffusion Coefficient				
	Known	Known Value			
	O Interpolation based on Tg	Diffusion Coefficient (cm^2/s): 1E-11			
	Piringer     Arrhenius     Customized Equation	Set to Default Values			
	O Brandsch Equation				
	O Welle Equation				
	Apply Same Mode to This Laye	Set All to Default Value Apply Same Mode to All L	ayers		
6 20 I 22 bit					

**FIG. 4 -** Introducing diffusion coefficient (if known, here le-ll is a default value) or selection of an estimation method (e.g. Piringer). In this example the Welle equation is marked in red because its use is impossible due to the lack of parameters required in this method.

🔜 😮 🗊 🍷 💥 📼 LDPE-Ethanol 10% (Package 1) - SML v 6.20 —	□ ×
Package Properties Output Calculation	_ @ ×
Image: Save Package       Image: Deckage       Image: Deckage	
Package Article Prediction F	
Surface (cm^2) 600 Article UDPE Contact Medi POLVETHVLE Ethanol 10% Migrant 1 OCTADECY F(2,263E:10) 0.0001 Concentration Diffusion Coefficient Partition Coefficient Solubility Add Migrant(s) Add Migrant(s) Migrant (Migrant 1) Diffusion Coefficient Example Temperature (*C): 20 Nnown Diffusion based on Tg Piringer Calculation Parameters Interpolation based on Tg Piringer Calculation Parameters Interpolation based on Tg Piringer Calculation Parameters Migrant Molecular Weight (g/mo)): 530.9 Migrant Molecular Weight (g/mo)): 530.9	Add Layer(s)
6.20132-bit	



<b>A O O O O O O O O O O</b>	LDPE-Ethanol 10% (Package 1) - SML v 6.20	- 🗆 X
Deduce Departies Output Coloridation		
Package Properties Output Calculation Open Package Properties Output Calculation Open Package Open Package Close Package Save Package Save Package </td <td>LDPF-Ethanol 10% (Package 1) - SML v 6.20 es Prediction on This Article Popen Article Duplicate Article Import Initial Concentration POLYETHYLE Ethanol 10% Import Initial Concentration POLYETHYLE Ethanol 10% Import Initial Concentration POLYETHYLE Ethanol 10% Import Initial Concentration IDPE Contact Medi POLYETHYLE Ethanol 10% Import Initial Concentration IDPE Contact Medi POLYETHYLE Ethanol 10% Import Initial Concentration Import Initial Concentration Import Initial Concentration Import Initial Contact Medi POLYETHYLE Import Initial Contact Medi POLYETHYLE Import Initial Concentration Import Initial Contact Medi POLYETHYLE Import Initial Contact Medi POLYETHYLE Import Initial Contact Medi Import Initial Contact Medi POLYETHYLE Import Initial Concentration Import Initial Concentration Import Initial Concentration Import Initial Concentration Import Initial Import Initial Contact Medi Import Initial Concentration Import Initial Import Initial Impor</td> <td>- C X - C X -</td>	LDPF-Ethanol 10% (Package 1) - SML v 6.20 es Prediction on This Article Popen Article Duplicate Article Import Initial Concentration POLYETHYLE Ethanol 10% Import Initial Concentration POLYETHYLE Ethanol 10% Import Initial Concentration POLYETHYLE Ethanol 10% Import Initial Concentration IDPE Contact Medi POLYETHYLE Ethanol 10% Import Initial Concentration IDPE Contact Medi POLYETHYLE Ethanol 10% Import Initial Concentration Import Initial Concentration Import Initial Concentration Import Initial Contact Medi POLYETHYLE Import Initial Contact Medi POLYETHYLE Import Initial Concentration Import Initial Contact Medi POLYETHYLE Import Initial Contact Medi POLYETHYLE Import Initial Contact Medi Import Initial Contact Medi POLYETHYLE Import Initial Concentration Import Initial Concentration Import Initial Concentration Import Initial Concentration Import Initial Import Initial Contact Medi Import Initial Concentration Import Initial Import Initial Impor	- C X -
Diffusion Coefficie Known Interpolation based on Pringer Arrhenius Customized Equation Brandsch Equation Welle Equation In-Silco Apply Same Mode to This	nt       Example Temperature (*C):       20         Piringer Calculation Parameters         g       Layer       A'p:       11.5         Tau:       0         Migrant       Molecular Weight (g/mol):       530.9         ayer       Set All to Default Value       Apply Same Mode to All Layers	

FIG. 6 - Selection of partition coefficient.

🔜 🕜 🟮 🕈 💥 📼		LDPE-Ethanol 10% (Package 1) - SML v	6.20		_		×
Package Properties Output	t Calculation					_	∂ ×
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Package 1	Surface (cm ^2) 500 Article Thickness (um) Migrant 1 OCTADECYL C Add Migrant(s) (i) Layer (Contact Medu Partition coefficient ( © Known Solubility Van't Hoff Pow Polarity scale Set All to Default Value? Applied	Mucle  LDPE Contact Medi POLYETHYLE Ethanol 10% 1000 1.667E04  m 0)  Migrant (Migrant 1)  (Kp)  Known Value  1  pply Same Mode to All Layers and Migrants	ition Coefficient	Solubility		Add Lav	(s) Off
6.20132-bit							

**FIG. 7** - Introducing of partition coefficient (if known) or selection of an estimation method (e.g. Octanol /Water partition coefficient). In this example the Polarity Scale is marked in red and is not available because of missing polarity scale parameters. Generally, two arbitrary selected partition coefficients according to the JRC guideline are used for upper limit calculations: kpF = 1 if the migrant is soluble in the food contact material/ simulant and kpF = 1000 if the migrant is not soluble in the food contact material/ simulant. The 'POW' method uses the relationship between log POW (derived from the polarity of the migrant) and log kpF and provides a more precise partition coefficient.



FIG. 8 - Partition coefficient based on Octanol/Water method.

#### MIGRANTS CALCULATION

When all properties of an article are introduced, it is possible to proceed with prediction calculations by clicking on the "Run Prediction" button.

The predictions of the migration can be performed for different temperature profiles:

- Isothermal
- Non-Isothermal
- Stepwise
- Modulated
- Shock
- Worldwide
- ► STANAG
- Customized

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Package Properties Outpu	t Calculation			_ @ ×
<ul> <li>Rew Package</li></ul>	Package 📊 Save All Packages kage age As 🛛 🖓 Package Details	Image: Second	<b>X</b>	
Packa	age	Article Prediction	File	•
Package 1	Surface (cm^2) [600 Article Migrant 1 OCTADECYL .	LDPE         Contact Medi           POLYETHYLE         Ethanol 10%           1000         1.667E04           POLETO         Prile10		Add Layer(s)
				Set-Off
	Add Migrant(s)	Run Prediction		
	Layer (Contact Medi	um 0) 🚡 Migrant (Migrant 1) 🦧 Data (Partition Coefficient)		
	Partition coefficient	(Кр)		
	() Known	Pow Calculation Parameters		
	Osolubility	$Kpf(-) = 10^{(B + A * log(Pow(-)))}$		
	○ Van't Hoff	Food A: 1		
	Pow	Food B: -3		
	O Polarity scale	rigrant LogPow: 13.41		
		Note: The estimation of Kpf based on Pow is limited to temperature below 60°C		
	Set All to Default Value?	pply Same Mode to All Layers and Migrants		
6.20   32-bit				

**FIG. 1 -** Prediction of Migration.

		20		
	PP-Ethanol 10% (Package I) - SiviL V 0	.20	_	L
Package Properties Output Calculation				_ 0 ×
Image: Source of the second	New Article         Save Article           Open Article         Duplicate Article	Predict	ion on This Article	
🔚 Save Package 📓 Save Package As	🐖 Import Article 🕃 Close Article	Concentration	Ion on All Articles 🛞	
Package	Article	P	rediction File	^
Predictions				× ×
Iso Non-Iso Step N	Iodulated Shock Worldwide	STANAG Custom	ized Repeated Use	
Isothermal Conditions			Time May 10 day	, , , , , , , , , , , , , , , , , , ,
	]		Without Statistics	~ ///
Temperature = 20 °C			Monte Carlo Runs	
ΔT = 20 °C			Number of Runs 10	-
Number of Teathering - 1			Include Sobol Run	is
			O Fast Distribution	
Final Temperature = 20 °C			O Family Approach	
			🕞 Save 📂 Lo	ad
	Number of steps	for this output: 100	🖌 OK 🗙 Car	ncel
Set All to Default Value?	Apply Same Mode to All Layers and Migrants			
6.20   32-bit				

**FIG. 2 -** Prediction of Migration occurring under isothermal conditions (during 10 days at 20°C).



**FIG. 3** - Concentration profile of migrant (Octadecyl 3-(3,5-di-tert-butyl-4-hydroxyphenyl) propionate) in the contact medium over time, no migration of migrant to food simulant 'Ethanol 10%' is found.



**FIG. 4 -** Concentration profile of migrant over layer thickness and time (no migration to food simulant).



**FIG. 5 -** Apply the option 'Duplicate Article' to modify the article properties in a new simulation.

🔜 🕜 🚺 🌻 💥 🔻			PP-Ethanol 109	6 (Package 1) - SML v 6	i.20		-			
Package Properties Output	Calculation							_ 8 ×		
😨 New Package 🛛 🚔 Duplicate F	Package 🔚 Save Al	ll Packages	New Article	Save Article		🔎 Prediction on This Article	8			
Save Package Save Packa	age	e Details	Import Article	Close Article	Import Initial	🔎 Prediction on All Articles	8			
Packa	ae		in port intere	Article	Concentration	Prediction	File	~		
Package 1	Surface (cm^2) 5	00						4		
✓	Article		LDPE Con	itact Medi						
	Thi	ickness (µm)	1000 1.6	67E04				Add Layer(s)		
	Migrant 1 OC	TADECYL	500 0					-0		
	Concentration         Diffusion Coefficient         Partition Coefficient         Solubility         Concentration         Set-Off           Add Migrant(s)         Add Migrant(s)									
	Add Migrant(s)     Set-Off       Image: Layer (LDPE)     Image: Migrant									
	📗 🛛 Layer (LD	OPE) 🧴	Migrant 📢	Data						
	< >	X	Copy From	Reset Layer 💄 Se	et to User Defined	📄 Database				
	Type:	Polymer	O Contact Me	dium						
	Thickness (µm):	1000								
	Density (g/cm^3):	0.925								
	Layer Abbreviation:	LDPE								
	Material:	POLYETHYL	ENE, LOW DENSITY (	PE)						
	Layer Details									
	Molecular Weight (	(g/mol): 15	500 G	lass Transition Temperatu	ure (°C): -125					
	Log Pow:	N/	A							
Peckage Properties Output Calculation -										
	Upper I	Limit: A'*p	: 11.5	Tau: 0	A*p: 11.5					
	🔿 Realisti	ic Case: A'p:	10	Tau: 0	Ap: 10					
( 201 22 L 2										
0.20   32-DIT										

**FIG. 6 -** Selection of the polymer layer.

🔜 🕜 📵 🌻 💥 📼			PP-Ethanol 10% (Package 1) - SML v 6.20	-	
Package Properties Output 0	Calculation				_ @ ×
Rew Package 🔮 Duplicate Package 🔮 Duplicate Package 😭 Close Packa Rew Package 😭 Save Package Save Package	ackage 📊 Save / ige ge As 🛜 Packa	All Packages ige Details	New Article     Duplicate Article     Move Article     Duplicate Article     Import Initial     Concentration     Article     Article	<ul> <li>(1)</li> <li>(2)</li> <li>(3)</li> <li>(3)</li> <li>(3)</li> <li>(4)</li> <li>(5)</li> </ul>	
Packag	Surface (cm^2)	500	Article Prediction	File	
Package I LDPE-Ethanol 10% 	Article Migrant 1	hickness (µm)	IDPE         Contact Medi           POL/TEHYLE         Ethanol 10%           1000         1.667E04           500         0		Add Layer(s)
		Co	ncentration Diffusion Coefficient Partition Coefficient Solubility		
	💧 Add Mig	rant(s)	مر Run Prediction		Set-Off
r	📗 Layer (l	DPE) 🧴	Migrant 🕰 Data		
	< >	×	Copy From Reset Layer 💄 Set to User Defined 📄 Database		
	Type:	Polymer	O Contact Medium		
	Thickness (µm):	1000			
	Density (g/cm^3)	0.925			
	Layer Abbreviatio	n: LDPE			
	Material:	POLYETHYL	ENE, LOW DENSITY (PE)		
	Layer Details				
	Molecular Weigh	t (g/mol): 15	00 Glass Transition Temperature (°C): -125		
	Log Pow:	N/	A		
	Material specifi	constants for	estimation of diffusion coefficients according to Piringer		
	Uppe	r Limit: A'*p	: 11.5 Tau: 0 A*p: 11.5		
	Realise	stic Case: A'p:	10 Tau: 0 Ap: 10		
< >>					
6.20   32-bit					.a

FIG. 7 - Selecting a new polymer from the database.

									-	~
📰 😢 👥 🌹 🔆 🔻			PP-Ethanol 10%	6 (Package 1) - SM	L v 6.20			_		×
Package Properties Output	t Calculation								— ć	×
<ul> <li>New Package Puplicate</li> <li>Open Package Close Pac</li> <li>Save Package Save Package</li> </ul>	Package kage age As 🔐 Packag	ll Packages ge Details	New Article	Save Article	icle Import Initi Concentrati	م Predictio ial ion م Predictio	on on This / on on All Al	Article 🕅 rticles 🛞		
Packa	age			Article		Pre	ediction	File		^
Package 1 ✓ - [] LDPE-Ethanol 10% ↓ - [] Iso(20°C , 10d) ↓ - [] PP-Ethanol 10%	Surface (cm^2)		Selecting I	_ayer Ma	terial(s)	- 0	×		Add Laye	<b>*</b> (s)
	Migrant 1 0	Brows	e Database						-0	
	💧 Add Mig	Reference N CAS Number	umber:		Name: Molecular Weight:	polypropylene			Set-Of	f
	🚺 🛛 Layer (l				Type:	POLYMER	~			
	Type:	Mas	sterDB (1938)	UserDE	3 (1)	Filt	er			
	Thickness (µm):	Name			CAS Number	Reference Number	F( ^			
	Density (g/cm^3)	CELLULOSE			0009004-34-6	14500; 43280	5!			
	La serie de la ser	CELLULOSE	ACETATE		0009004-35-7	14505				
	Layer Abbreviatio	CELLULOSE	ACETATE BUTYRATE		0009004-36-8	43300;14508; 43	. 5!			
	Material:	CELLULOSE	ACETATE PROPIONAT	TE .	0009004-39-1	14512				
					0009004-57-3	10925; 53280	5:		_	
	Layer Details	NITROCEU	ULOSE	DROATPENTAIN	00000181-31-3	22450-43330	5/			
	Molecular Weigh	POLYBUTAD	DIENE		0009003-17-2	23515				
	Log Pow:	POLYBUTAD	DIENE, EPOXIDIZED			23518				
		POLY(1,4-B	UTYLENEGLYCOL)		0025190-06-1	23530; 76570				
	Material specific	POLYDIMET	HYLSILOXANE (polyme	er)	0009016-00-6					
	Uppe	POLYHYDRO	DXYBUTYRATE		0029435-48-1	23615	~			
	O Reali	<			2000000 00 F	22222 21222	>			
	U recuit	Previewski	ous Layer 🔰 N	lext Layer		Assign 🛛 🗙 C	Close			
< >										
6.20   32-bit										

FIG. 8 - Searching for 'polypropylene'.

🔳 🙆 🔒 🔶 👳			PP-Ethanol 10%	(Package 1) - SML	v 6.20				_		×
											- v
Package Properties Output	t Calculation Package	ll Packages	New Article	Save Article		🞺 Pred	liction on Th	is Article		-	
Save Package Save Package	age As 🔐 Packag	ge Details	Import Article	Close Article	Import Initi Concentrati	ial 🦯 🎾 Pred ion	liction on All	l Articles	8		
Packa	ige			Article			Prediction	7	File		^
Package 1 ↓ LDPE-Ethanol 10% ↓ Jiso(20°C , 10d) ↓ PP-Ethanol 10%	Surface (cm^2) Article		selecting I	Layer Mat	erial(s)		×			Add Lay	er(s)
	Add Mig	Reference Nu CAS Number:	umber:	N	ame: Iolecular Weight:	polypropylen	e			Set-C	) Iff
	/ 📗 Layer (l			т	ype:	POLYMER	$\sim$				
	< >				Clas	ar Eiltere	Filter				
	Type:	Ma	sterDB (26)	UserDB (	0)	al l'illers	Titter				
	Thickness (µm):	Name		C	AS Number	Reference Num	ber F( ^				
	Density (g/cm^3)	POLYESTER	S OF 1,2-PROPANEDI	OL AND/OR 1,3		76866	7:				
	Layer Abbreviatio	POLYPROPY	LENEGLYCOL ADIPATI	E 0	025101-03-5	80820					
	Material:	POLYPROPY METHYL MET	LENE, homopolymer ( THACRYLATE-BUTYL A	PP) 0 CRYLATE-GRAFT 0	009003-07-0 121510-09-6	80760					
	Layer Details	POLYPROPY	LENE, AMORPHOUS								
	Molecular Weigh	POLYPROPY	LENE GLYCOL PHTHAL LENE, MALETC ANHYD	ATE 0	037228-86-7						
	Log Pow:	Siloxanes ar POLYPROPY	nd silicones, dimethyl, LENE, heterophasic co	methylhydrogen opolymer with et 0	009010-79-1	80760	-1				
	Material specifi	POLYPROPY	LENE, random copolyr	mer with ethylen 0	009010-79-1	80760					
	Uppe	Siloxanes ar	nd Silicones, dimethyl,	Me hydrogen, p 0	068037-64-9		~				
	O Realit	<			000010 00 F		>				
		Previo	bus Layer 🔰 N	Vext Layer		Assign	K Close				
< >											
6.20   32-bit											

FIG. 9 - Selection of 'polypropylene'.

🔜 🕜 🚺 🍷 💥 🔻	PP-Ethano	l 10% (Package 1) - SML v 6	5.20		-		×
Package Properties Output Calculation						-	Β×
Swe Package      Puplicate Package     Lose Package     Save All Pa     Save Package     Save Package Save Package As     Package	etails	le 🕞 Save Article cle 🗇 Duplicate Article ticle 🔀 Close Article Article	Import Initial Concentration	o Prediction on Thi مر Prediction on All Prediction	Articles 8		^
Package 1     Surface (cm^2)					1		<u>42</u>
Preckage 1         Source (cit 2)         Source (cit 2)           V = LOPE-Ethanol 10%         Article           PP-Ethanol 10%         Migrant 1	Selectin Browse Database	g Layer Mate	erial(s)	– – ×		Add Lay	(er(s)
smt							×
I Sill Mi	issing Paran	neters					
Lee Devreet eveilebl	a ia tha databasa		Paguirod for				
Eog Pow not available	e in the uatabase		Required for				
Please enter log Pow			larity scale				
Molecular weight not	t available in the datab	ase	<b>Required for</b>				
Please enter molecul	lar weight	(g/mol)	Estimation of pa	rtition coefficients with Br	randsch and In-si	lico	
					🖌 ОК	X	Cancel
Meteriar. ME	THYL METHACRYLATE-BU	TYL ACRYLATE-GRAFT 012	1510-09-6				
Layer Details PO	LYPROPYLENE, AMORPHO	DUS	7000 06 7				
Molecular Weigh	ULTEROPTLENE GLYCOL PH DLYPROPYLENE, MAI FTC A	NHYDRIDE ADDUCT	/228-86-/				
Log Pow: Silo	oxanes and silicones, dime	thyl, methylhydrogen					
PO	LYPROPYLENE, heteropha	sic copolymer with et 000	9010-79-1 8076	50			
Material specific PO	DLYPROPYLENE, random co	polymer with ethylen 000	9010-79-1 8076	50			
Uppe	v v oro v b	anyi, me nyarogen, p 000	2012 02 5	×			
🔾 Realit				>			
	Previous Layer	Next Layer	Assig	n 📉 K Close			

FIG. 10 - Adding of missing parameters (if known).

🔜 🕜 🕕 🍷 X 🗧 PP-Ethanol 10% (Package 1) - SML v 6.20	-	
Package Properties Output Calculation		_ 8 ×
Image: Save Package       Image: Duplicate Package       Image: Save All Package       Image: Pack	💓 M S File	~
Package 1 Surface (cm^2) 600		4
V         [] LDPE-Ethanol 10%         LDPE         Contact Medi           [] Iso(20°C, 10d)         Article         LDPE         Contact Medi           [] PP-Ethanol 10%         POLYPROPYL         Ethanol 10%           [] Migrant 1         OCTADECYL         500         0		Add Layer(s)
Concentration Diffusion Coefficient Partition Coefficient Solubility		
Add Migrant(s)		Set-Off
🔰 Layer (LDPE) 👗 Migrant 🥰 Data		
🔇 🔪 🗙 Copy From Reset Layer 💄 Set to User Defined 📄 Database		
Type:      Polymer      Contact Medium		
Thickness (µm): 1000		
Density (g/cm^3): 0.91		
Layer Abbreviation: LDPE		
Material: POLYPROPYLENE, homopolymer (PP)		
Laver Details		
Molecular Weight (g/mol): N/A Glass Transition Temperature (°C): -20		_
Log Pow: N/A		
Material specific constants for estimation of diffusion coefficients according to Piringer		
Upper Limit: A <sup>re</sup> p: 13.1 Tau: 1577 A <sup>e</sup> p: 7.721		
O Realistic Case: A'p: 9.4 Tau: 1577 Ap: 4.021		
< >>		
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**FIG. 11 -** Layer abbreviation should be accordingly corrected in case of changing the polymer.

🔜 🕜 📵 🌻 💥 🔻		PP-Ethanol 10% (Package 1) - SML v 6.20	- 🗆	×			
Package Properties Output	Calculation		-	∂ ×			
🔁 New Package 🛛 💣 Duplicate P	Package 🔚 Save All Packages	New Article     Save Article     Sove Article     Sove Article     Sove Article     Sove Article					
Save Package Save Packa	age As Package Details	Import Initial					
Packa	ae	Article Prediction	File	~			
Package 1	Surface (cm^2) 600			42			
✓	Article	PP Contact Medi					
PP-Ethanol 10% POLYPROPYL. Ethanol 10% Add Laver(s)							
	Migrant 1 OCTADECYL	500 0					
	-	opcontration Diffusion Coefficient Partition Coefficient Solubility		3			
			Set-0	off			
	Add Migrant(s)	<sup>O</sup> Run Prediction					
	🚺 Layer (PP) 🧴	Migrant 🕰 Data					
	< > X	Copy From Reset Layer 💄 Set to User Defined 📄 Database					
	Type:      OPolymer	O Contact Medium					
	Thickness (µm): 1000						
	Density (g/cm^3): 0.91						
	Layer Abbreviation: PP						
	Material POLYPROF	YI FNE homonolymer (PP)					
	Find Children	The star from open final (FT)					
	Layer Details						
	Molecular Weight (g/mol): N	A Glass Transition Temperature (°C): -20					
	Log Pow: N	/A					
	Material specific constants for	estimation of diffusion coefficients according to Piringer					
	Upper Limit: A'*	p: 13.1 Tau: 1577 A*p: 7.721					
	<ul> <li>Realistic Case: A'p</li> </ul>	9.4 Tau: 1577 Ap: 4.021					
< >							
6.20   32-bit							

FIG. 12 - Layer abbreviation changed to 'PP'.

Pickage Propertie       Output Calculation	🔜 🕜 🚹 🕈 💥 💷		PP-Ethanol 10% (Package 1) - SML v 6.20	_					
New Package       Duplicate Package       Save All Package       Save Anticle       Open Article       Open Article       Open Article       Open Article       Open Article       Prediction on All Article       % Prediction on All Article         Save Package       Save Package as       Package       Concentration       Prediction on All Article       % Prediction on All Article       % Prediction on All Article       % Prediction on All Article         Package       Save Package       Save Article       Prediction on All Article       % Prediction on All Article       % Prediction on All Article         Package       Save Article       Prediction on All Article       % Prediction on All Article       %         Mide       Prediction on All Article       % Prediction on All Article       %       %         Package       Save Article       Prediction on All Article       %       %         Mide       Prediction on All Article       %       %       %       %         Mide       Prediction on All Article       % </td <td>Package Properties Output</td> <td>Calculation</td> <td></td> <td></td> <td>_ @ ×</td>	Package Properties Output	Calculation			_ @ ×				
Package 1 Article Prediction Pried Prediction Prediction Prediction Prediction Pried Prediction Predictin Predictin Prediction Prediction Prediction Prediction Predi	<ul> <li>New Package Pupilicate F</li> <li>Open Package Close Pack</li> <li>Save Package Save Package</li> </ul>	Package 🕌 Save All Packages age ige As 🛜 Package Details	Import Article         Import	) )) ()					
surface (am <sup>-</sup> /2) <u>au</u> <u>Lipe Ethanol 10%</u> <u>Prethanol 10%</u> <u>Prethanol 10%</u> <u>Mgrant 1 OctraDECt <u>Pfs 1666:10</u> <u>Contact Med</u> <u>POLYPROPV Ethanol 10%</u> <u>Mgrant 1 OctraDECt <u>Pfs 1666:10</u> <u>Contact Med</u> <u>POLYPROPV Ethanol 10%</u> <u>Mgrant 1 OctraDECt <u>Pfs 1666:10</u> <u>Contact Med</u> <u>Mgrant Mgrant Mgrant 1</u> <u>Contact Med</u> <u>Mgrant Mgrant Mgrant 1</u> <u>Mgrant 1</u> <u>Mgrant Mgrant 1</u> <u>Mgrant 1 1</u> <u>Mgrant 1 1 <u>Mgrant 1 1 Jugrant 1 Jugrant 1 Jugrant 1 1 Jugrant 1 Jugrant 1 Jugrant 1 Jugrant 1 1 Jugrant </u></u></u></u></u></u></u></u></u></u></u></u></u>	Packa	ge	Article Prediction	File					
Add Angrant(s)  Add Angrant(s)  Migrant (Migrant 1)  Diffusion Coefficient  Example Temperature (*C): 20  Nown  Interpolation based on Tg  Pringer Calculation Parameters  Layer A'p: 13.1  Tau: 1577  Migrant Molecular Weight (g/mol): 530.9  Customized Equation  Brandsch Equation  In-Sieco  Apply Same Mode to This Layer  Set All to Default Value  Apply Same Mode to All Layers  620132-bit	Package 1     ✓	Artide Thickness (µm) Migrant 1 OCTADECYL Cc	PP Contact Medi POLYPROPY Ethanol 10% 1000 1.667E04 P(5.166E-12) 0.0001 prcentration Diffusion Coefficient Partition Coefficient Solubility		Add Layer(s)				
Oknown     Piringer Calculation Parameters       Interpolation based on Tg     Layer     A'p:     13.1       Image: Piringer     Tau:     1577       Archenius     Higrant     Molecular Weight (g/mol):     530.9       Ocustomized Equation     Brandsch Equation       In-Silco     In-Silco       Apply Same Mode to This Layer     Set All to Default Value     Apply Same Mode to All Layers	Add Migrant(s)  Migrant (Migrant 1)  Add (Diffusion Coefficient)  Data (Diffusion Coefficient  Example Temperature (%): 20								
620132-bit		Known         Interpolation based on Tg         Piringer         Arrhenius         Customized Equation         Brandsch Equation         Welle Equation         In-Silco         Apply Same Mode to This Layer	Piringer Calculation Parameters         Layer       A'p:       13.1         Tau:       1577         Migrant       Molecular Weight (g/mol):       530.9         Set All to Default Value       Apply Same Mode to All Layers						
	6.20   32-bit								

**FIG. 13 -** Diffusion coefficient will be automatically updated if estimation procedure is available (Methods highlighted in red cannot be chosen because of missing required parameters).



**FIG. 14 -** Partition coefficient will also be automatically updated if estimation procedure is available.



FIG. 15 - Migration calculation (click Run Prediction).

🔜 🕜 🟮 🍷 🔆 📼	PP-Ethanol 10% (Package 1) - SML v 6.20		- 🗆 ×						
Package Properties Output Calculation			_ 8						
<ul> <li>New Package</li> <li>Duplicate Package</li> <li>Save All Packages</li> <li>Close Package</li> <li>Save Package</li> <li>Save Package</li> <li>Save Package As</li> <li>Package</li> </ul>	Import Article         Import Article           Import Article         Duplicate Article           Import Article         Concentration           Article         Article	ッダ Prediction on This Article 、ダ Prediction on All Articles Prediction	<ul> <li>Image: Second second</li></ul>						
Predictions     Temperature Profiles			× ×						
Iso Non-Iso Step M	lodulated Shock Worldwide STANAG	Customized Repeated	Use						
Isothermal Conditions		Time Max 10	day 🗸						
Temperature = 20 PC		Without Statisti	ics						
		O Monte Carlo Ru	ins						
ΔT = 20 °C		Number of Run	IS 10 ÷						
Number of Isotherms = 1		Include So	bol Runs						
Final Temperature = 20 °C		Family Approad	h						
Number of steps for this output:       100       Image: Cancel         Set All to Default Value?       Apply Same Mode to All Layers and Migrants									
620132-bit									

**FIG. 16** - Prediction of migration of migrant (Octadecyl 3-(3,5-di-tert-butyl-4-hydroxyphenyl) propionate) into the contact medium under isothermal conditions (here during 10 days at 20°C).



FIG. 17 - Concentration profile of migrant (Octadecyl 3-(3,5-di-tert-butyl-4-hydroxyphenyl) propionate) over time to food simulant 'Ethanol 10%'. Note negligible concentration of migrant in food simulant being lower than 5E-8 mg/kg what indicates that the migration does not occur.





🔜 🕜 🚺 🌻 💥 🔻		5	5ML v 6.20			-	
Package Properties Output O	Calculation						– 🗗 🗙
😭 New Package 📑 Duplicate Pa Den Package 🎇 Close Packa Gave Package 🌠 Save Package	ackage 🕌 Save All Packages ige ge As 🛛 Package Details	New Article	Save Article	Import Initial Concentration	ッ <sup>®</sup> Prediction on This Article ッ <sup>®</sup> Prediction on All Articles	<ul> <li>N</li> <li>N</li> <li>N</li> </ul>	
Packag	e		Article		Prediction	File	^ 
	Surface (cm^2) 600 Article Migrant 1 OCTADECYL Add Migrant(s) Layer (Contact Medi	PP Inta POLYPROPYL Ethe 1000 1.66 500 0 oncentration Diffu: uum 0) <u>     M</u> Copy From	at Medium 0 Inol 10% Ision Coefficient Parti grant & Data Reset Layer	tion Coefficient	Solubility		Add Layer(s)
	Type: OPolymer Thickness (µm): 16667 Density (g/cm^3): 0.98 Layer Abbreviation: Contact Me Contact Medium Details Food group (according to Annee Ethanol 10% - food simulant ( Simulant Ethanol 10% Parameters required for estima @ Upper Limit A: 1 O Realistic Case A: 107	Contact Med     Contact M	lum I) 10/2011 and some mor alcoholic foods < 6%) / 1 cient based on Pow: 22	e) Ethanol 10% - Leber	smittelsimulanz (nicht alkoholische l	Lebensr	nittel oc 🗸
6.20   32-bit							3



🔜 🕜 🚹 🌻 💥 📼		SML v 6.20			_				
Package Properties Output	Calculation					_ @ ×			
😨 New Package 🛛 Duplicate P Dopen Package 🔗 Close Pack 🙀 Save Package 📝 Save Packa	Package 🕌 Save All Packages age ge As 🛜 Package Details	Image: Sevential sevent	Import Initial Concentration		<b>)</b>				
Packa	ge	Article		Prediction	File	^			
V Package 1	Surface (cm^2) 600					4			
	Artide Thickness (µm) Migrant 1 OCTADECYL	PP         Intact Medium 0           POLYPROPYL         Ethanol 10%           1000         1.667E04           500         0				Add Layer(s)			
	C	concentration Diffusion Coefficient Partit	tion Coefficient	Solubility		Cat Off			
	Add Migrant(s)								
	🚺 🛛 Layer (Contact Medi	ium 0) 🧴 Migrant 🖧 Data							
	Layer (contact Heading 0)       Layer Reset Layer         Type:       O Polymer       © Contact Medium         Thickness (um):       16667          Density (g/cm^3):       0.98          Layer Abbreviation:       Contact Medium 0								
	Contact Medium Details								
	Food group (according to Anne	ex III of Regulation (EU) 10/2011 and some more	2)						
	Ethanol 10% - food simulant ( Simulant	(non-alcoholic foods or alcoholic foods < 6%) / E	thanol 10% - Leben	ismittelsimulanz (nicht alkoholische L	.ebensr	nittel oc 🗸			
	Ethanol 10%					$\sim$			
	Parameters required for estima <ul> <li>Upper Limit</li> <li>A: 1</li> <li>Realistic Case</li> <li>A: 1.07</li> </ul>	bition of partition coefficient based on Pow:           B:         -3           B:         -1.82							
6.20   32-bit									

FIG. 20 - Selection of the food group (click on current food group).

🔜 🕜 🟮 🍷 💥 👳			SML v 6.20			_	
Package Properties Output Calculation							_ @ ×
📸 New Package 💣 Duplicate Package 🕌 🎾 Open Package 🍘 Close Package 🔚 Save Package 📓 Save Package As	New Article	G Save Article	Import Initial Concentration	ダ Prediction on This Article ダ Prediction on All Articles	) )) ()		
Package			Article		Prediction	File	^ _
▼ Package 1         Surface (r           ▼         DPE-thanol 10%         Article           ↓         Iso(20°C, 10d)         Article           ↓         DP-thanol 10%         Migrant 1           ↓         DP-thanol 10%         Migrant 1           ↓         DP-thanol 10%         Migrant 1	Thickness (µm OCTADECYL	PP         Cor           POLYPROPYL         Eth           ) 1000         1.6           .         500         0           Concentration         Diffu           lium 0)         4         M	ntact Medi anol 10% 67E04 usion Coefficient Part	ition Coefficient	Solubility		Add Layer(s)
Type: Type: Thickness Density (g Layer Abt Food gr Ethano Not gr Uvgetal Lipophi Ethano Ethano Ethano Ethano	Polyme     Polyme	Copy From r e Copy From r e Copy Erom e Copy Erom r e Copy Erom e Copy E	Reset Layer dium U) 10/2011 and some mor r alcoholic foods < 6%) // Inpohlie Lebenomitel (FG margarine, etc.) / Pfana xoducts, sour cream, etc.) margarine, etc.) / Pfana water emulsions) / Lebens 5.) / Essigsaure 3% - Leb Schokaladerprodukte	e) Ethanol 10% - Leber Ite und Ole, freie Fe I - Lebersmittels ) / Jiopohle Lebens mittelsmulanz (loo mittelsimulanz (sa ensmittelsimulanz (sa	nsmittelsimulanz (nicht alkoholische I tte an der Oberfläche) mudanz (Oliveno), Sonnenblumenol, vittel - ol in Wasser Film hile Lebensmittel - ol in Wasser Film olische Lebensmittel - ol in Wasser Film olische Lebensmittel pH < 4,5)	.ebensr Margar ch und I	nittel oc ine, etc Vilchprov i)
6.20   32-bit							

**FIG. 21 -** Changing the food group from 'Ethanol 10%' to 'lipophilic foods'.

🔜 🕜 🟮 🌻 💥 🔻		SML v 6.20			-	
Package Properties Output	Calculation					– 🗗 🗙
<ul> <li>New Package Puplicate P</li> <li>Open Package Close Pack</li> <li>Save Package Save Package</li> </ul>	ackage 🕌 Save All Packages age ge As 🛛 Package Details	Image: Seve Article         Image: Seve Article           Open Article         Duplicate Article           Import Article         Close Article	Import Initial Concentration	$\[equation] \[equation] \[eq$	) )) (8)	
Packa	ge	Article		Prediction	File	~
Package 1	Surface (cm^2) 600 Article Thidoness (um) Migrant 1 OCTADECYL Cr Add Migrant(s) Layer (Contact Piedi Contact Medium Details Food group (according to Ame	PP Contact Med., POLVPROPYL Ethanol 10% 1000 1.667E04 500 0 concentration Diffusion Coefficient Partit um 0)  Migrant Copy From Reset Layer  Copy From Reset Layer	ion Coefficient  s	Solubility		Add Layer(s)
	Simulant	free fat on surface) / lipophile Lebensmittel (Fet	te und Ole, freie Fet	te an der Oberflache)		~
	User Defined					~
	Parameters required for estima Upper Limit A: 0 Realistic Case A: 0	tion of partition coefficient based on Pow: B: 0 B: 0				
6.20   32-bit						

FIG. 22 - Selection of a food simulant.

🔜 🕜 🜖 🌻 💥 =		SN	VIL v 6.20			-		×
Package Properties Output Calculation						-	∂ ×	
😨 New Package 💣 Duplicate P 🎓 Open Package 🍘 Close Packa 😱 Save Package 📝 Save Package	ackage 📊 Save All Packages age ge As 🖓 Package Details	New Article  Open Article  Import Article	🚡 Save Article 🗇 Duplicate Article 🌋 Close Article	import Initial Concentration	<sup>メ</sup> ダ Prediction on This Article <sup>メ</sup> ダ Prediction on All Articles	<b>)</b>		
Packag	je		Article		Prediction	File		^
	Surface (cm^2) 600 Article Migrant 1 OCTADECYL Add Migrant(s) Add Migrant(s) Ca Add Migrant(s) Ca Add Migrant(s) Ca Add Migrant(s) Ca Add Migrant(s) Ca Add Migrant(s) Ca Add Migrant(s) Ca Add Migrant(s) Ca Add Migrant(s) Ca Ca Ca Ca Ca Ca Ca Ca Ca Ca	PP Conta POLYPROPYL Ethan 1000 1.667 500 0 concentration Diffusi um 0) Copy From F © Contact Mediu       	ct Medi ol 10% E04 on Coefficient  Parti rant & Data Reset Layer 	tion Coefficient  s	Solubility		Add Lay	er(s)
	Simulant							
	User Defined User Defined Vegetable oil Upper Limit A: 0 Realistic Case A: 0	B: 0 B: 0						
6.20   32-bit								.3

FIG. 23 - Selection of 'vegetable oil' as a food simulant.

Package Properties Output Calculation - 5	×
Import Article       Import Article       Import Article       Import Initial Concentration       Import Initial Concentration	~
Surface (m^/2)         Bull           Article         PP           Comparison - 1         Migrant 1           OCTADECYL         P(5.1688-12)           Migrant 1         OCTADECYL	(s)
Concentration Diffusion Coefficient Partition Coefficient Solubility       Set-Off         Add Migrant(s)	
Oknown       Piringer Calculation Parameters         O Interpolation based on Tg       Image: Tau: 13.1 Tau: 1577         Order Pringer       Arbenius         O customized Equation       Migrant Molecular Weight (g/mol): 530.9         Welle Equation       Image: Tau: 1577         O Interpolation based on Tg       Set All to Default Value         Apply Same Mode to This Layer       Set All to Default Value	

FIG. 24 – Evaluation of diffusion coefficient by Piringer method.

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Package Properties Output Calculation					
Save Package 🚰 Uuplicate Package 🕌 Save All Packages	Image: New Article         Image: Save Article         ✓         ✓         Prediction on This Article           Image: Article         Image: Save Article         Image: Save Article         ✓         Prediction on This Article           Image: Article         Image: Close Article         Image: Save Article         ✓         Prediction on All Articles           Article         Article         Prediction on All Articles         Prediction on All Articles	In the second se			
V Package 1 Surface (cm^2) 600			4		
Article     DPE-Ethanol 10%     DPE-Ethanol 10%     Pe-Ethanol 10%     Diso(20°C, 10d)     Migrant 1 OCTADECYL.     PP-olive oil	Article PP Contact Medi POLYPROPYL Vegetable oil Thickness (µm) 1000 1.667E04 Migrant 1 OCTADECYL PP(0.0) Conconstration Diffusion Confisiont Confision Confisiont Confision Confision				
Add Migrant(s)	Add Migrant(s)				
Laver (Contact Medi	um 0) Migrant (Migrant 1) R Data (Partition Coefficient)				
Partition coefficient	(Кр)				
() Known	Pow Calculation Parameters				
◯ Solubility	$Kpf(-) = 10^{(B + A + \log(Pow(-)))}$				
O Van't Hoff	Food A: 0				
Pow     Polarity scale	Migrant Log Pow: 13.41				
	Note: The estimation of Kpf based on Pow is limited to temperature below $60^\circ\text{C}$				
Set All to Default Value?	pply Same Mode to All Layers and Migrants				
6.20   32-bit					

**FIG. 25** – Evaluation of partition coefficient by Octanol/ Water method.



FIG. 26 - Migration calculation (click Run Prediction).

Package Properties       Output Calculation       — 5         Image: Save Package       Image: Save Article       Image: Save Article
Import Article       Import Article       Import Article       Import Initial       Prediction on This Article         Import Article       Import Article       Import Article       Import Initial       Impo
Predictions
Iso Non-Iso Step Modulated Shock Worldwide STANAG Customized Repeated Use
Isothermal Conditions Time Max 10 day ~ ff
Without Statistics
Temperature = 20 °C
ΔT = 20 °C. Number of Runs 10
Number of Isotherms = 1 Indude Sobol Runs
O Fast Distribution
Final Temperature = 20 °C
Save
Number of steps for this output: 100
Set All to Default Value? Apply Same Mode to All Layers and Migrants

**FIG. 27 -** Prediction of migration under isothermal conditions (here during 10 days at 20°C).



**FIG. 28 -** Migration profile of Octadecyl 3-(3,5-di-tert-butyl-4-hydroxyphenyl) propionate over time in 'vegetable oil'. The significant migration takes place, note continuous increasing of concentration of migrant in olive oil.





### **RESULTS / COMPLIANCE CERTIFICATE** -

The output window shows the results of the simulated predictions. Following results may be displayed:

- ► The results grid
- ► The c(t) chart
- ► The c(x, t) chart
- Comparison Output
- Sum Output
- Compliance Certificate

🔜 🕜 1 🌻 💥 🕫		Output - SN	IL v 6.20	_	
Package Properties Output	t Calculation				_ @ ×
<ul> <li>New Comparison Output</li> <li>New Sum Output</li> <li>New Global Comparison Output</li> </ul>	Save Delete Output Output	Import Export Migration c(t) Migration c(t)	Import Concentration c(x,t) Concentration profile	Compliance	~
✓ - Package 1     ✓ - LDPE-Ethanol 10%     ✓ - ISO(20°C, 10d)     ✓ - PP-Ethanol 10%     ✓ - ISO(20°C, 10d)		▶ 📄 😅 王 → 📘 Display unit mg/kg 🗸 ⊙ c rface	(t) : draw mean concentration ○ c(t) : draw concentrat	ration at 0	
	Article	PP     POLYPROPY Thiddness (µm) OCTADECYL S00 Concentration Diffusion Cod	Contact Medi Ethanol 10% 1.667E04 4.643E-08		
	<ul> <li>         • c(t) - PP-Ethanol 10         <ul> <li>c(x,t) - PP-Ethanol</li> </ul> </li> </ul>	0% - Iso(20°C ,10d) 10% - Iso(20°C ,10d)			
	Ĩ		— Migrant 1		
	500 450 450 350 300 250 150 100 0 0				
	0	500	1,000 Layer Thickness (μm)	1,500	2,00
					10 (days)
6.20   32-bit					

FIG. 1 - Selection 'Output calculation'.







**FIG. 3** - Migration results show no migration of migrant from both polymers ('LDPE' and 'PP') to food simulant 'Ethanol 10%'.



FIG. 4 - Selection of comparison output.



**FIG. 5 -** Migration profile over time for 'vegetable oil' (in red) and 'Ethanol 10%' (in blue). No migration is observed for ethanol solution.



**FIG. 6 -** Click on 'Compliance' to generate the compliance certificate according to legislation conformity.



**FIG. 7 -** Compliance certificate for the system: polypropylene-olive oil- Octadecyl 3-(3,5-di-tert-butyl-4-hydroxyphenyl) propionate.

🔜 🕜 🚺 🍷 💥 😑	Legislation - SML v 6.20	-		×
Package Properties Output	t Calculation		-	∂×
Package 1	Initial concentration			<u></u>
Iso(20°C ,10d)	PP : 500mg/kg			
✓ - E PP -Ethanol 10%	PP / Contact Medium 0 : 0.01 (POW based)			
Comparison - 1	Diffusion coefficient at initial temperature			
V PP -olive oil	PP : 5.168E-12 cm^2/s (Piringer based)			
Iso(20°C , 10d)	Contact Medium 0 : 1.000E-04 cm^2/s (Known)			
	Time/Temperature conditions :			
	10 day(s)			
	Iso 20°C			
	Migration :			
	9M (mg/kg of contact medum): Specific Migration Limit QM (mg/kg of packaging): Quantity Maximum QMA (mg/km <sup>2</sup> of packaging): Quantity Maximum per Area			
	DL (mg/kg of contact medium): Detection Limit Green : Compliant			- 14
	Red: Not compliant			
	Migrant 1 / 7 079E-01 mg/kg 433 / 0002092-70-3 / OCTADECVI 2-/3 5-D1-bart-BI ITVI -4-HVDD OVVDHENVI \ DD ODTONATE			
	El European Linion : Regulatory : (El ) No 10/2011 amended un to (El ) No 2018/831			
	SML QM QMA DL			
	□ Switzerland : Regulatory : SR 817.023.21 (2016)			
	SML QM QMA DL			
	6			
	El European Union : Regulatory : 2002/72/EC			
	SML QM QMA DL			
				~
6.20   32-bit				

**FIG. 8** - Compliance certificate: Comparison of migration calculation (7.078e-01 mg/kg) and food regulations (SML: 6 mg/kg) is marked in red. Green colour indicates that specific migration limit is not exceeded.

# FOR FURTHER INFORMATION VISIT: www.akts.com/sml







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