



# SPECIFIC MIGRATION LIMITS Software (SML)

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

**CONTENT** AKTS 用テキスト

### www.akts.com/sml/e-learning

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#### **AKTS E-LEARNING**

SPECIFIC MIGRATION LIMITS ソフトウェア (SML) を使用すると、さまざまな形状や多層構造を持つ複雑な 材料の特定の移行評価が可能になります。移行プロセスのシミュレーションは、閉鎖系の隣接する層間または 接触媒体間の分割を考慮したフィックの第2拡散法則に基づいています。このソフトウェアには、2万を超える 化学物質のデータベースが含まれており、拡散係数と分配係数の 包括的な推定手順を提供します。必要なパ ラメータが欠落している場合、ソフトウェアは推定方法を赤でマークし、欠落しているパラメータを示しま。 SML ユーザーは、これらのパラメータを手動で追加するか(わかっている場合)、別の方法を選択する必要が あります。

SPECIFIC MIGRATION LIMITS ソフトウェア(SML)の解析作業は、次の4つのステップで進めることができます。



ワークフローには以下の4つの主要なステップがあります。

1-パッケージのさまざまな記事を作成してパッケージを定義し、それらのプロパティを紹介します。 2-さまざまな温度プロファイル(iso、non-iso、世界的な気候など)を使用して移行を予測します。 3-.計算された出力を分析します。

4-.結果が対応する法律に適合しているかどうかを確認します。

# \_\_\_\_\_ パッケージ構造 \_\_\_\_\_

パッケージは、それぞれが異なるレイヤー・プロパティを持つ異なる品目のグループです。 たとえば、ボトルは、ボトルキャップとボトル本体の 2 つの物品として扱うことができます。 品目は、異なるサイズとプロパティの1つ以上のレイヤーで構成されます。 注: Article を品目と和訳します。



FIG.1-複数の品目(蓋と容器)で構成されるパッケージを想定します。



FIG.2 - Start\_SML をクリックすると SML が起動します。SML スタートの"開けゴマ"です。

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Package Properties Output Calculation				
New Package      Duplicate Package     Save All Package     Save Package     Save Package     Save Package As     Package	es New Article Save Article Open Article Duplicate Article Import Article Close Article Article	ッダ Prediction on This Article ダ Prediction on All Articles Prediction	∭ ∭ ⊗ File	~
Package	Article	Prediction	File	^
6.20   32-bit				



🔜 🕜 🚺 🌻 💥 🔻	SML v 6.20			_	×
Package Properties Output Calculation					
Wew Package         Implicate Package         Save All Package           Open Package         Implicate Package         Implicate Package           Save Package         Implicate Package         Implicate Package	New Article Save Article Open Article Import Article Close Article Article Article	Import Initial Concentration	ッグ Prediction on This Article ッグ Prediction on All Articles		
Package	Апісіе		Prediction	File	~
Create a new empty package. A package is a group of different					
6.20   32-bit					



		SMI	v 6 20				_		×
Package Properties Output	Calculation	51112	¥ 0.20					_	- ×
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Package 1	Surface (cm ^2) 600 Article Article Add Migrant(s)	oncentration Diffusion	Atuce	tion Coefficient	Package 1 Geometry Rectangular Contact Surfar Volume of Con Width (cm): Height (cm): Length (cm): Surface and m Articles Sur Article 1 600 Total surface of all articles (	ce (cm^2): 10 10 10 10 10 10 10 cm^2): cm^2): witch Package in Fittin	600 600 600	200 000 e 2))	e
6.20 32-bit									

FIG.5 - パッケージのジオメトリ(例:立方体)を選択します。

🔜 🕜 🚺 🌻 💥 🔻		SM	L v 6.20			-	
Package Properties Output	Calculation						– 8 ×
😨 New Package 💣 Duplicate F Dipon Package 🝘 Close Pack Gin Save Package 🚮 Save Packa	Package 🙀 Save All Packages cage age As 🖓 Package Details	New Article	Save Article Duplicate Article Close Article	Import Initial Concentration	ッダ Prediction on This Article ッダ Prediction on All Articles	) )) (8)	
Packa	ge		Article		Prediction	File	~
Package 1	ge Surface (cm ^2) 600 Article Add Migrant(s)	ant 🕰 Data	Article	ition Coefficient	Solubility		Add Layer(s)
6 20   32 bit							

FIG. 6 - パッケージには、1つまたは複数の物品(ボトル本体とその蓋など)を含めることができます。

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Pac	kage			Article		Prediction	File		~
✓ - Package 1	Surface (cm^2) 600	0 Conc	centration Diffu	ision Coefficient Part	ition Coefficient	Solubility		Add La	yer(s)
	💧 Add Migran	it(s)				Run Prediction		Set-	Off
	Layer	💧 Migrant	: 💰 Data	3					
6.20132-bit									

FIG.7 - レイヤーを加えることにより品目の構成をします。

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Package 1 Surface	e (cm^2) 600	Diffusion Coefficient	Partition Coefficient	Solubility		Add Layer(s)
	Add Migrant(s)	ant Coefficient ant Coefficient ayer(s) flayer(s) to add: 2	Cancel	Aur Prediction		Set-Off
6.20   32-bit						

#### FIG. 8 - レイヤーの数を設定します。

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Packa		Article		Prediction	File		^
Package 1	Surface (cm^2) 500 Article Thickness (um) C Add Migrant(s)	Layer 1 Layer 2 Not Defined Not Defined 100 100 oncentration Diffusion Coefficient Parti	tion Coefficient	Solubility		Add Lay	er(s)
	Type:	Copy From Reset Layer Contact Medium Contact Med	re (°C): N/A Pringer A*p: N/A Ap: N/A	Detabase			
6.20   32-bit							

FIG.9 - ポリマー層の特性はデータベースから選択できます。

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Packad	- ge		Article	concentration	Pre	ediction	File	
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	Add Mig Layer ( CAS Number Type:	Number:	Nan Mol Typ	ne: [ ecular Weight: [ e: [	POLYMER			Set-Off
	Thickness (µm): Mame	asterDB (1938)	UserDB (1)	Number Re	eference Number	FLA		
	CELLULOS	E	000	9004-34-6 14	1500; 43280	5!		
	Layer Abbreviatio CELLULOS	E ACETATE	000	9004-35-7 14	1505			
	Material: CELLULOS CELLULOS	E ACETATE BUTYRATE E ACETATE PROPIONAT	000 TE 000	9004-36-8 43 9004-39-1 14	3300; 14508; 43 1512	. 5!		
	Layer Details 3-HYDRO	LULOSE (YBUTANOIC ACID-3-H)	000 DROXYPENTAN 008	9004-57-3 16 0181-31-3 18	925; 53280 8888	5! 74		
	Molecular Weigh NITROCEL	LULOSE	000	9004-70-0 22	2450; 43330	56		
	Log Pow: POLYBUTA POLYBUTA	ADIENE ADIENE, EPOXIDIZED	000	9003-17-2 23	3515 3518			
	Material specific POLY(1,4-	BUTYLENEGLYCOL)	002	5190-06-1 23	3530; 76570			
	Uppe POLYDIME	THYLSILOXANE (polyme	er) 000	9016-00-6				
		KOXTBUTYRATE	002	9935-98-1 23	i615	>		
	Pre-	vious Layer 🔪 N	lext Layer	As	sign 🗙 C	Close		
6.20   32-bit								

FIG. 10 - ポリマー特性の検索には、いくつかのオプションを適用できます(CAS 番号、名前など)。

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Package 1	Surface (cm^2)	Selecting Layer N	Naterial(s)	- C X		Add Layer(s)
	CAS Numbe	r:	Molecular Weight:	OLYMER V		
	Density (g/cm^3) Name CELLULOSE		CAS Number Refi 0009004-34-6 145	erence Number F( ^ 00: 43280 5:		
	Layer Abbreviatio CELLULOSE Material: CELLULOSE	ACETATE ACETATE BUTYRATE	0009004-35-7 145 0009004-36-8 433	05 00;14508; 43 5!		
	Layer Details	E ACETATE PROPIONATE ULOSE	0009004-39-1 145 0009004-57-3 169 0080181-31-3 188	12 25; 53280 5!		
	Molecular Weigh NITROCELI Log Pow: POLYBUTA	LULOSE DIENE	0009004-70-0 224 0009003-17-2 235	50; 43330 5t 15		
	Material specifi Uppe Realt	DIENE, EPOXIDIZED BUTYLENEGLYCOL) THYLSILOXANE (polymer) OXYBUTYRATE	235 0025190-06-1 235 0009016-00-6 0029435-48-1 236	i18 i30; 76570 i15 ···································		
6 20 1 32-bit	Prev	Next Layer	Assig	IT Close		

**FIG. 11 -** 名前または特定のプロパティによるポリマーの検索 (この例では、検索キーワードは「低密度」です)。

🔜 🕜 🚺 🌻 💥 🔻		SML v 6.20			_	
Package Properties Output C	alculation					_ @ ×
<ul> <li>New Package Puplicate Participation</li> <li>Open Package Close Package</li> <li>Save Package</li> <li>Save Package</li> <li>Package</li> </ul>	ckage 📊 Save All Packages ge e As 🖓 Package Details e	Image: Several state         Image: Several state           Open Article         Duplicate A           Import Article         Close Article           Article         Article	e 👸 urticle Import Initial Concentration	ッジ Prediction on This Arti ッダ Prediction on All Artic Prediction	cle les $\otimes$ File	~
Package 1     End LDPE-Ethanol 10%	Article Brows	Gelecting Layer M	aterial(s)	X		Add Layer(s)
	Add Mig CAS Number:	asterDB (3) User	Name: 00 Molecular Weight: Type: P( Clear Filt DB (0)	DLYMER V Filter		Set-Off
	Density (g/cm^3)         Name POLYETHYLI           Layer Abbreviatio         POLYETHYLI           Material:         Ultra-high m           Layer Details         Molecular Weigh           Log Pow:         Image: Comparison of the second	ENE, LOW DENSITY (PE) ENE, LINEAR LOW DENSITY iolecular weight siloxane polymer dispe.	CAS Number Ref 0009002-88-4 769 0009002-88-4 769 	erence Number FCM   50; 80000 549 51; 76950; 80		-
6 20 1 32- kit	Material specifi	bus Layer Next Layer	Assig	n X Close		

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Package 1	Artide Brows	Belecting Layer Material(s)	- X	Add Layer(s)
	CAS Number	Molecular Weight:		
	Fill Missin	g Parameters		×
	Log Pow not available in the	database Required to	or	
	Please enter log Pow	Estimation of	f partition coefficients with Polarity scale	2
				OK Cancel
	Layer Details			
	Molecular Weigh			
	Log Pow:			
	Material specific			
	Uppe			
	O Realit		>	
	Previo	ous Layer > Next Layer	Assign 🔀 Close	
6.20   32-bit				

**FIG. 13 -** 不足しているパラメーターを入力します(わかっている場合)。 この例では、 LogPow がありません。

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Package Properties Output	Calculation					_ @ ×			
😨 New Package 🛛 Duplicate P Dopen Package 🎆 Close Package 😭 Save Package 📝 Save Package	ackage 🕌 Save All Packages age ge As 🛜 Package Details	Image: Save Article         Image: Save Article           Open Article         Image: Duplicate Article           Image: Image: Image: Save Article         Image: Close Article	Import Initial Concentration	ッジ Prediction on This Article ッグ Prediction on All Articles	<b>)</b>				
Packag	je	Article		Prediction	File	^			
<ul> <li>Package 1</li> <li>LDPE-Ethanol 10%</li> </ul>	Surface (cm^2) 600 Article Thickness (um)	Layer 1 Layer 2 POLYETHYLE Not Defined 100 Diffusion Coefficient  Part	ition Coefficient	Solubility		Add Layer(s)			
	Add Migrant(s)			Run Prediction		Set-Off			
Layer (Layer 1)       Mgrant       Data         Image: Copy From       Reset Layer       Set to User Defined       Database         Type:       Image: Polymer       Contact Medium       Trideness (um):       Image: Polymer         Density (g/cm^3):       Image: Polymer       Contact Medium       Image: Polymer       Density (g/cm^3):       Image: Polymer         Density (g/cm^3):       Image: Polymer       Contact Medium       Image: Polymer       Image: Polymer         Layer Abbreviation:       Layer 1       Image: Polymer       Image: Polymer       Image: Polymer         Material:       POLYETHYLENE, LOW DENSITY (PE)       Image: Polymer       Image: Polymer       Image: Polymer         Layer Details       Molecular Weight (g/mol):       1500       Glass Transition Temperature (*C):       -125         Log Pow:       Image: N/A       Image: Polymer       A*D:       11.5									
6.20   32-bit	Realistic Case: A'p:	10 Tau: 0	Ap: 10						



sm] 🕐 🕛 🌹 🏹 🔻		SML v 6.20			_	ЦХ
Package Properties Output	t Calculation					– 8 ×
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🎧 Save Package 🛛 🔏 Save Packa	age As	🔄 Import Article 🐹 Close Article	Concentration	> reaction on An Andres	$\otimes$	
Packa	age	Article		Prediction	File	· · ·
Package 1	ge Surface (cm^2) 500 Article Thickness (um) Add Migrant(s) Add Migrant(s) Layer (Layer 1) C Type: Polymer Thickness (um): 1000 Density (g/cm^3): 0.925 Layer Abbreviation: Syser3 Material: POLYETHY Layer Details Molecular Weight (g/mol): 11 Log Pow: N Material specific constants for © Upper Limit: A"# C Realistic Case: A'p:	Article  Article Article  Article Article Article Article Article Article Article Article Article Article Article Article Article Article Article A	ition Coefficient et to User Defined re (°C): -125 o Piringer A*p: 11.5 Ap: 10	Solubility	File	Add Layer(s)
6.20   32-bit						

FIG. 15 - レイヤーの名前は変更できます(要求された場合)。

		Ch4L 6 20					_
📼 😈 U T 🏊 📍		SIVIL V 0.20			_	ц )	Ì.,
Package Properties Output	Calculation					- 8	×
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Packa	ge	Article		Prediction	File		~
✓	Surface (cm^2) 600					4	
一庐 LDPE-Ethanol 10%	Article Thickness (um)	LDPE Layer 2 POLYETHYLE Not Defined 1000 100				Add Layer(s)	)
	Co	ncentration Diffusion Coefficient Parti	tion Coefficient	Solubility		Г	
	Add Migrant(s)			Run Prediction		Set-Off	
	Layer (LDPE)	Migrant 💰 Data					
		Copy From Reset Layer 💄 Se	t 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 Temperatu	re (°C): -125				
	Log Pow: N/A	Ą					
	Material specific constants for	estimation of diffusion coefficients according to	Piringer				
	<ul> <li>Upper Limit: A'*p.</li> <li>Realistic Case: A'p:</li> </ul>	: 11.5 Tau: 0 10 Tau: 0	A*p: 11.5 Ap: 10				
6.20   32-bit							

**FIG. 16 -** 拡散の推定に必要な Piringer 法による物質特定係数の導入。 Piringer 法の値には「上限値」または「現実的なケース」がある。

# 食品グループと食品疑似溶媒

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Packa	ge	Article		Prediction	File		^
✓	Surface (cm^2) 600 Article Thickness (µm)	LDPE Layer 2 POLYETHYLE Not Defined 1000 100				Add Lay	er(s)
	C	oncentration Diffusion Coefficient Parti	tion Coefficient	Solubility		-6	3
	Add Migrant(s)			Run Prediction		Set-O	off
	Layer (LDPE) 🧴	Migrant 🕰 Data					
	< > X	Copy From Reset Layer	et to User Defined	📄 Database			
	Type:      O Polymer	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): 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				
	Realistic Case: A'p:	10 Tau: 0	Ap: 10				
6.20   32-bit							

FIG.1 - 次のレイヤー「レイヤー2」の選択

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Package Properties Output	Calculation					_ @ ×
Rew Package 💣 Duplicate F P Open Package 🔗 Close Pack R Save Package 📝 Save Packa Packa	Package 📊 Save All Packages age age As 🛜 Package Details ge	New Article     Open Article     Import Article     Close Article     Article     Article	Import Initial Concentration	ッダ Prediction on This Article ノダ Prediction on All Articles Prediction	💓 M S File	~
Packa Package 1	ge Surface (cm^2) 600 Article Thickness (um) Ca Add Migrant(s) () Layer (Layer 2) Ca Type:  Polymer Thickness (um):  Do Density (g/cm^3):  N/A Layer Abbreviation: Layer 2 Material:  Not Defined Layer Details Molecular Weight (g/mol):  N/ Log Pow:  O Density (g/cm constants for O Dense Linger Lingt: A <sup>*</sup> D D Dense Lingt: A <sup>*</sup> D D D D D D D D D D D D D D D D D D D	Article  LOPE LOPE LOPE OVETHYLE Not Defined 1000 100 DOCENTRATION Diffusion Coefficient Parti Copy From Reset Layer Contact Medium Composition Contac	tion Coefficient   to User Defined re (°C): N/A >Pringer A*D: N/A	Solubility Solubility Database	File	Add Layer(s)
6.20   32-bit	O Realistic Case: A'p:	N/A Tau: N/A	Ap: N/A			

FIG. 2 - レイヤー2は食品疑似溶媒と設定されているので、「ポリマー」から「接触媒体」への変更が必要です

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Package Properties Output	Calculation					-	₽ ×
😭 New Package 🛛 🚔 Duplicate P 🍺 Open Package 🎇 Close Pack	Package 🕌 Save All Packages	Image: New Article         Image: Save Article           Image: Open Article         Image: Duplicate Article		, o Prediction on This Article			
🎧 Save Package 🛛 📓 Save Packa	ige As Trackage Details	🐖 Import Article 🞇 Close Article	Concentration	Prediction on All Articles	8		
Packa	ge	Article		Prediction	File		~
✓ 🚍 Package 1	Surface (cm^2) 600						4
— ि LDPE-Ethanol 10%	Article Thickness (um)	LDPE Contact Medi POLYETHYLE User Defined 1000 1.667E04				Add Laye	er(s)
	C	ncentration Diffusion Coefficient Partit	ion Coefficient	Solubility		ГС	\$
	Add Migrant(s)			Run Prediction		Set-O	ff
	/ 📗 Layer (Contact Medi	um 0) 🧴 Migrant 🕰 Data					
	< > X	Copy From Reset Layer					
	Type: OPolymer	Contact Medium					
	Thickness (um): 16667						
	Density (= (m 0.2)						
	Density (g/ciii · 5): 0.98						
	Layer Abbreviation: Contact Me	dium 0					
	Contact Medium Details						
	Food group (according to Appe	v III of Regulation (EU) 10/2011 and some more	)				- 1
	Not Defined	Citt of Regulation (EO) 10/2011 and some more	,			~	7
	Simulant						
	User Defined					~	
	Parameters required for estima	tion of partition coefficient based on Pow:					
	Upper Limit A: 0	B: 0					
	Realistic Case A: 0	B: 0					
6.20   32-bit							

**FIG.3**-食品グループで検索して接触媒体を定義する。 ([未定義]をクリックして食品グループを選択します)。

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Package Properties Output	Calculation					_	∂ ×
😨 New Package 🛛 Duplicate P 🥟 Open Package 🎇 Close Packa 😭 Save Package 📝 Save Packa	Package 🕌 Save All Packages age ge As 🛜 Package Details	Image: Sevential sevent	Import Initial Concentration	ッ <sup>d</sup> Prediction on This Article 、 <sup>d</sup> Prediction on All Articles	) )) (8)		
Packag	ge	Article		Prediction	File		^
Package 1	Surface (cm^2) 600 Artide Thickness (um)	LDPE Contact Medi POLYETHYLE User Defined 1000 1.667E04 oncentration Diffusion Coefficient Partit	tion Coefficient	Solubility		Add Lay	yer(s)
	Add Migrant(s)	ium 0) 🧴 Migrant 🥵 Data		Run Prediction		Set-O	Off
Copy From     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: Ethanol 10% - food simulant ( lipophilic foods (fats and olis, 1 Vegetable oil - food simulant (o Lipophilic foods - oil in water en Ethanol 20% - food simulant ( Ethanol 20% - food simulant ( Acetic acid 3% - food simulant ( Chacelate and chacelate prod Ethanol 20% - food simulant ( Chacelate and chacelate prod Ethanol 20% - food simulant (	x III of Regulation (EU) 10/2011 and some more (non-alcoholic foods or alcoholic foods < 6%) / E free fat on surface /  loophile Lebensmittel (Fer- tilve oil, sunflower oil, margarine, etc.) / Pfanze usion (milk and mik products, sour oream, etc.) ipophile foods - oil in water emulsions/) (Lebens alcohole foods - 20%) (Ethanol 20% - Lebens alcohole foods - 20%) (Ethanol 20% - Lebens ucts / Schokolader und Schokoladerprodukte non-alcoholic foods or alcoholic foods < 6%) / E	e) ithanol 10% - Leber endi - Lebers noi - Lebersmitteise mitteismularz (logo nitteismularz (alkoh nomitteismulanz (sc thanol 10% - Leber	nsmittelsimulanz (nicht alkoholische I tte an der Oberfläche) mulanz (Olivenöl, Sonnenblumenöl, titel – O in Wasser Emulosnen (Mil hile Lebensmittel – O In Wasser Em olische Lebensmittel so 20%) uzw Lebensmittel soft – 4,5) ismittelsimulanz (nicht alkoholische I	Lebensr Margar ch und I ulsioner	nittel oc ine, etc Vilchprov I) nittel od	5 < 5
6.20   32-bit							

FIG. 4 - 要求された食品グループの選択(英語とドイツ語)。

		Ch41 ( 20					
smi 🖤 👥 🕇 🛝 👘		SIVIL V 6.20	—				
Package Properties Output	t Calculation			– 🗗 🗙			
😨 New Package 🛛 🖆 Duplicate	Package 🕌 Save All Package kage	New Article     Save Article     Sove Article     Predice     Open Article     Duplicate Article     Import Initial     of Destin	tion on This Article				
🔚 Save Package 🛛 📓 Save Packa	age As	Import Article 🔀 Close Article Concentration	ion on All Articles				
Packa	ige	Article	rediction File	^			
✓	Surface (cm^2) 600			4			
LDPE-Ethanol 10%	Article Thickness (un	LDPE         Contact Medi           POLYETHYLE         User Defined           1 000         1.667E04		Add Layer(s)			
		Concentration Diffusion Coefficient Partition Coefficient Solubility		-a			
Add Migrant(s)							
	Layer (Contact Me	lium 0) 🧴 Migrant 🥰 Data					
	< > X	Copy From Reset Layer					
	Type: OPolym	r Ocontact Medium					
	Thickness (um): 16667						
	Density (g/cm^3): 0.98						
	Layer Abbreviation: Contact	1edium 0					
	Contact Medium Details						
	Food group (according to the	av III of Degulation (EII) 10/2011 and some more)					
	Ethapol 10% food cimulan	ex III of Regulation (EO) 10/2011 and some more)	az (nicht alkaholischa Labons	nittel er v			
	Simulant		12 (High alkoholische Lebensi	littlei oc 🔹			
	User Defined			~			
	User Defined						
	Ethanol 10%	PL D					
		B: 0					
	C Realistic Case A: 0	B: U					
6.20   32-bit							

FIG.5-接触媒体としての「エタノール10%」の選択。

🔜 🕜 🚺 🌹 💥 🔻		SML v 6.20			-		$\times$
Package Properties Output	t Calculation					-	₽ ×
😭 New Package 🔮 Duplicate I 🏷 Open Package 🍘 Close Pack 😭 Save Package 📓 Save Packa	Package 🕌 Save All Packages kage age As 🖓 Package Details	New Article     Save Article     Open Article     Import Article     Close Article	Import Initial Concentration	್ಲಳೆ Prediction on This Article ್ಲಳೆ Prediction on All Articles	<ul> <li>(1)</li> <li>(2)</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	- ige	Article	concentration	Prediction	File		~
Package 1	Surface (cm^2) 600	LDPE Contact Med POLYETHYLE Ethanol 10%					*
	Thickness (µm)	1000 1.667E04				Add Lay	er(s)
	C	oncentration Diffusion Coefficient Parti	ition Coefficient	Solubility		-6	3
	Add Migrant(s)			Run Prediction		Set-C	off
	/ 📗 Layer (Contact Medi	um 0) 🧴 Migrant 🥰 Data					
	< > X	Copy From Reset Layer					
	Type: OPolymer	Contact Medium					
	Thickness (um): 16667						
	Density (a/cm (3))						
	Density (g)chi 3). 0.30						
	Layer Abbreviation: Contact Me	edium 0					
	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 I	Lebensr	nittel oc	1
	Simulant						
	Ethanol 10%					`	-
	Parameters required for estimation	tion 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							3

**FIC.6**-オクタノール/水の推定に必要なパラメータの導入 「上限値」または「現実的なケース」法による分配係数が選択できます。

移行

移行物質プロパティパネルでは、現在選択されている移行物質のプロパティを定義できます。 移行物質がユー ザー定義として設定されている場合、そのプロパティを手動で入力することができます。 それ以外の場合、移 行物質がデータベースからロードされると、そのプロパティは自動的に入力されます。

データベースでは、既知の移行物質(20,000 を超える化学物質:添加剤、モノマー、光重合開始剤、顔料、溶 剤など)を 閲覧できます。

🔜 🕜 🕕 🅈 💥 🔻		S	ML v 6.20			-		$\times$
Package Properties Outp	ut Calculation						_	e ×
😨 New Package 💣 Duplicat 🥟 Open Package 🧱 Close Pa 🚛 Save Package 📝 Save Pac Pac	e Package ickage :kage As Package Details kage	New Article	Gave Article	Import Initial Concentration	್ಲಳೆ Prediction on This Article ್ಲಳೆ Prediction on All Articles Prediction	∭ ∭ ⊗ File		^
✓	Surface (cm^2) 600							4
니슈 LDPE-Ethanol 10%	Article Thickness (um)	LDPE Cont POLYETHYLE Etha 1000 1.66 Diffus	act Medi nol 10% 7E04 sion Coefficient Parti	tion Coefficient	Solubility		Add Lay	yer(s)
	Add Migrant(s)				Run Prediction		Set-(	Dff
	Layer (Contact Medi	<b>um 0) 🚺 🔬</b> Mig	grant 💰 Data					
	< > X	Copy From	Reset Layer					
	Type: OPolymer	Contact Med	ium					
	Thickness (µm): 16667							
	Density (g/cm^3): 0.98							
	Layer Abbreviation: Contact Me	edium 0						
	Contact Medium Details							
	Food group (according to Anne	x III of Regulation (EU	) 10/2011 and some more	e)				
	Ethanol 10% - food simulant (	non-alcoholic foods or	alcoholic foods < 6%) / E	Ethanol 10% - Leber	nsmittelsimulanz (nicht alkoholische l	lebensr	nittel oc	~
	Simulant							
	Ethanol 10%							~
	Parameters required for estima	tion of partition coeffic	ient based on Pow:					
	Opper Limit A: 1	B: -3	2					
	C Realistic Case A: 1.07	B: -1.8	2					
6.20   32-bit								

FIG.1 - 移行物質の数を定義する操作のために Adding\_Migrants をクリックします。

🔜 🕜 📵 🌻 💥 📼		SML v 6.2	20		-	
Package Properties Output	t Calculation					_ 8 ×
😨 New Package 💣 Duplicate 🍃 Open Package 🍘 Close Pack 🕞 Save Package 🛃 Save Packa	Package 🕌 Save All Package cage age As 🛜 Package Detail	A New Article Save	e Article licate Article e Article e Article	$\[eq: \phi]{}^{\phi}$ Prediction on This Article $\[eq: \phi]{}^{\phi}$ Prediction on All Articles	) )) (8)	
Packa	ige	4	Article	Prediction	File	^
V Package 1	Surface (cm^2) 600					4
LUPE-Ethanoi 10%	Article Thickness (	LDPE Contact Medi POLYETHYLE Ethanol 10% 1000 1.667E04				Add Layer(s)
		Concentration Diffusion Coe	efficient Partition Coefficient	Solubility		-a
	Add Migrant(s)			Run Prediction		Set-Off
	Layer (Contact I	edium 0) 🚺 Migrant	🕰 Data			
	Type: OPoly	Copy Fro Sm Add Migrant(s	) s) to add:	×		
	Thickness (µm): 16667 Density (a/cm^3): 0.98		V OK	Cancel		
	Laver Abbreviation: Conta	Madium 0				
	Layer Abbreviation.	medium o				
	Contact Medium Detai	5				
	Food group (according to A	nex III of Regulation (EU) 10/201	1 and some more)			
	Ethanol 10% - food simul	nt (non-alcoholic foods or alcoholic	foods < 6%) / Ethanol 10% - Leber	nsmittelsimulanz (nicht alkoholische L	.ebensr	nittel oc $ \sim $
	Simulant					
	Ethanol 10%					~
	Parameters required for es	mation of partition coefficient base	ed on Pow:			
	Upper Limit A: 1	B: -3				
	O Realistic Case A: 1	7 B: -1.82				
6.20   32-bit						

FIG. 2 - 移行物質の数を定義します。

🔜 🕜 🚺 🌻 💥 📼			SML v 6.20			_		×
Package Properties Output Calculation							- 1	s ×
Son New Package 🚽 Duplicate Package 🕌 Den Package 😸 Close Package Save Package 🛃 Save Package As Save Package	Save All Packages Package Details	Rew Article Open Article Import Article	Gave Article Duplicate Article Close Article Article	Import Initial Concentration	メ <sup>ø</sup> Prediction on This Article メ <sup>ø</sup> Prediction on All Articles Prediction	💓 M Sile		^
Package 1 LDPE-Ethanol 10% Migrant 1 Migrant Ab Migrant 2 Migrant 2 Mig	\[     \begin{aligned}     begin{aligned}     begin{a	LDPE Con     POLYETHYLE Eth     1000 1.6     0 0     concentration Diffu rant (Migrant 1)     Copy From     igrant 1     ot Defined     (A     (A     (A	tact Medi and 10% 57E04 sion Coefficient Parti Reset Migrant Melting Point (°C): Button 1 Log Pow:	tion Coefficient  s	Solubility		Add Lays	★ r(s) if
6.20   32-bit								

FIG. 3 - データベースの中から移行物質の特性を見ることができます。

🔜 🕜 🕕 🕈 💥 📼		SML v 6.20			-	
Package Properties Output	t Calculation					_ @ ×
<ul> <li>New Package Puplicate I</li> <li>Open Package Close Pack</li> <li>Save Package Save Package</li> </ul>	Package 🕌 Save All Package kage age As 🛜 Package Details ige	<ul> <li>New Article Save Article</li> <li>Open Article Duplicate A</li> <li>Import Article Close Article</li> </ul>	e 👸 vrticle Import Initial Concentration	ッダ Prediction on This Articl ッダ Prediction on All Article Prediction	e s File	~
Package 1	Surface (cm^2)	Selecting Migrant	(s)	- 🗆 X		Add Layer(s)
	Add Mig Layer	Number: 68320	Name: Molecular Weight: Type: A			Set-Off
	Migrant Abbreviat Migrant:	asterDB (24080) User	DB (3)			
	Migrant Detail Abietic Ad	id EHYDE	0000514-10-3 100	30 3·		
	Molecular Weight		0000064-19-7 100	90; 30000; 30 1:		
	Density (g/cm^3)	NHYDRIDE	0000108-03-4 101 0000108-24-7 101 0000108-24-7 101	50; 30280 2:		
	Molecular Volume ACETOP ACETOP ACETOP ACIDS, F ACIDS, F ACIDS, F ACIDS, F ACIDS, F Prev	New Migrant Next Migrant	0000974-02-5 101 0000974-86-2 101 0000074-86-2 102 0061788-89-4 105 0068783-41-5 105 0000079-06-1 106 0000079-06-1 106	57 10 1: 80 99/90; 10599 7( 99/924; 1105 7: 30 1: x Close		
6.20   32-bit						

**FIG. 4 -** この事例では Reference 番号を入力してデータベースの中から移行物質を探索します。 その他 CAS No.を使うことをお勧めします。

Package Propertie Output Calculation	SIVIL V 0.20	
New Package  Duplicate Package  Open Package  Sove Article  Open Article  Open Article  Duplicate Article  Package  Sove Packag	Package Properties Output Calculation	_ @ ×
Other (III 2)       Selecting Migrant(S)         Made (III 2)       Browse Database         Reference Number:       58320         Add Mig       CAS Number:         Migrant Abbrevia       MasterDB (1)         UserDB (1)       UserDB (1)         Migrant Abbrevia       MasterDB (1)         Migrant Abbrevia       MasterDB (1)         Migrant Abbrevia       MasterDB (1)         UserDB (1)       UserDB (1)         UserDB (1)       UserDB (1)         UserDB (1)       UserDB (1)         Migrant Abbrevia       MasterDB (1)         Migrant Betail       OCTADECYL 34(3;5D1+sert-BUTYL-4+HYDROXYPHE 0002082:79-3         Molecular Weight       Density (g/cm ^3)         Molecular Volume       Frevious Migrant         Migrant I       Next Migrant         Assign       Close	Import Article       Import Article       Import Article       Import Article       Import Article         Package       Save Package As       Package Details       Import Article	
Migrant Abbreviat MasterDB (1)   Migrant Abbreviat MasterDB (1)   UserDB (1) UserDB (1)   Migrant 2 Name   CAS Number Reference Number   FCM OCTADECYL 3-(3,5-DI-tert-BUTYL-4+HYDROXYPHE   Molecular Weight Density (g/cm^3)   Molecular Volume Molecular Volume	Article (uni <)  Article Selecting Migrant(s)  Migrant 1  Reference Number: 68320  Name:  CAS Number:  Molecular Weight:  Type:  ALL	Add Layer(s)
	Migrant Abbreviat       MasterDB (1)       UserDB (1)         Migrant Abbreviat       MasterDB (1)       UserDB (1)         Higrant Detail       OCTADECYL 3-(3,5-DI-tert-BUTYL-4+HYDROXYPHE 0002082-79-3       68320         Molecular Weight       Density (g/cm^3)       Molecular Volume         Molecular Volume       Image: Case of the second s	

FIG. 5 - 要求される移行物質を選択したら Assign ボタンをクリックします。

🔜 🕜 🚺 🅈 🔆 🔻		SML v 6.20		- 🗆 ×
Package Properties Output	t Calculation			_ 8 ×
Rew Package Puplicate Duplicate Dopen Package Close Pack Gave Package Save Pack Pack	Package 🕌 Save All Packages kage age As 😭 Package Details age	New Article     Open Article     Duplicate Article     Import Article     Article     Article	بين المعادي المعادي معادي المعادي معادي معادي المعادي معادي معادي معادي معادي معاد معادي معادي	Article Articles File
V Package 1	Surface (cm^2)			4
LDPE-Ethanol 10%	Article Signature Signatur	Selecting Migrant(s)	- U X	Add Layer(s)
	sml			×
	⑦ Fill Missin	g Parameters		
	Molecular volume not availa	ble in the database	Required for	
	Please enter molecular volur	ne	Estimation of diffusion coefficients with We	lle
				✓ OK Cancel
	Migrant Detail			
	Molecular Weight			
	Density (g/cm^3)			
	Molecular Volume	us Migrant 🔹 Next Migrant	Assign X Close	
6.20   32-bit				

FIG. 6 - 欠落しているパラメータ、ここではモル体積を加えます。(モル体積が分かっている場合)

🔜 🕜 🗓 🍷 🛠 🔻	LDPE-Ethanol 10% (Package 1) - SML v 6.20	- 🗆 X
Package Properties Output Calculation		_ & ×
😨 New Package 🔮 Duplicate Package 🕌 Save All Package 🌝 Open Package 🍘 Close Package 🙀 Save All Package Edition and the same set of the s	s I wew Article I Save Article i Duplicate Article I mport Initial Concentration Article I Pre- i Import Article I Concentration Article I Market Article I Market I Article I Market I Article I Market I Article I Market I Article I	diction on This Article
Package	Article	Prediction File ^
Package 1     Surface (cm^2) [600     Article     Thickness (u     Migrant 1     OCTADECYL     Add Migrant(s)     Migrant 2     Add Migrant(s)	LDPE Contact Medi POLYETHYLE Ethanol 10% ) 1000 1.657E04 0 0 Concentration Diffusion Coefficient Partition Coefficient Solubility grant (Migrant 1)	Add Layer(s)
Migrant Abbreviation: Migrant : Migrant Details Molecular Weight (g/mol): Density (g/m^3): Molecular Volume (Å^3):	Copy From Reset Migrant Log Point (*C): 241.01 230.88 241.01 242.0 241.01 2530.88 2	abase
6.20   32-bit		

FIG.7 - 品目のレイヤーと移行物質(migrant)を定義します。

## 移行特性(濃度、拡散、分配係数)

移行プロセスを予測するには、移行者の主要なパラメータを導入する必要があります。

- ▶ 濃度
- ▶ 拡散係数
- ▶ 分配係数

🔜 🕜 🕕 🌻 💥 🔻		LDPE-Ethanol 10	% (Package 1) - SML v	6.20		_		$\times$
Package Properties Output	Calculation						-	₽ ×
😨 New Package 🛛 🚽 Duplicate I Dopen Package 🎆 Close Pack 😱 Save Package 🚮 Save Packa Packa	Yackage 🙀 Save All Packages iage ige As 😭 Package Details ige	New Article	🕞 Save Article 🗇 Duplicate Article 🎉 Close Article Article	Import Initial Concentration	ッダ Prediction on This Article ッダ Prediction on All Articles Prediction	Image: Second secon		^
Package 1	Surface (cm~2) 600 Article Thickness (um) Mgrant 1 OCTADEC/L Add Migrant(s) (0 Layer (LDPE) Extended Properties Concentration (mg/kg) 0	LDPE Con POLYETHYLE Ethi 1000 1.66 oncentration Diffu	tact Medi and 10% sion Coefficient  Part	ition Coefficient	Solubility		Add Lav	er(s)
6.20 32-bit								

FIG.1 - 移行物質の濃度を定義する。(移行物質の含有量が既知であることが必須条件です。)

🔜 🕜 🚹 🌻 💥 📼			LDPE-Ethanol 10	% (Package 1) - SML v	6.20		_		×
Package Properties Output	Calculation							_	σ×
🗟 New Package 💣 Duplicate F 🍺 Open Package 🔮 Close Pack 😭 Save Package 🛃 Save Packa Packa	Package 📊 Save All lage lige As 🛜 Packagi ge	ll Packages ge Details	New Article Open Article	E Save Article	Import Initial Concentration	ッグ Prediction on This Article ッグ Prediction on All Articles Prediction	X M X File		~
Packa	ge Surface (cm^2) 6	500		Article		Prediction	rile		<b>8</b> 2
Fackage 1     LDPE-Ethanol 10%	Artide Migrant 1 OC	nickness (µm) CTADECYL	LDPE Cor POLYETHYLE Eth 1000 1.6 500 0	anol 10% 67E04				Add Lay	rer(s)
		Co	ncentration Diffu	sion Coefficient Part	ition Coefficient	Solubility			<b>)</b>
	👗 Add Migra	ant(s)				or Run Prediction		Set-C	лт
	Laver (LDF	PE)	Migrant (Migrant	1) 🔏 Data (0	Concentration)				
	Extended Pro	operties /kg) 500							
6 20 1 22 1-2									

**FIG. 2 -** 移行濃度の単位を mg / kg (ppm) で設定します。

🔜 🕜 🟮 🕈 💥 📼		LDPE-Ethanol 10% (Package 1) - SML v	6.20		-	
Package Properties Output	t Calculation					_ @ ×
Swew Package Puplicate Duplicate Dopen Package Close Pack Grand Save Package Save Package Package Package	Package 🙀 Save All Packages kage age As 😭 Package Details ige	New Article     Save Article     Open Article     Duplicate Article     Import Article     Article     Article	Import Initial Concentration	ッダ Prediction on This Article ッダ Prediction on All Articles Prediction	<ul><li>Image: Second second</li></ul>	~
Package 1	Surface (cm ^2) 500 Article Thickness (um) Migrant 1 OCTADEC/L Add Migrant(s) (C Add Migrant(s) (C Add Migrant(s) (C Concentration (mg,kg) 500	LDPE Contact Medi POLVETHYLE Ethanol 10% 1000 1.667E04 500 0 oncentration Diffusion Coefficient Partia Migrant (Migrant 1) & Data (C	tion Coefficient	Solubility		Add Layer(s)
6.20   32-bit						

FIG.3 - 拡散係数の選択します。

🔜 🕜 🚺 🌹 🔆 🔻	LDPE-Ethanol 10% (Package 1) - SML v 6.20	_	
Package Properties Output Calculation			– 🗗 🗙
<ul> <li>New Package Duplicate Package</li> <li>Open Package Close Package</li> <li>Save All Package</li> <li>Save Package</li> <li>Save Package Save Package As</li> <li>Package</li> </ul>	yes Several Article Save Article Save Article Duplicate Article Import Initial Concentration Article Article Article Scherol Article Article Article Scherol Article Article Article Article Article Scherol Article A	∭ ∭ ⊗ File	^
Package 1 V Package 1 Surface (cm^2) [600 Article Migrant 1 OCTADEC Add Migrant (s) Diffusion Coefficie © Known Interpolation based on Pringer Arthenius Customized Equation Brandsch Equation Welle Equation In-Silco Apply Same Mode to This	Article Prediction  IDPE Contact Medi POLYPEHYLE Ethanol 10% I.667E04 I IE-11 0.0001 Concentration Diffusion Coefficient Partition Coefficient Solubility  Concentration Diffusion Coefficient Partition Coefficient Migrant (Migrant 1) Data (Diffusion Coefficient)  Int  Known Value Diffusion Coefficient (cm^2/s): IE-11 Set to Default Value Apply Same Mode to All Layers		Add Layer(s)
6 20 L 22 bit			

**FIG. 4** - 拡散係数の導入(既知の場合、ここでは le-ll がデフォルト値です)または推定方法の選択(例: Piringer)。 この例では、Welle equation で推定する必要なパラメータが不足しているために使用できないために、Welle 方程式は赤 でマークされています。Version5.2以降に追加された機能です。

Package Properties       Output Calculation       -	_ @ ×
Image: Save Package       Puplicate Package       Image: Save All Package       <	
Package 1         Surface (cm^2)         600           Image: International 10%         Article         IDPE         Contact Medi           POLVETHYLE         Ethanol 10%         Add Lave         Add Lave	^
Article LDPE Contact Medi POLYETHYLE Ethanol 10% Add La	4
Indoness (um) 1000 106/204 Migrant 1 OCTADECYL P(2/2052-10) 0.0001 Concentration Diffusion Coefficient Partition Coefficient Solubility Add Migrant(s) Add Migrant(s) Diffusion Coefficient Example Temperature (*C): 20 Norun Interpolation based on Tg Arrhenius Customized Equation Brandsch Equation Brand	Layer(s)
6.20   32-bit	

**FIG. 5** – Piringer 法に基づく拡散係数の評価に必要な計算パラメータ(Ap および Tau)の導入

🔜 🕜 🚺 🅈 💥 📼			LDPE-Ethanol 10	)% (Package 1) - S	SML v 6.20		-		$\times$
Package Properties Output	Calculation							-	∂ ×
Swew Package 🚽 Duplicate P Dopen Package 😸 Close Pack Close Package 🛃 Save Package	Package 📊 Save tage age As 🛜 Packa	All Packages age Details	New Article	Gave Article	ticle Import Initial Concentration	م Prediction on This Article أربع Prediction on All Articles	<ul> <li>(3)</li> <li>(4)</li> <li>(4)</li> <li>(5)</li> <li>(5)</li> <li>(6)</li> <li>(6)</li> <li>(7)</li> <li>(7)</li></ul>		
Раска	ge			Article		Prediction	File		-
✓ · ── Package 1 LDPE-Ethanol 10%	Surface (cm^2)	600							<u> </u>
	Article		LDPE Cor	apol 10%					
		Thickness (µm)	1000 1.6	67E04				Add La	yer(s)
	Migrant 1	OCTADECYL	P(2.263E-10) 0.0	001				1	-
		Co	oncentration Diffu	ision Coefficient	Partition Coefficient	Solubility			9
	1					d		Set-	Off
	Add Mig	grant(s)				Run Prediction			
	Layer (I	LDPE) 🧴	Migrant (Migran	t1) 🔏 🛛	ata (Diffusion Coefficie	ent)			
	<b>〈</b> 〉								
	Diffusion C	oefficient	Example Tempera	ture (°C): 20					
	Known		Piringer Calcula	tion Parameters	5				
		based on To	Layer A'p:		11.5				
	Piringer	based on ty	Tau:		0				
	Arrhenius		Migrant Molec	ular Weight (g/mol)	): 530.9				
	Customized E	quation							
	Brandsch Equ	ation							
	O Welle Equatio	n							
	O In-Silico								
	Apply Same Mo	de to This Layer	Set All to De	efault Value	Apply Same Mode to All Li	ayers			
6.20   32-bit									

FIG. 6 - 分配係数の選択

Package Properties       Output Calculation	🔜 🕜 🟮 🕈 💥 📼		LDPE-Ethanol 10% (Package 1) - SML v 6.20	20	-	
Import Article   Impor	Package Properties Outp	ut Calculation				_ @ ×
Package 1       Surface (cm^2) 600         Article       LDPE         Contact Mediu       POLYETHYLE Ethanol 10%         Migrant 1       OCTADECYL         OCTADECYL       I         Concentration       Diffusion Coefficient         Set-Off       Set-Off         Image: Contact Medium 0)       Migrant (Migrant 1)         Image: Contact Medium 0)       Migrant (Migrant 1)	Rew Package 💣 Duplicate Popen Package 🔗 Close Package Save Package 🥁 Save Package Package	e Package ckage kage As Package Details kage	New Article     Deen Article     Doen Article     Import Article     Article     Article	بی Prediction on This Article Import Initial Concentration به Prediction on All Articles Prediction	<ul><li>Image: Second second</li></ul>	
Known Value                  Solubility                  Van't Hoff                  Pow                  Polanty scale            Set All to Default Value?           Apply Same Mode to All Layers and Migrants	Package 1     Ethanol 10%	Surface (cm^2) 600 Article Thickness (um) Migrant 1 OCTADECYL C Add Migrant(s) Migrant (s) C Add Migrant(s) Partition coefficient ( © Known Solubility Van't Hoff Powy Polerity scale Set All to Default Value? A	LDPE Contact Medi POLYETHYLE Ethanol 10% 1000 1.667E04 1 oncentration Diffusion Coefficient Partitio m 0)  Migrant (Migrant 1) (Kp) Known Value 1	n Coefficient Solubility		Add Layer(s) Set-Off

6.20 | 32-bit

FIG.7 - -分配係数の入力(分配係数がわかっている場合)または推定方法の選択(例:オクタノール/水分配係数)。 この例では、極性スケールは赤でマークされており、極性スケールのパラメータが欠落しているため使用できません。 一般に、JRC ガイドラインに従って任意に選択された2つの分配係数が上限計算に使用されます。 移行物質が食品接触材料/模擬物質に可溶である場合、kpF=1とします。

移行物質が食品接触材料/模擬物質に溶解しない場合、kpF=1000。

オクタノール・水の分配係数を利用する「POW」方式は、log POW(移行物質の極性から導出)と log kpF の間の関係 を 使用し、より正確な分配係数を提供します。



FIG.8-オクタノール/水法に基づく分配係数。



品目のすべてのプロパティが導入されたら、「Run\_Prediction 予測の実行」ボタンをクリックして予測計算 を進めることができます。

移行の予測は、さまざまな温度プロファイルに対して実行できます。

- ▶ 等温
- ▶ 非等温
- ▶ 段階的
- ▶ 変調
- ▶ ショック
- ▶ 世界気候 世界都市の気候温度条件
- ▶ STANAG NATO の軍規格 SML では使用しません。
- カスタマイズ

🔜 🕜 🕕 🍷 💥 📼		LDPE-Ethan	ol 10% (Package 1) - SML v	6.20		-		×
Package Properties Output	Calculation						_	∂ ×
😨 New Package 🛛 Package Package Package Package Package Package Package Package Packa	Package 🕌 Save All Packages age ige As 😭 Package Details ge	New Artic	le 🕞 Save Article cle 🗊 Duplicate Article ticle 🕃 Close Article Article	Import Initial Concentration	ッダ Prediction on This Article ッダ Prediction on All Articles Prediction	) M (S) File		^
Padage 1	Surface (cm ^2) 500 Article Thickness (um) Mgrant 1 OCTADECYL C Add Migrant(s) Dartition coefficient ( Known Solubility Van't Hoff © Powi Polarity scale Set All to Default Value? Ag	LDPE POLYETHYLE 1000 oncentration [] m 0) (Kp) Pow Calcula Kpf(-) = 10 <sup>(K)</sup> Food A Food B Migrant L Note: The e	Contact Medi           Ethanol 10%           1.667E04           P(1E10)           Diffusion Coefficient           Part           Migrant (Migrant 1)           ation Parameters           8 + A * log(Pow(-)))           t:         1           ::         -3           og Pow:         13.41           stimation of Kpf based or           to All Layers and Migrants	ition Coefficient	Solubility Solubility tition Coefficient) temperature below 60°C		Add La	er(s)
6.20   32-bit								

FIG.1-移行物質の移行量(溶出量)の予測

🔜 🕜 🟮 🌪 💥 🗢 🛛 PP-Et	anol 10% (Package 1) - SML v 6.20	- 🗆 X
Package Properties Output Calculation		_ @ ×
New Package      Duplicate Package     Save All Package     Dopen Package     Save Package     Save Package     Save Package     Save Package     Package	Article 🕞 Save Article Article 🗇 Duplicate Article t Article 🕃 Close Article Article	
Predictions     Temperature Profiles		× 3
Iso Non-Iso Step Modulated	Shock Worldwide STANAG	Customized Repeated Use
Isothermal Conditions		Time Max 10 day 🗸
		Without Statistics
		O Monte Carlo Runs
ΔT = 20 °C		Number of Runs 10
Number of Isotherms = 1		Include Sobol Runs
Final Temperature - 20 °C		
		Save
	Number of steps for this output:	100 VK XCancel
Set All to Default Value? Apply Same ?	de to All Layers and Migrants	

FIG.2-等温条件下で発生する移行の予測(20°Cで10日間)。



FIG. 3 - 接触媒体中の移行物質(オクタデシル 3- (3,5-ジ-tert-ブチル-4-ヒドロキシフェニルプロピオネート)の濃度プロ ファイルは、時間の経過とともに、移行物質の食品疑似溶媒「エタノール10%」への移行は見られません。



FIG. 4 - 層の厚さと時間にわたる移行物質の濃度プロファイル(食品疑似溶媒への移行なし)。

🔜 🕜 🚺 🌻 💥 🔻	lso(20°	, 10d) (Package 1) - SML v 6.20		-		×
Package Properties Output	Calculation				— ć	7 ×
😨 New Package 🛛 🚔 Duplicate 🍺 Open Package 🔗 Close Pac 🚛 Save Package 🛛 Save Pack Pack	ackage in Save All Packages age ge As Package Details ge As	icle Grave Article ticle Duplicate Article Article Close Article Article	ダ Prediction on This Article ダ Prediction on All Articles Prediction	Image: Second secon		~
Package 1	Q     Q     E     ••     E     ••       Temperature : 20 (°C)     Display unit     mg/r       % of thickness from surface	Duplicate Article Create a clone of the currently selected article.	) : draw concentration at 0			
	- Grid					
	Artide Thickness (um) Migrant 1 OCTADECYL	LDPE         Contact Medi           POLYETHYLE         Ethanol 10%           1000         1.667E04           500         4.719E-08				
	Concentration	Diffusion Coefficient Partition Coefficient	Solubility			-
	c(t) - LDPE-Ethanol 10% - Iso(20°C ,10	i)				
	c(x,t) - LDPE-Ethanol 10% - Iso(20°C ,	0d)				
	ĩo	— Migrant 1				
	5.0E+2 4.0E+2 3.0E+2 2.5E+2 2.5E+2 1.0E+2 1.0E+2 5.0E+1 0 4.0E+2 1.0	500 1000	1500			
	U	500 1,000 Layer Thickness (μm	1,500		2	,001
					10 (day	/s)
6.20   32-bit						

FIG. 5 - [品目の複製]オプションを適用して、新しいシミュレーションで品目のプロパティを変更します。 Duplicate Article は頻繁に使用する機能です。品目を複製した場合、後日に何を解析しようとしたが判るようにその都度 その名称を丁寧に変更することが不可欠です。SML6 を効率的に使用する場合に非常に重要なことです。

🔜 🕜 🚺 🌻 💥 🔻			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 OCTADECYL 500 0								-0
		Co	oncentration Diffu	sion Coefficient Part	ition Coefficient	Solubility		Set-Off
	💧 Add Migra	ant(s)				Run Prediction		Secon
	📗 🛛 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					
	Material specific (	constants for	estimation of diffusio	n coefficients according to	o Piringer			
O Upper Limit: A <sup>th</sup> 11.5 Tau: A A <sup>th</sup> : 11.5 Tau: A <sup>th</sup> : 11.5								
	🔿 Realisti	ic Case: A'p:	10	Tau: 0	Ap: 10			
( 201 22 L 2								
0.20   32-DIT								

FIG.6-ポリマーレイヤーの選択

Package Properties       Output Calculation	🔜 🕜 🚺 🌻 💥 📼		PP-Ethanol 10% (Package 1) - SML v 6.20		_	
New Package       Duplicate Package       Swe Atticle       Swe Atticle       Open Package       Prediction on This Atticle       Prediction on All Atticle         Swe Package       Swe Package       Package Details       Package Atticle       Open Atticle       Open Atticle       Prediction on All Atticle       Prediction on All Atticle         Package I       Swe Package Atticle       Package Atticle       Package Atticle       Prediction on All Atticle       Prediction on All Atticle         Package I       Swe fackage       Swe fackage       Swe fackage       Swe fackage       Package Atticle       Prediction on All Atticle       Prediction on All Atticle         Package I       Swe fackage (on ^2)       Souther Contact Med       Prediction on All Atticle       Prediction on All Atticle         Package I       Swe fackage (on ^2)       Souther Contact Med       Prediction on All Atticle       Prediction on All Atticle         Package I       Swe fackage       Souther Contact Med       Prediction on All Atticle       Prediction on All Atticle         Package I       Souther Contact Med       Souther Contact Med       Prediction on All Atticle       Souther Contact Med	Package Properties Output 0	Calculation				_ @ ×
Package 1       Surface (m^2) 500       Image: Contact Med         PD/XETHYLE       Contact Med       PD/XETHYLE       Ethanol 10%         Article       DEFENDING       Image: Contact Med       PD/XETHYLE       Ethanol 10%         Migrant 1       OCTADECYL       500       0       Image: Contact Med       PD/XETHYLE       Ethanol 10%         Migrant 1       OCTADECYL       500       0       Image: Contact Med       PD/XETHYLE       Ethanol 10%       Image: Contact Med         Migrant 1       OCTADECYL       500       0       Image: Contact Med       I	New Package 💣 Duplicate Package 🚰 Duplicate Package 😰 Close Packa Close Package 📓 Save Package Pac	ackage ge ge As Package Details e	New Article     Open Article     Duplicate Article     Import Article     Kricle     Article	الله من المناطقة من من المناطقة من المناطقة من المناطقة من من المناطقة من المناطقة من المناطقة من المناطقة من المناطقة من المناطقة من من المناطقة من المناطقة من المناطقة من من المناطقة من المناطقة من	∭ ∭ ⊗ File	^
< >> 6.20132-bit	Package 1 Package 1 DPE-Ethanol 10% PP-Ethanol 10%	e Surface (cm^2) 500 Article Thickness (um) Migrant 1 OCTADECYL Co Add Migrant(s) Layer (LDPE) Type: Polymer Thickness (um): 100 Density (g/cm^3): 0.925 Layer Abbreviation: LDPE Material: POLYETHYL Layer Details Molecular Weight (g/mol): 15 Log Pow: N/ Material specific constants for ① Upper Limit: A**p ○ Realistic Case: A'p:	Article  Art	er Defined Database  r -125 r 11.5 10		Add Layer(s)
	< >> 6.20 32-bit					

**FIG.7**-ポリマーのデータベースから新しいポリマーの選択

🔜 🕜 🟮 🌻 💥 💷			PP-Ethanol 10%	6 (Package 1) - SML	. v 6.20			_		×
Package Properties Output	Calculation								_	∂×
<ul> <li>New Package</li> <li>Duplicate I</li> <li>Open Package</li> <li>Close Pack</li> <li>Save Package</li> <li>Save Package</li> </ul>	Package 📊 Save Al kage age As 🛜 Packag	ll Packages je Details	New Article	Gave Article	le Import Initi Concentratio	al A Predictio	on on This Articl on on All Article	e s File		~
Package 1     ✓ □ LDPE-Ethanol 10%     ↓↓↓ Iso(20°C ,10d)     □ PP-Ethanol 10%	Surface (cm^2) Article Migrant 1	Brows	Selecting	Layer Ma	terial(s)		×		Add Lay	Yer(s)
	Add Mig	Reference N CAS Number	umber:		Name: Molecular Weight: Type:	polypropylene			Set-	off
	Type:	Ma	sterDB (1938)	UserDB	(1)	Filte	er			
	Density (g/cm^3)	Name CELLULOSE			CAS Number 0009004-34-6	Reference Number 14500: 43280	F( ^			
	Density (grein b)	CELLULOSE	ACETATE		0009004-35-7	14505	-			
	Layer Abbreviatio	CELLULOSE	ACETATE BUTYRATE	-	0009004-36-8	43300;14508; 43	5!			
	Material:	ETHYLCELL	ILOSE		0009004-39-1	14512	5!			
	Laver Details	3-HYDROX	BUTANOIC ACID-3-H)	DROXYPENTAN	0080181-31-3	18888	7			
		NITROCELL	ULOSE		0009004-70-0	22450; 43330	56			
	Molecular Weigh	POLYBUTAD	DIENE		0009003-17-2	23515				
	Log Pow:	POLYBUTAL	DIENE, EPOXIDIZED		0025100-06-1	23518				
	Material specific	POLYDIMET	HYLSTLOXANE (polyme	er)	0023190-06-1	23530; 76570				
		POLYHYDR	DXYBUTYRATE		0029435-48-1	23615				
		<		010		22222 24222	> V			
	C Realt	Previ	ous Layer 📏 N	Vext Layer	4	Assign 🔀 C	lose			
< >										
6.20   32-bit										



🔜 🕜 🟮 🕈 💥 📼			PP-Ethanol 10%	(Package 1) - SML v	6.20					-		×
Package Properties Output	t Calculation										_	a x
New Package Puplicate Open Package Close Pack Save Package Save Pack Package	😨 New Package 🛛 Puplicate Package 🕌 Save All Packages 🎾 Open Package 🦉 Close Package 🔚 Save Package 📓 Save Package As 🖓 Package Details Package			E Save Article	Import Concent	Initial	Predicti مُہر Predicti مُہر Pr	ion on Th ion on All rediction	is Article Articles	∭ ∭ ⊗ File		^
Package 1 ✓ □ LDPE-Ethanol 10% ↓ ↓ ↓ ↓ ↓ ↓ ↓ ↓ ↓ ↓ ↓ ↓ ↓ ↓ ↓ ↓ ↓ ↓ ↓	Surface (cm^2) Article Migrant 1	Browse	Selecting L	ayer Mate	erial(s)	)		×	]		Add Lay	er(s)
	Add Mig	Reference Ni CAS Number:	umber:	Na Mc Ty	ime: plecular Weigh pe:	poly it: POL	propylene YMER	v ter			Set-C	) )ff
	Type:	M-	storDR (26)	LinerDR (0								
	Thickness (um):		ISCEIDD (20)	USEIDD (U	<b>/</b>			-	1			
	Density (g/cm^3)	Name POLYESTER:	S OF 1,2-PROPANEDIC	OL AND/OR 1,3	AS Number	Refere 76866	ence Number	7:				
	Layer Abbreviatio	POLYPROPY	LENEGLYCOL ADIPATE	. 00	25101-03-5 29408-67-1	80820 80845						
	Material:	POLYPROPY METHYL MET	LENE, homopolymer (F THACRYLATE-BUTYL A	P) 00 CRYLATE-GRAFT 01	09003-07-0 121510-09-6	80760						
	Layer Details	POLYPROPY	LENE, AMORPHOUS LENE GLYCOL PHTHAL	ATE 00	37228-86-7							
	Molecular Weigh	POLYPROPY	LENE, MALEIC ANHYD	RIDE ADDUCT								
	Log Pow:	POLYPROPY	LENE, heterophasic co	polymer with et 00	09010-79-1	80760						
	Material specific	POLYPROPY	LENE, random copolyn	ner with ethylen 00	09010-79-1	80760						
	Uppe	Siloxanes ar	d Silicones, dimethyl, I	Me hydrogen, p 00	68037-64-9			~				
	O Reali	<						>				
		Previo	bus Layer 📏 N	lext Layer	[	Assign	X	Close				
< >												
6.20   32-bit												

**FIG.9** - Polypropylene を選択し、Assign をクリックします。

🔜 🙆 🚹 🌻 💥 👳		PP-Ethanol 10	)% (Package 1) - SML v 6	5.20		_		×
Package Properties Output	t Calculation		-				_	σ×
😨 New Package 💣 Duplicate I 🕝 Open Package 🦉 Close Pack 😭 Save Package 🚮 Save Packa Packa	Package in Save All Packages kage age As Package Details sge	New Article	E Save Article	Import Initial Concentration	ッ <sup>ゆ</sup> Prediction on Thi ッ <sup>ゆ</sup> Prediction on All Prediction	is Article		^
Package 1 ↓ DPE-Ethanol 10% ↓ DPE-Ethanol 10% ↓ Iso(20°C, 10d) ↓ PP-Ethanol 10%	Surface (cm^2)	Selecting e Database	Layer Mate	erial(s)	– – X		Add La	yer(s)
Fill Missing Parameters								
	Please enter log Pow			Estimation of par	tition coefficients with Po	larity scale		
	Molecular weight not availal	ble in the databas	e	Required for				
	Please enter molecular weig	ht	(g/mol)	Estimation of par	rtition coefficients with B	randsch and In-	silico	
< >>	Materials Molecular Weigh Log Pow: Material specifi @ Uppe Realt Pol/PROP Pol/PROP Pol/PROP Pol/PROP Siloxanes a Siloxanes a Siloxanes a Pol/PROP Pol/POL/POL/POL/POL/POL/POL/POL/POL/POL/POL	THACRYLATE-BUTYL LENE, ANGRPHOUS LENE GLYCOL PHTH LENE, MALEIC ANH nd silcones, dimethy LENE, heterophasic LENE, random copol nd Silcones, dimethy coo	ACRYLATE-GRAFT 012 ALATE 003 TORIDE ADDUCT ( ), methylhydrogen copolymer with ethylen 000 1, Me hydrogen, p 006 1, Me hydrogen, p 006 Next Layer	1510-09-6 7228-86-7 9010-79-1 8076 9010-79-1 8076 8037-64-9 9010-00-5 Assig	50 50 > n X Close	ОК	] ×	Cancel
6.20   32-bit								

**FIG. 10 -** 入力されていないパラメータの入力が催促されます。 入力されない場合、解析モードによっては解析が不可能な場合が出てきます。

= 🕺 🔋 🕐 🗧		PP-Ethanol 10% (Package 1) - SML v 6.	20		-		×
Package Properties Outp	ut Calculation					- 8	1.3
😨 New Package 🛛 🚔 Duplicati 🏠 Open Package 🦉 Close Pa 🚛 Save Package 🛛 Gave Pac Paci	e Package 🕌 Save All Packages ckage kage As 🔐 Package Details kage	Image: New Article         Image: Save Article           Image: Open Article         Image: Duplicate Article           Image: Image: Article         Image: Close Article           Article         Article	Import Initial Concentration	ッダ Prediction on This Article ッダ Prediction on All Articles Prediction	X X X File		
Package 1	Surface (cm^2) 600	Ande		reaction	- The	ح	Ŷ
<ul> <li>✓ - EDPE-Ethanol 10%</li> <li>☐ Iso(20°C , 10d)</li> <li>☐ PP-Ethanol 10%</li> </ul>	Artide Thickness (µm) Migrant 1 OCTADECYL	LDPE         Contact Medi           POLYPROPYL         Ethanol 10%           1000         1.667E04           500         0				Add Layer(	(s)
	C.	oncentration Diffusion Coefficient Parti	tion Coefficient	Solubility		to	
	Add Migrant(s)			Run Prediction		Set-Off	
	🚺 Layer (LDPE) 💰	Migrant 🕰 Data					
	< > X	Copy From Reset Layer 💄 Se	t to User Defined	😸 Database			
	Type:  Polymer Thickness (µm): 1000 Density (g/cm^3): 0.91 Layer Abbreviation: LDPE	Contact Medium					
	Material: POLYPROP	YLENE, homopolymer (PP)					
	Lawer Details						
	Molecular Weight (g/mol): N/	A Glass Transition Temperatu	re (°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				
	O Realistic Case: A'p:	9.4 Tau: 1577	Ap: 4.021				
< >							
6.20   32-bit							-

FIC.11 - ポリマーを変更する場合は、それに応じてレイヤーの略語を修正する必要があります。LDPE⇒PP へ

🔜 🕜 💽 🌻 💥 🔻		PP-Ethanol 10% (Package 1) - SML v 6.20	-	
Package Properties Output	Calculation			– 8 ×
New Package      Duplicate P     Dipen Package      Close Package     Save Package     Save Package	Package 📊 Save All Packages age ige As 🔐 Package Details	New Article     Duplicate Article     Import Article     Mort Article		
Packa	ge	Article Prediction	File	~
Package 1	Surface (cm^2) 600			4
✓	Artide	PP Contact Medi POLYPROPYL Ethanol 10%		Add Laver(s)
	Thickness (µm)	1000 1.667E04		Add Edyci (3)
	Migrant I OCTADECTE			r G
	C	oncentration Diffusion Coefficient Partition Coefficient Solubility		Set-Off
	Add Migrant(s)	Run Prediction		
	/ 📗 Layer (PP) 🧴	Migrant 🕰 Data		
	< > X	Copy From Reset Layer 💄 Set to User Defined 📄 Database		
	Type:      Polymer	O Contact Medium		
	Thickness (µm): 1000			
	Density (g/cm^3): 0.91			
	Layer Abbreviation: PP			
	Material: POLYPROP	YLENE, homopolymer (PP)		
	Laver Details			
	Molecular Weight (g/mol): N	A Glass Transition Temperature (°C): -20		
	Log Pow: N	A		
	Matarial and if a constants for			
	Upper Limit: A'*	esumation of an usion coefficients according to Pringer		
	Realistic Case: A'n:	9.4 Tau 1577 Apr 4.021		
	C Inclusion claser, Mp.	APP 100, 1077 m Mp. 4,021		
< >				
6.20   32-bit				

FIG. 12 - レイヤーの略語が PP に変更されました。

🔜 🙆 🚹 🕈 🗶 👳		PP-Ethanol 10% (Package 1) - SML v 6.20	_	
Package Properties Output	Calculation			_ @ X
Source of the second seco	Package 🕌 Save All Packages rage age As 😭 Package Details	New Article     Save Article     Open Article     Duplicate Article     Import Initial     Concentration     Article     Article	💓 🔊 Nile	~
Package 1	Surface (cm^2) 600			4
✓ LDPE-Ethanol 10%     ↓ Iso(20°C , 10d)     PP-Ethanol 10%	Article Thickness (µm) Migrant 1 OCTADECYL	PP         Contact Medi           POLYPROPYL         Ethanol 10%           1000         1.667E04           P(S.1668E-12)         0.0001		Add Layer(s)
	Co	oncentration Diffusion Coefficient Partition Coefficient Solubility		Set-Off
	Add Migrant(s)	📈 Run Prediction		
	Layer (PP) 🧴	Migrant (Migrant 1) 🛛 🦧 Data (Diffusion Coefficient)		
	Diffusion Coefficient	Example Temperature (°C): 20		
	⊖ Known	Piringer Calculation Parameters		
	Interpolation based on Tg  Pringer Arrhenius Customized Equation Brandsch Equation Welle Equation In-Silico Apply Same Mode to This Layer	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** - 推定手順が利用できる場合、拡散係数は自動的に更新されます。 (赤で強調表示されている方法は、必要なパラメータが不足しているため選択できません)

		DD Februard 10% (Declares 1) CMI + 6.20					
		PP-Ethanol 10% (Package 1) - Sivil V 0.20		~			
Package Properties Output	Calculation			– 8 ×			
😪 New Package 🛛 🚔 Duplicate P 🗁 Open Package 🦉 Close Packa	ackage 🕌 Save All Packages	New Article         Save Article           Open Article         Duplicate Article	Prediction on This Article     Operativities on All Articles				
🔚 Save Package 🛛 📓 Save Packag	ge As	Import Article 🦉 Close Article Con	icentration	8			
Packag	ge	Article	Prediction	File ^			
✓	Surface (cm^2) 600			4			
✓	Artide Thickness (µm) Migrant 1 OCTADECYL	PP Contact Medi POLYPROPYL Ethanol 10% 1000 1.667E04 P(1E10)		Add Layer(s)			
	G	ncentration Diffusion Coefficient Partition C	Coefficient Solubility				
	Add Migrant(s)		Run Prediction	Set-Off			
	Layer (Contact Mediu	n 0) 🚺 Migrant (Migrant 1) 🦧	Data (Partition Coefficient)				
	Partition coefficient (	Κρ)					
	() Known	Pow Calculation Parameters					
		$Kpf(-) = 10^{(B + A * log(Pow(-)))}$					
	🔿 Van't Hoff	Food A: 1					
	Pow	Food B: -3					
	O Polarity scale	Migrant Log Pow: 13.41					
		Note: The estimation of Kpf based on Pow is	s limited to temperature below 60°C				
Set All to Default Value? Apply Same Mode to All Layers and Migrants							
6 20   32-bit							

FIG. 14 - 推定手順が利用できる場合、分配係数も自動的に更新されます

🔜 🕜 🚹 🕈 💥 🗉		PP-Ethanol 10% (Package 1) - SML v 6	i.20		_	
Package Properties Output	Calculation					_ @ ×
<ul> <li>Rew Package</li> <li>Duplicate F</li> <li>Open Package</li> <li>Close Pack</li> <li>Save Package</li> <li>Save Package</li> </ul>	Package 🕌 Save All Packages iage ige As 😭 Package Details ge	New Article         Save Article           Open Article         Duplicate Article           Import Article         Close Article           Article         Article	Import Initial Concentration	メ <sup>ø</sup> Prediction on This Article メ <sup>ø</sup> Prediction on All Articles Prediction	∭ ∭ ⊗ File	~
Package 1 V-E LOPE-Ethanol 10% Iso(20°C, 10d) PP-Ethanol 10%	Surface (cm^2) 600 Article Thickness (um) Migrant 1 OCTADECYL C Add Migrant(s) Migrant(s) Migrant (s) Migrant (s) Partition coefficient ( Known Solubility Van't Hoff @ Pow Polarity scale	PP         Contact Medi           POLYPROPYL         Ethanol 10%           1000         1.667E04           P(1E10)            oncentration         Diffusion Coefficient         Part           m 0) <u>A</u> Migrant (Migrant 1)             Kp()              Pow Calculation Parameters               Kp(f(·) = 10 (B + A * log(Pow(-))))            Food              A: 1               Food B: -3            Migrant              Log Pow: 13.41            Note: The estimation of Kpf based on	ition Coefficient	Solubility		Add Layer(s)
6.20   32-bit	Set All to Default Value? A	oply Same Mode to All Layers and Migrants				

FIG.15 - 移行の計算([予測の実行]をクリックします)

🔜 🕜 🟮 🌻 💥 🔻	PP-Ethanol 10% (Package 1) - SML v 6.20	- 🗆 X
Package Properties Output Calculation		_ & ×
<ul> <li>Wew Package Puplicate Package</li> <li>Open Package Close Package</li> <li>Save All Package</li> <li>Save Package</li> <li>Save Package As</li> <li>Package</li> </ul>	ages	
Predictions     Temperature Profiles		× 1 er(s)
Iso Non-Iso Step	Modulated Shock Worldwide STANAG	Customized Repeated Use
Isothermal Conditions         Temperature =       20       ℃         ∆T =       20       ℃         Number of Isotherms =       1         Final Temperature =       20       ℃		Time Max     10     day     ff <ul> <li>Without Statistics</li> <li>Monte Carlo Runs</li> <li>Number of Runs</li> <li>Include Sobol Runs</li> <li>Fast Distribution</li> <li>Family Approach</li> <li>Family Approach</li> <li>Load</li> </ul>
Set All to Default Value?	Number of steps for this output: Apply Same Mode to All Layers and Migrants	100 V K Cancel

FIC. 16 - 等温条件下(ここでは 20°C で 10 日間)の接触媒体への移行物質

(オクタデシル 3- (3,5-ジ-tert-ブチル-4-ヒドロキシフェニルプロピオネート))の移行量(溶出量)の予測。



FIG. 17 - 食品疑似溶媒「エタノール10%」に対する経時的な移行(オクタデシル 3-(3,5-ジ-tert-ブチル-4-ヒドロキシフ ェニルプロピオネート))の濃度プロファイル。食品疑似溶媒中の移行物質の濃度は 5E-8mg/kg 未満であることに注意 してください。移行が発生しないことを示します。



**FIG. 18 -** 移行物質の濃度プロファイル(オクタデシル 3-(3,5-ジ-tert-ブチル-4-ヒドロキシフェニルプロピオネート) 層の厚さと時間にわたって、食品疑似溶媒への移行は観察されません。

🔜 🕜 🚹 🌻 💥 👳		SML v 6.20			_	
Package Properties Output	Calculation					_ 8 ×
<ul> <li>New Package Puplicate F</li> <li>Open Package Close Pack</li> <li>Save Package Save Packa</li> </ul>	Package 🕌 Save All Packages age ge As 😭 Package Details	New Article         Save Article           Open Article         Duplicate Article           Import Article         Close Article           Article         Article	Import Initial Concentration	ダ Prediction on This Article ダ Prediction on All Articles Prediction	<ul><li>Image: Second second</li></ul>	~
Package 1	Surface (cm^2) 600	Anticie		Frediction	The	4
<ul> <li></li></ul>	Artide Thickness (µm) Migrant 1 OCTADECYL	PP         Intact Medium 0           POLYPROPYL Ethanol 10%         1000           1000         1.667604           500         0	ition Coefficient	Solubility		Add Layer(s)
		Diffusion Coefficient Part	tion coefficient	Solubility		Set-Off
	Add Migrant(s)			🔎 Run Prediction		
	/ 📗 🛛 Layer (Contact Medi	um 0) 🧴 Migrant 🕰 Data				
	Ype:     Polymer       Type:     Polymer       Thidness (µm):     16667       Density (g/cm^3):     0.98       Layer Abbreviation:     Contact Me	Copy From Reset Layer © Contact Medium  				
	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%) /	Ethanol 10% - Leber	nsmittelsimulanz (nicht alkoholische I	Lebensr	nittel oc $ \smallsetminus $
	Simulant					
	Parameters required for estima Upper Limit A: 1  Realistic Case A: 1.07	tion of partition coefficient based on Pow: B: -3 B: -1.82				
6.20   32-bit						

FIG. 19 - 接触媒体(食品疑似溶媒)の変更

🔜 🙆 🔒 荣 👳		SML v 6.20		- 🗆 X
Package Properties Output	Calculation			_ @ ×
Package Properties Output     Package Properties Output     Package Properties Output     Package Properties Output     Open Package Second Package     Package Save Packa     Package 1     Package 1     Package 1     DPE-Ethanol 10%     DPE-Ethanol 10%     PDE-Ethanol 10%     PDE-	Calculation Package age age age age age Surface (cm ^2) 600 Article Thickness (um) Mgrant 1 OCTADECYL Ca Add Migrant(s) Caper (Contact Medi Add Migrant(s) Caper (Contact Medi Add Migrant(s) Contact Medium Details Food group (according to Annee Ethanol 10% - food simulant ( Simulant Ethanol 10%	SML v 6.20  SML v	Around Sector Sect	- C × - C × File × Add Layer(s) Set-Off
	Parameters required for estimation	ion of partition coefficient based on Pow: B: -3		
	Opper Limit A: 1     Realistic Case A: 1.07	B: -3 B: -1.82		
6 20 I 32-bit				

**FIG. 20** - 食品グループからの選択(現在の Contact Medium 接触媒体グループをクリックします) 注: Contact\_Medium はデータベースが食品疑似溶媒 と食品グループの2種類に分けて登録されています。

🔜 🕜 🕕 🕈 💥 📼		SML v 6.20			_		×
Package Properties Output Calcula	tion					_	∂ ×
New Package Duplicate Package     Open Package Close Package     Save Package Save Package As     Package     Package	Gave All Packages	New Article Save Article     Open Article     Duplicate Article     Import Article     Article	Import Initial Concentration	ッダ Prediction on This Article ッダ Prediction on All Articles Prediction	💓 🔊 File		^
Comparison - 1     PP-olive oil	Thidkness (µm) ht 1 OCTADECYL Add Migrant(s) Layer (Contact Medi	PP Contact Med POLYPROPYL Ethanol 10% 1000 1.667E04 500 0 oncentration Diffusion Coefficient Partil time 0) 3 Migrant 3 Data	tion Coefficient	Solubility		Add Lay	rer(s)
Type: Thidd Densi Layer Foor Foor Not Veg	Polymer ess (µm): 16667 y (g/cm^3): 0.98 Abbreviation: Contact Me tact Medium Details group (according to Anne anol 10% - food simulant ( Defined Johic Foods (fats and ols), Johic Stods (fats and ols),	Copy From Reset Layer © Contact Medium    edium 0       	e) ithanol 10% - Leber te und Ole, free Fee	smittelsimulanz (nicht alkoholische I te an der Oberflache) mulanz (Oliverflache)	.ebensn Margari	nittel oc	× •
6.20   32-bit	shilic foods - oil in water er and 50% - food simulant ( nol 20% - food simulant ( cic acid 3% - food simulant colate and chocolate prod colate and chocolate prod	nulson (mik and mik products, sour cream, etc. Ipophilic foods - oil in water emulsions) / Lebens alcohole foods - 20%) / Ethanol 20% - Lebens (acidic foods, pH < 4.5) / Essigsäure 3% - Lebe Lucts / Schokoladenprodukte	) / lipophile Lebensm mittelsimulanz (lipop nittelsimulanz (alkoh ensmittelsimulanz (sa	iittel - Öl in Wasser Emulsionen (Mil hile Lebensmittel - Öl in Wasser Emu löche Lebensmittel < 20%) sure Lebensmittel pH < 4,5)	th und N	tilchpro: )	

FIG. 21 - 食品グループを「エタノール 10%」から「親油性食品」に変更します。

🔜 🕜 🚺 🌻 💥 📼		SML v 6.20			_	
Package Properties Output	Calculation					_ @ ×
New Package 💣 Duplicate f Popen Package 🦉 Close Pack Gave Package 🛃 Save Packa	Package 🕌 Save All Packages age 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		) )) (8)	
Packa	ge	Article		Prediction	File	^
V Package 1	Surface (cm^2) 600					4
<ul> <li>✓</li></ul>	Artide Thickness (µm) Migrant 1 OCTADECYL	PP         Contact Medi           POLYPROPYL         Ethanol 10%           1000         1.667E04           500         0				Add Layer(s)
	C	oncentration Diffusion Coefficient Part	ition Coefficient	Solubility		Set-Off
	Add Migrant(s)		_	Run Prediction		Sel-OII
	Layer (Contact Med	ium 0) 🚺 Migrant 🕰 Data				
	Ype:     Polymer       Tidcness (µm):     16667       Density (g/cm^3):     0.98       Layer Abbreviation:     Contact Mathematical M	Copy From Reset Layer Contact Medium  edum 0				
	Contact Medium Details					
	Food group (according to Anne	x III of Regulation (EU) 10/2011 and some mor	e)			
	lipophilic foods (fats and oils,	free fat on surface) / lipophile Lebensmittel (Fe	tte und Öle, freie Fe	tte an der Oberfläche)		~
	User Defined					~
	Our Defined     Parameters required for estima     Oupper Limit A: 0     Realistic Case A: 0	tion of partition coefficient based on Pow: B: 0 B: 0				
6.20   32-bit						

FIG. 22 - 食品疑似溶媒の選択

🔜 🕜 🗓 🌻 💥 📼	SML v 6.20			-	
Package Properties Output Calculation					_ @ ×
Image: Save Package       Image: Save Package<	ticle 🕞 Save Article Article 🗇 Duplicate Article Article 🞇 Close Article	Import Initial Concentration	ッグ Prediction on This Article ッグ Prediction on All Articles Prediction	X X X	
Package 1 Surface (cm^2) 600	Antice		Frediction	The	42
✓         DPE-Ethanol 10%         PP           ✓         Iso(20°C, 10d)         PP           ✓         PP-Ethanol 10%         PP           ✓         Iso(20°C, 10d)         Thideness (µm) 1000           ✓         Comparison - 1         OCTADECYL 500	Contact Med Ethanol 10% 1.667E04 0				Add Layer(s)
Concentration	Diffusion Coefficient Parti	tion Coefficient	Solubility		Set-Off
💧 Add Migrant(s)			Run Prediction		
Layer (Contact Medium 0)	🗴 Migrant 🛛 🕰 Data				
Type: Polymer  Copy From Type: Polymer  Copy From Thickness (um): 16667 Density (g/cm^3): 0.98 Layer Abbreviation: Contact Medium 0	keset Layer				
Contact Medium Details					
Food group (according to Annex III of Regula lipophilic foods (fats and oils, free fat on sur	ation (EU) 10/2011 and some mor face) / lipophile Lebensmittel (Fet	e) tte und Öle, freie Fe	tte an der Oberfläche)		~
Simulant			,		
User Defined					$\sim$
User Defined Vegetable oil					
O Upper Limit A: 0     Realistic Case A: 0	B: 0				
6.20   32-bit					

FIG. 23 - 食品疑似溶媒として vegitable\_oil を選択

		SMI ~ 6 20	
smi 🔮 😏 T 🎪 Y		SIVE V 0.20	
Package Properties Output	t Calculation		_ @ ×
😨 New Package 🛛 🚔 Duplicate I 🏠 Open Package 🖉 Close Pack	Package 🕌 Save All Packages cage	Image: Prediction         Image: Prediction           Image: Prediction         Image: Prediction           Image: Prediction         Image: Prediction	on This Article
🔚 Save Package 🛛 📓 Save Packa	age As 🛜 Package Details	Import Initial Article Close Article Concentration	on All Articles 🛞
Packa	ige	Article Predi	ction File 🔺
✓ · ── Package 1	Surface (cm^2) 600		4
<ul> <li>✓ - ELDPE-Ethanol 10%</li> <li>✓ Iso(20°C, 10d)</li> <li>✓ - PP-Ethanol 10%</li> <li>✓ Iso(20°C, 10d)</li> <li>✓ Comparison - 1</li> <li>Øperberd</li> </ul>	Article Thickness (um) Migrant 1 OCTADECYL	PP         Contact Medi           POLYPROPYL         Vegetable of           1000         1.667E04           P(S.1668E-12)         0.0001	Add Layer(s)
PP-olive oil	C	oncentration Diffusion Coefficient Partition Coefficient Solubility	
	Add Migrant(s)		Set-Off
	Layer (PP)	Migrant (Migrant 1) Cata (Diffusion Coefficient)	
	Diffusion Coefficient	Example Temperature (°C): 20	
	Known	Piringer Calculation Parameters	
	O Interpolation based on Tg	Layer A'p: 13.1	
	Piringer	Tau: 1577	
	O Arrhenius	Migrant Molecular Weight (g/mol): 530.9	
	O Customized Equation		
	O Brandsch Equation		
	O Welle Equation		
	O In-Silico		
	Apply Same Mode to This Laye	Set All to Default Value     Apply Same Mode to All Layers	
6.20   32-bit			

FIG. 24 - Piringer 法による拡散係数の評価。

🔜 😧 🕽 🌻 🔆 🔻	SML v 6.20		-	
Package Properties Output Calculation				_ @ ×
Image: Solution of the second seco	New Article     Save Article     Open Article     Duplicate Article     Import Initial     Import Article     Article	ッダ Prediction on This Article ッダ Prediction on All Articles Prediction	💓 🔊 File	•
Padage 1     DPE-Ethanol 10%     DP-Ethanol 10%     Doperational 10	PP Contact Med POLYPROPYL Vegetable ol 1.067E04 . P(0.01) Concentration Diffusion Coefficient Partition Coefficient um 0)  Migrant (Migrant 1)  Q Data (Par (Kp)	Solubility d Run Prediction littion Coefficient)		Add Layer(s)
<ul> <li>○ Known</li> <li>○ Solubility</li> <li>○ Van't Hoff</li> <li>● Pow</li> <li>○ Polarity scale</li> </ul>	Pow Calculation Parameters         Kpf(·) = 10 (B + A * log(Pow(-)))         Food       A:         Food       B:       -2         Migrant       Log Pow:       13.41         Note: The estimation of Kpf based on Pow is limited to         Apply Same Mode to All Layers and Migrants	• temperature below 60°C		
6.20   32-bit				

FIG. 25 - オクタノール/水法による分配係数の評価



FIG. 26 - 移行の計算([予測の実行]をクリックします)

🔜 🕜 🜖 🌪 💥 🗧 SML v 6.20		- 🗆	×
Package Properties Output Calculation		-	ð ×
<sup>1</sup> New Package <sup>1</sup> Duplicate Package <sup>1</sup> New Article <sup>1</sup> Save Article <sup>1</sup> Save Article <sup>1</sup> New Article <sup>1</sup> Save Article <sup>1</sup> Monothing	on This Article on All Articles	INE INE INE	~
	iction	X	4
Predictions			er(s)
Temperature Profiles Iso Non-Iso Step Modulated Shock Worldwide STANAG Customized	d Repeated U	se	
Isothermal Conditions	Time Max 10	dav 🗸	ff
	Without Statistic	:s	
Temperature = 20 °C	O Monte Carlo Rur	ns	
ΔT = 20 °C	Number of Runs	10 ÷	
Number of Isotherms = 1	Include Sol	bol Runs	
	Fast Distribution	l.	
Final Temperature = 20 °C (	Family Approach	1	
	Save	Coad	
Number of steps for this output: 100	🖌 ОК	Cancel	
Set All to Default Value? Apply Same Mode to All Layers and Migrants			

FIG. 27 - 等温条件下での移動の予測(ここでは 20°C で 10 日間)。



FIG. 28 - 植物油中のプロピオン酸オクタデシル 3- (3,5-ジ-tert-ブチル-4-ヒドロキシフェニル) の経時的な移行プロファイル



FIG. 29 - 「植物油」中の層の厚さと時間にわたるプロピオン酸オクタデシル 3- (3,5-ジ-tert-ブチル-4-ヒドロキシフェニル)の移行プロファイル。表示された予測は、「親油性食品」で移行が発生することを示しています。

# 結果/コンプライアンス証明書

出力ウィンドウには、シミュレートされた予測の結果が表示されます。 次の結果が表示される場合があります。

- ▶ 結果グリッド
- ▶ c (t) チャート
- ▶ c (x、t) チャート
- ▶ 比較出力
- ▶ 合計出力
- ▶ コンプライアンス証明書

🔜 🕜 🚺 🅈 🛠 🕫		Output - SM	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 Export Concentration c(x,t) Concentration c(x,t)	t)	~
		• E ⇔ 조 → L Display unit mg/kg ∨ ⊙ cl	(t): draw mean concentration () c(t): draw concentratio	centration at 0	
	Artice	PP     POLYPROPY Thickness (µm) 1000 OCTADECYL 500 Concentration Diffusion Coe	Contact Medi Ethanol 10% 1.667E04 4.643E-08 efficient Partition Coefficient Solubility		
	<ul> <li>E c(t) - PP-Ethanol 10</li> <li>E c(x,t) - PP-Ethanol</li> </ul>	1% - Iso(20°C ,10d) 10% - Iso(20°C ,10d)			
	ĨOÌ		— Migrant 1		
	500 450 450 300 250 100 100 0 0				
	0	500	1,000 Layer Thickness (µm)	1,500	2,00
6.20   32-bit				•	10 (days)

**FIG.1**- 「出力計算」を選択します。



FIG.2-「比較出力」により、次の移行プロファイル間の比較が可能になります。

「LDPE」と「PP」の層に含まれるプロピオン酸オクタデシル 3-(3,5-ジ-tert-ブチル-4-ヒドロキシフェニル)。



**FIG.3**-移行計算結果は、両方のポリマー(「LDPE」と「PP」) から食品疑似溶媒「エタノール10%」への移行物質の移行を示していません。



FIG. 4 - 比較出力の選択。



FIG.5 - 「植物油」(赤)と「エタノール10%」(青)の経時的な移行プロファイル。 エタノール溶液では移動は観察されません。



FIG.6 - [Compliance]をクリックして、法律の適合性に従ってコンプライアンス証明書を生成します。



FIG.7-システムのコンプライアンス証明書:

ポリプロピレン-オリーブオイル-オクタデシル 3- (3,5-ジ-tert-ブチル-4-ヒドロキシフェニル)プロピオネート。

**FIG. 8 -** 適合証明書:移行計算(7.078e-01 mg/kg)と食品規制(SML:6 mg/kg) の比較は赤でマークされています。 緑色は、特定の移行制限を超えていないことを示します。