SML seminar　Migration Modelling

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場所：東京・茅場町 スペースまる八

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materials | database | simulation

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IT Solutions

- ► complianceBASE (compliance management database)

  コンプライアンス管理データベース

- ► comBASE (communication in the supply chain)

  供給チェーンにおけるコミニュケーション

- ► chemprofiler (substance inventory & regulations)

  chemprofiler 物質の詳しい表と規制

- ► SML Software (migration modeling)

  SML5/6 ソフトウエア（移行モデルによる計算）

Content *セミナー講演内容*

- ► Interaction Packaging <> contact medium 容器相互作用<>接触媒体
- ► Legal Background 法的背景
- ► Migration Modelling / Law of Diffusion 移行モデル計算/拡散の原理
- ► Functional barrier 機能性バリア
- ► Experimental determination of diffusion coefficients (D_P) & partition coefficients ($K_{P,M}$)
  拡散係数(D_P）と分配係数($K_{P,M}$)の実験データによる決定
- ► Estimation of diffusion coefficients (D_P) & partition coefficients ($K_{P,M}$)
  拡散係数（D_P)と分配係数($K_{P,M}$）の推定
- ► SML Software 操作方法

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Interaction packaging <> contact medium
(food/pharmaceuticals/cosmetics)

容器包装の相互作業　<>　接触媒体

(食品/医薬品/化粧品cosmetics)

Interaction packaging food - mass transfer

容器と食品の相互作用　　質量移動

source 放出　< > sink 吸収

<u>driving force 原動力</u>:

concentration difference between materials and media in direct contact to each other　(difference in chemical potential)

お互いに接触する物質と媒体間の濃度差（化学ポテンシャルの差）

⇒ to be considered for each substance !
それぞれの物質が考慮されること

⇒ It is not the question <u>if</u> migration occurs but only <u>to which extent</u> !

移行が起きるとして、どの範囲に及ぶかどうか課題である。

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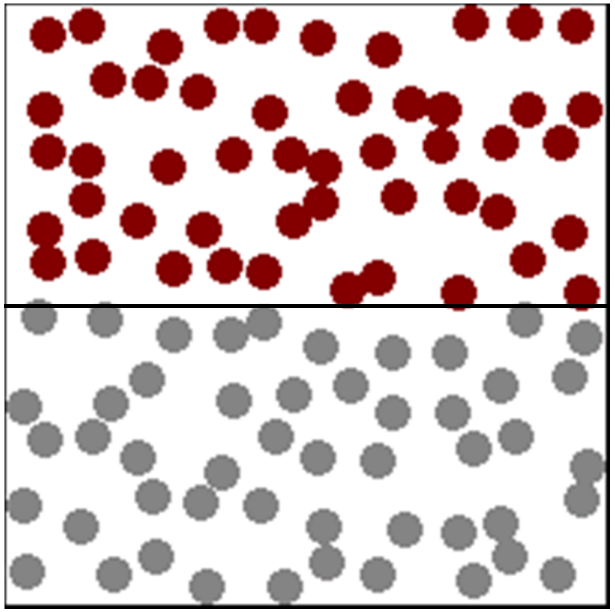
Diffusion process

» temperature induced random walk of molecules

温度に誘起されるランダムな動き

» driving force is the difference in chemical potential

化学ポテンシャルの差による原動力



Mass Transport *質量の移動*

▶ **Permeation** (passing through) 浸透（透り抜ける）

- Transport of a substance through the packaging: **物質が包装を通り抜けて輸送**
  - from environment into filled good 環境から充填された製品へ
  - from filled good into environment **充填された製品から環境へ**

▶ **Migration** **移行**

- Transport of a substance 物質の移行
  - from packaging into filled good
  - from filled good into packaging

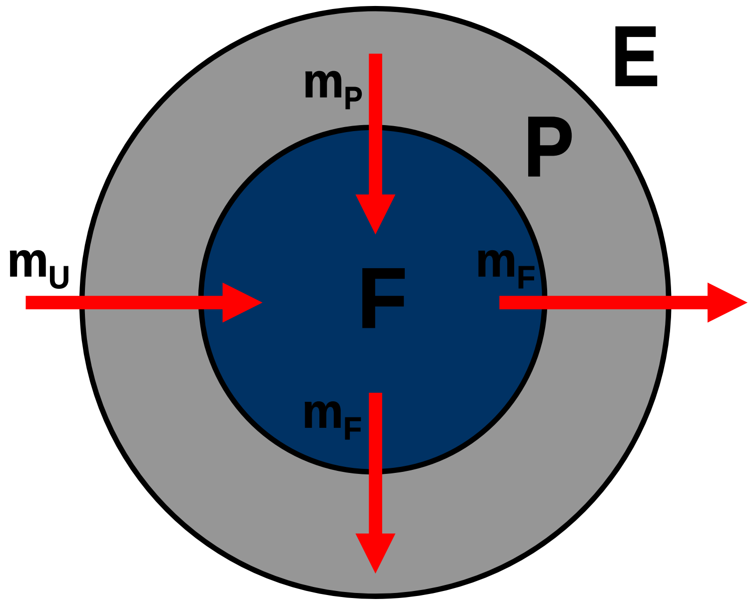
  包装から充填された商品へ

  充填された商品から包装容器へ

E - environment

P - packaging

F - filled good



Examples

- Permeation of oxygen from the environment into the packaging, e.g. beer
- 環境から包装への酸素の浸透　例：ビール
- Permeation of CO_2 from the packaging into environment, e.g. soft drinks
  環境から包装への炭酸ガスの浸透　例：ソフトドリンク
- Migration of low molecular mass packaging components into filled good, e.g. additives, plasticizer, oligomers, etc. with molar mass < 1000 g/mol
  包装材料の低分子量の構成物の充填食品への移行
  例：添加剤、軟化剤、オリゴマーや他1000g/モル以下の分子量の物質

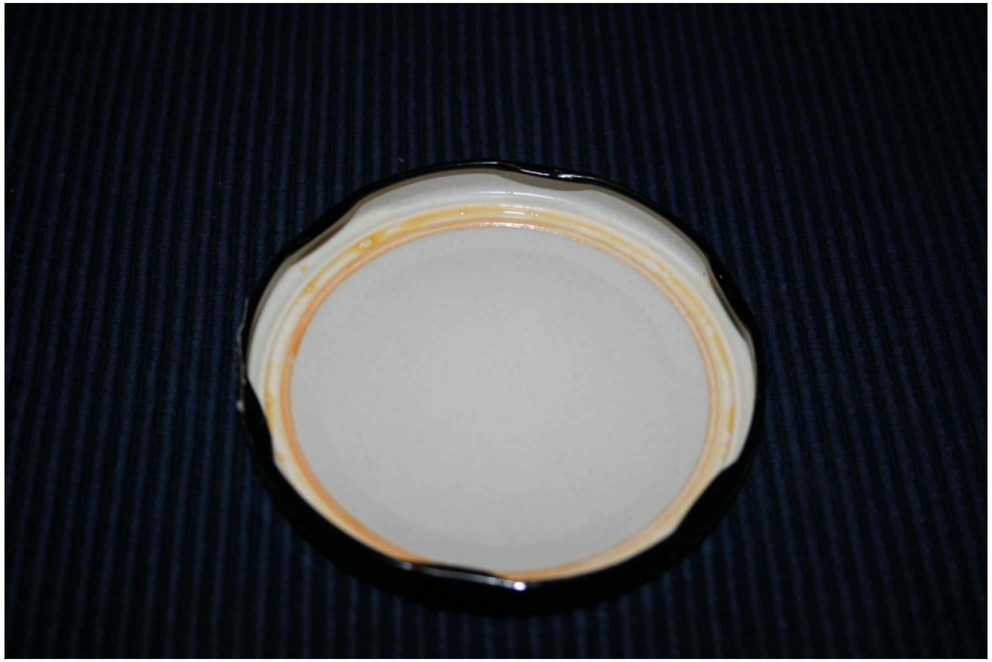
Examples

- Migration of aroma components from the filled good in the packaging or the environment, e.g. loss of aroma from soft drinks and coffee or loss of active component from pharmaceuticals
- 充填食品から環境や包装材から芳香物の移行
  例：ソフトドリンクからの香りの消失
  医薬品から活性物質が消失

Color change due to interaction

e.g. Lycopin from paprika in sealing

シールにパプリカ（食品）からリコピン（色素）が



red colored sealing due to similar polarity

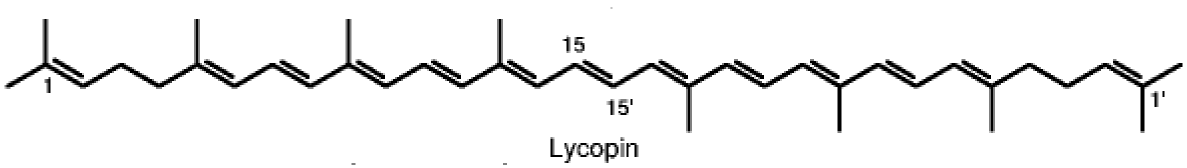
似た極性によりシールが赤色になる。

Color change due to interaction *(相互作用による色変化)*

natural dye (fat soluble) 自然染料(脂溶性)

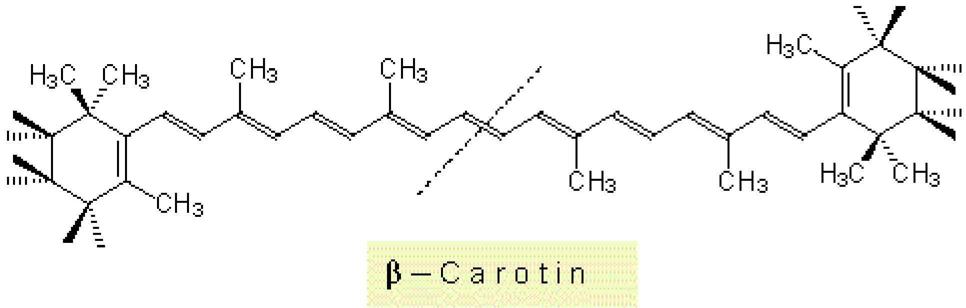
Lycopin: red dye in paprika and tomatoes

リコピン: 赤色染料（パプリカやトマトに含まれる）



β-Carotin: yellow/orange dye in carrots

B-カロチン: 黄色オレンジ色染料（カボチャに含まれる）



No color change due to interaction (相互作用があっても色変化なし)

e.g. chlorophyll from spinach in packaging (Board/PE)
容器(板状/PE)中のほうれん草からクロロフィル

no green colored PE layer due to opposite polarity 反極性のためPE層は緑色にならない。

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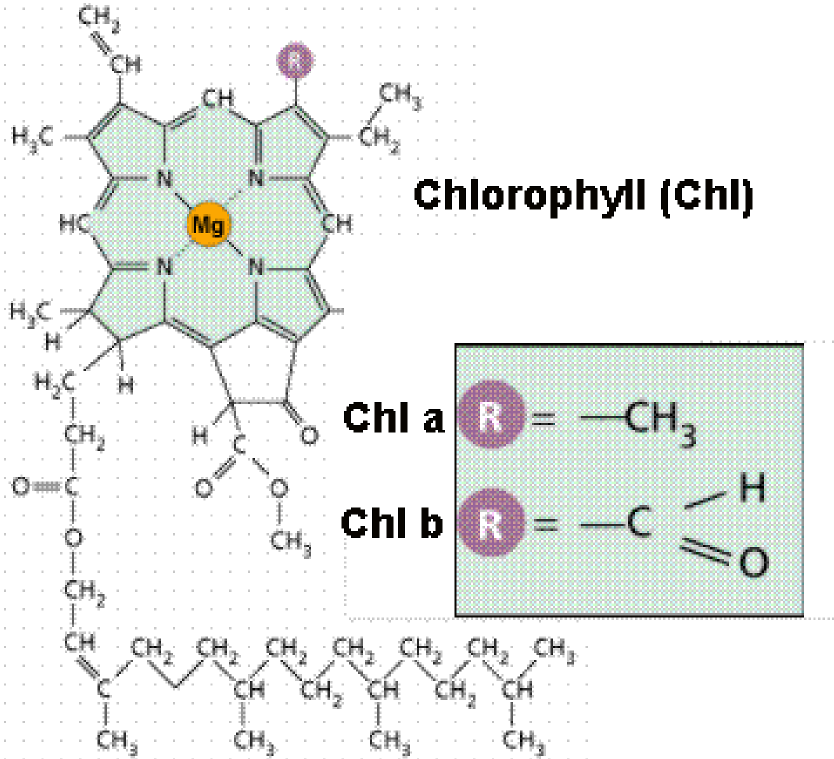
Color change due to interaction

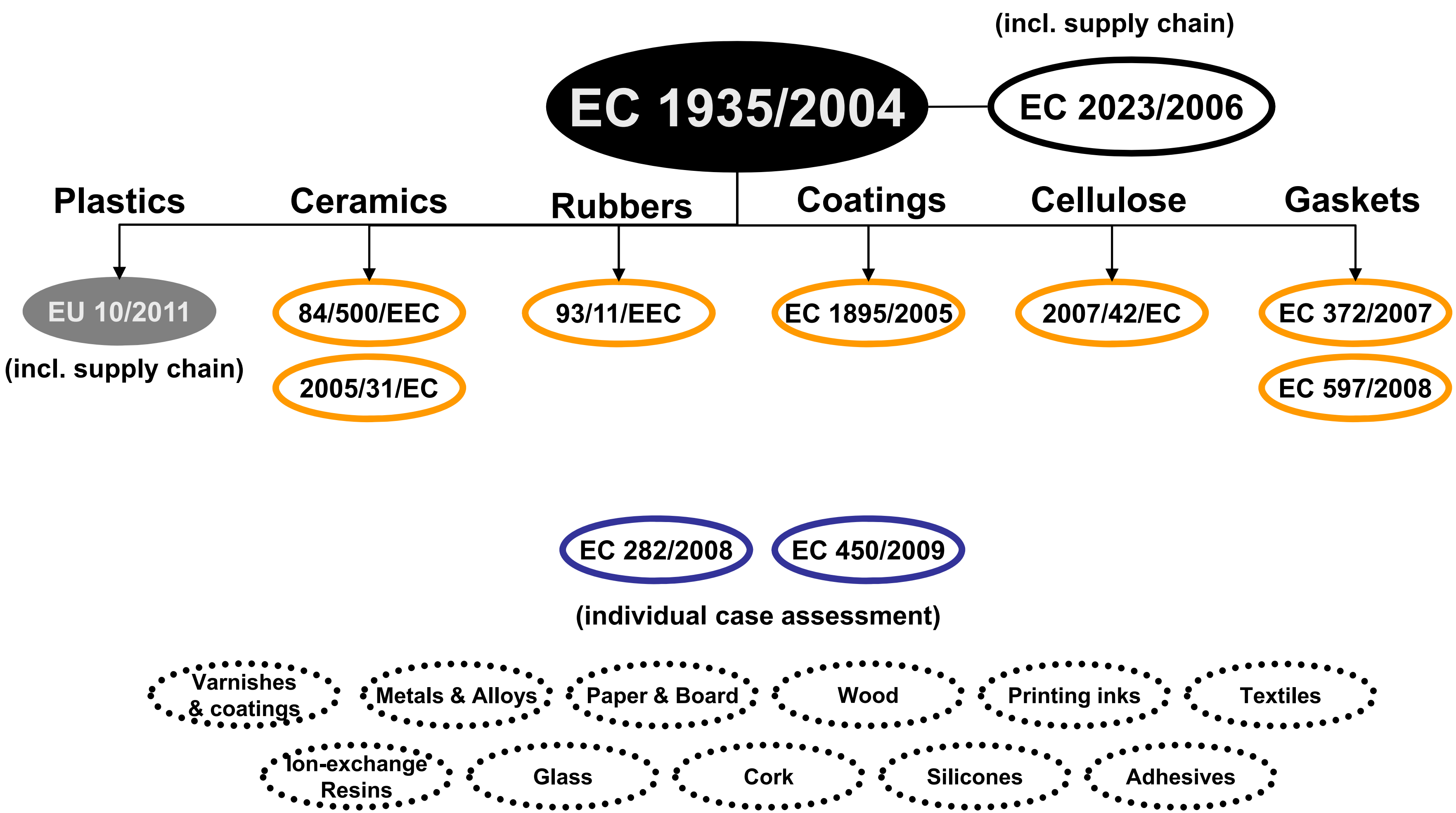
natural dye (water soluble)　自然染料（水溶性）

Chlorophyll :green dye in spinach クロロフィル:緑色染料（ほうれん草）



► Migration Modeling / legal background EU Annex V to Regulation (EU) No 10/2011

EU Regulations for FCM (Regulations & Directives)



EU Regulations - specific regulations ***EU規制 - 特殊な法令***

- ▶ Framework Regulation (EC) No 1935/2004,
  GMP (EC) No 2023/2006 and specific measures (Regulations & Directives)

- ▶ e.g. Plastics Regulations (EU) No. 10/2011 **プラスチック施行規則**
  - positive list (limitations) ポジティブリスト（制限）
  - functional barrier 機能性バリア
  - specific migration (SM) 特定移行量
  - overall migration (OM)
  - screening approaches (e.g. migration modeling)
  - migration testing 移行試験
    - ● food simulants 食品擬似物
    - ● time / temperature 暴露/時間と温度

- ▶ if a component from the material in contact with food is not covered by the positive list, a petition at EFSA(**欧州食品安全機関**) is required

  食品と接触する物質の

Important national regulations *重要な数々の国家規制*

- DE: BfR Reccomendation 独：BfR 独連邦リスク評価研究所-勧告
  - XXXVI Paper & board
  - XV Silicones
  - XXI Rubber
- FR: 仏
  - Circulaire no 176 Pigments 色素
  - Brochure no.1227 (summary food contact legislation 食品接触法令の概要)
- NL: Warenwet 蘭
  - Coatings
  - Rubbers
- IT: D.M. 21-3-1973 伊

Other references for evaluation *他の評価基準*

- Opinion of the Bundesinstitut für Risikobewertung (BfR)
  e.g. mineral oil (2009) 独連邦リスク評価研究所の見解
- Opinion of the European Food Safety Authority (EFSA)
  e.g. ITX (2005) 欧州食品安全機関の見解
- Guidelines of the EU-Commission EU委員会のガイドライン
  e.g. Migration Modelling 移行モデルによる計算
- Guidelines from Industry Associations 業界団体のガイドライン
- Standards 標準 基準
- Toxicological evaluations (TDI) 毒性評価**Tolerable Daily Intake**一日耐容摂取量
- etc.

EU legislation – Reg. (EU) No 10/2011, Annex V

2.2 Screening approaches スクリーニングへの取組み
2.2.3. Migration modelling 移行モデルによる計算

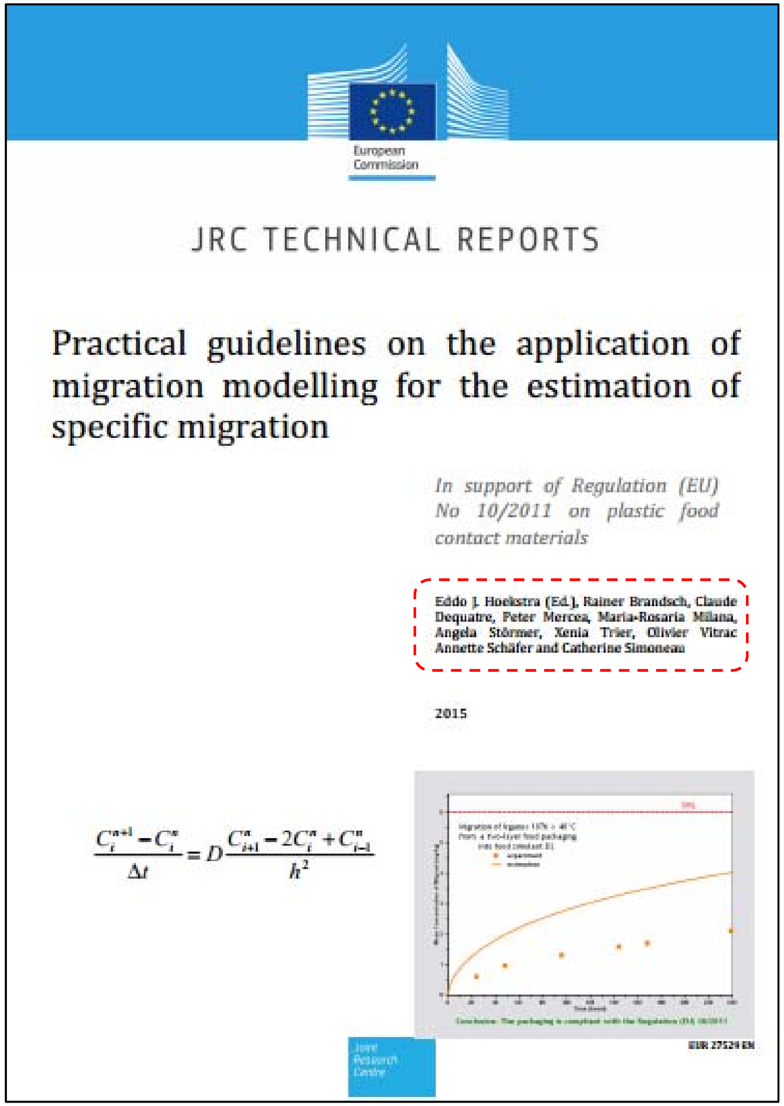
To screen for specific migration the migration potential can be calculated based on the residual content of the substance in the material or article applying generally recognized diffusion models based on scientific evidence that are constructed such as to overestimate real migration.

科学的物証に基づき、実際の移行量よりも過大に移行量を推定するように構成された拡散モデルが次第に認知されています。

▶ residual amount / initial concentration of migrant needs to be **known** !

移行物質の初期濃度/残存量が判明していることが必要

Guideline on migration modelling



European Commission

JRC TECHNICAL REPORTS

Practical guidelines on the application of migration modelling for the estimation of specific migration

In support of Regulation (EU) No 10/2011 on plastic food contact materials

Eddo J. Hoekstra (Ed.), Rainer Brandsch, Claude Dequatre, Peter Mercea, Maria-Rosaria Milana, Angela Störmer, Xenia Trier, Olivier Vitrac Annette Schäfer and Catherine Simoneau

2015

$$\frac{C_i^{n+1}-C_i^n}{\Delta t}=D\frac{C_{i+1}^n-2C_i^n+C_{i-1}^n}{h^2}$$

EUR 27529 EN

Joint Research Centre

移行モデルの応用による特定移行量を
推定するための実用的ガイドライン

JRCとは　Joint Research Centre

欧州委員会の委員会直属科学サービス組織 として、共同研究センター（JRC)の任務は EUの政策に独立的で実証に基く科学および 技術的支援を全政策サイクルにわたり一貫 して提供することである。

政策担当総局（DG）と密接に協力するJRC は主要な社会的変化を研究対象とすると同 時に、新たな方法、ツールや基準の開発、 自組織の持つノ ウハウのEU加盟国、科学者 コミュニティーや国際的提携先との共有を 通して革新を推進している。

JRC_JapanのHPより　抜粋

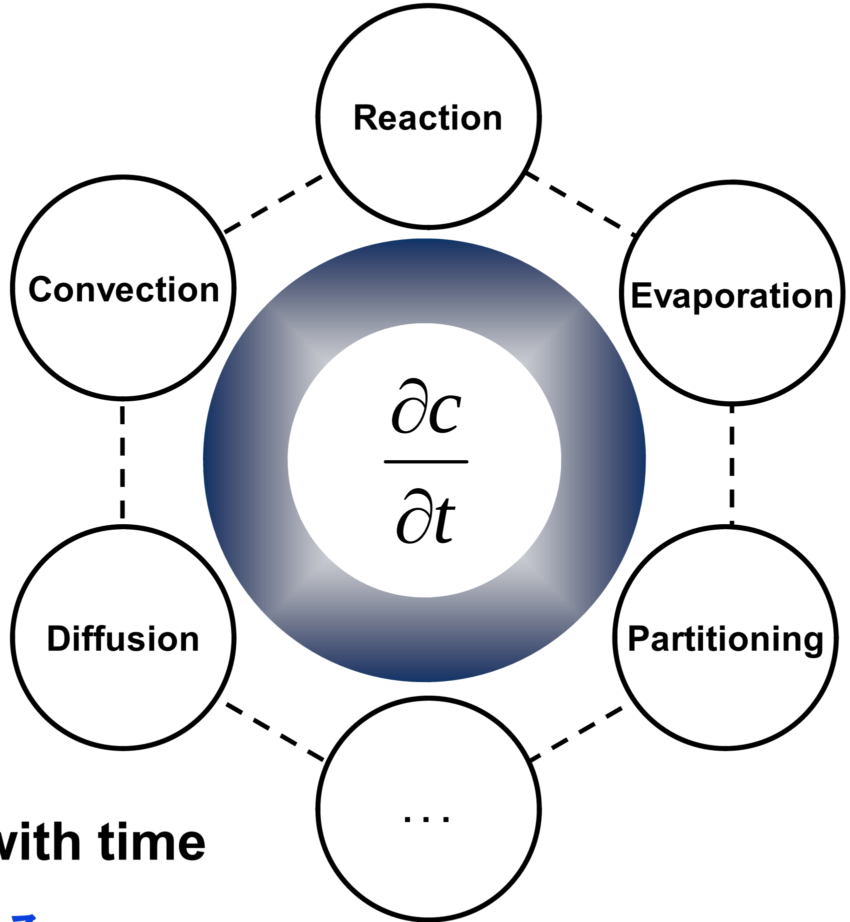
赤破線内の参加メンバーの名前が別資料の8ページにあります。

► Migration Modelling / Law of Diffusion

移行モデル　/　拡散法則

Mass transfer ***質量移送***

Diffusion	拡散
Convection	対流
Evaporation	蒸発
Reaction	反応
Partitioning	分配



>>> change of concentration with time

時間とともに濃度が変化する

Transport equation 輸送式

$$-\left|\frac{\partial c}{\partial t}\right|_{total} = -D\left(\frac{\partial^2 c}{\partial x^2}+\frac{\partial^2 c}{\partial y^2}+\frac{\partial^2 c}{\partial z^2}\right)+\left(v_x\frac{\partial c}{\partial x}+v_y\frac{\partial c}{\partial y}+v_z\frac{\partial c}{\partial z}\right)+k_r c^n + k_e\sigma$$

$$\frac{\partial c}{\partial t}$$

= **Diffusion** + **Convection** + **Reaction** + **Evaporation**

Migration process *移行プロセス*

Migration ~ Diffusion

移行（溶出）　　　拡散

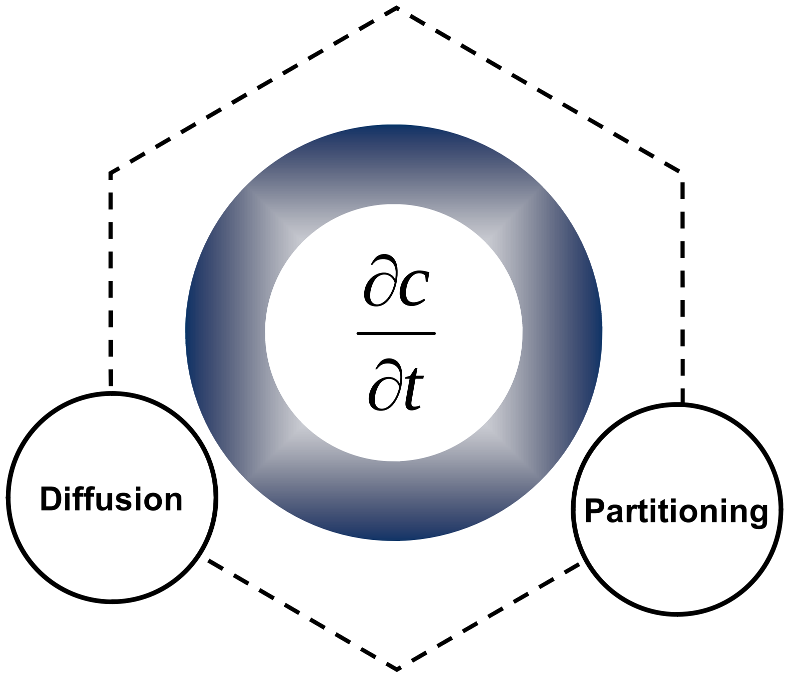
simplifying assumption

簡略化した仮定

拡　散
Diffusion

＋

分配係数
Partioning



Migration (mass transport processes)

溶出(移行)プロセス（質量移動プロセス）

Migration ~ Diffusion　**移行～拡散**

- Diffusion process is determined by:

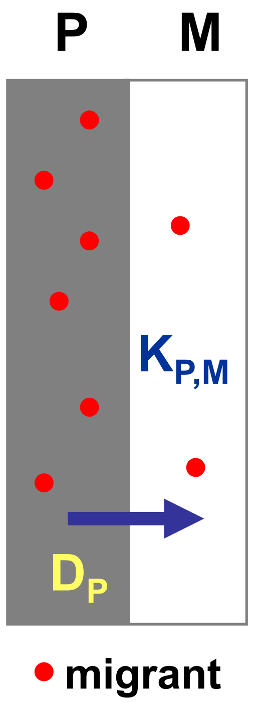
  - mobility of the polymer　**ポリマーの移動性**
    (A_P, polymer specific constant)　A_P　**ポリマー特定定数**

  - size of the migrant　**溶出(移行)物質のサイズ**
    (M_r, molecular weight)　Mrelative　**相対分子量**

  - temperature　**温度**
    (T, temperature)

A_P value :　A_P'- polymer specific constant　(Piringer)

Mass transport = Migration ~ Diffusion



P - polymeric material

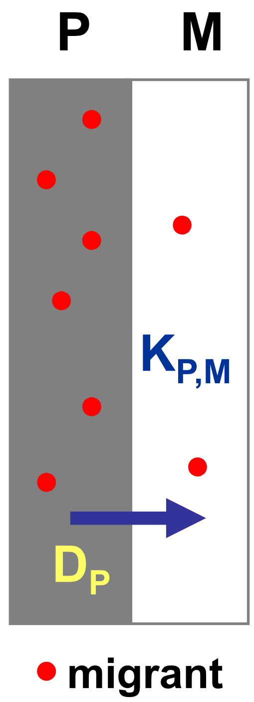
M - contacting medium

Fick's 2nd law of diffusion (one dimensional):

$$\frac{\partial c_F}{\partial t} = \mathbf{D} \cdot \frac{\partial^2 c_P}{\partial x^2}$$

c - concentration [mg/kg] (food/packaging)
t - time [s]
x - distance [µm]
D - diffusion coefficient [cm²/s]

Diffusion models



» monolayer materials
(monolayer) 単層

D/K

» multilayer materials
(multilayer) 複層

$\mathbf{(D/K)_n}$

» general diffusion model

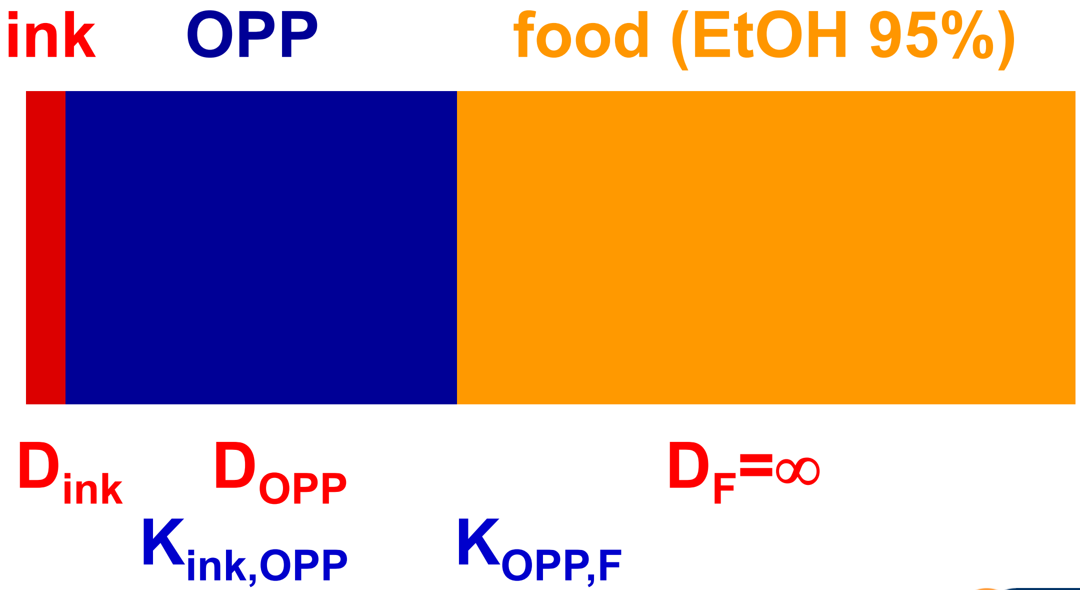
$\mathbf{(D/K)_n/D_F}$

D,K - mass transfer constants

質量移動定数

Migration in Multilayer Materials

$$\frac{d_{tot}^2}{D_{tot}} = \frac{d_1^2}{D_1} + \frac{d_2^2}{D_2} + \cdots + \frac{d_n^2}{D_n}$$



Diffusion coefficient

- **Arrhenius relationship - "how fast"** いかに速く拡散するか？
(temperature dependence)

$$D = D_0 \cdot e^{\frac{-E_A}{RT}}$$

D - Diffusion coefficient [cm²/s]
D_0 - pre-exponential factor
E_A - activation energy [J]
R - gas constant [8,314 J/molK]
T - temperature [K]

- **Piringer equation (estimation of diffusion coefficients)**

$$D_P = D_0 \exp\left(A_P - 0.1351 \cdot M_r^{2/3} + 0.003 \cdot M_r - \frac{R \cdot 10454}{R \cdot T} \right)$$

Piringer式（拡散係数の推定）　A_P　Mr　相対分子量

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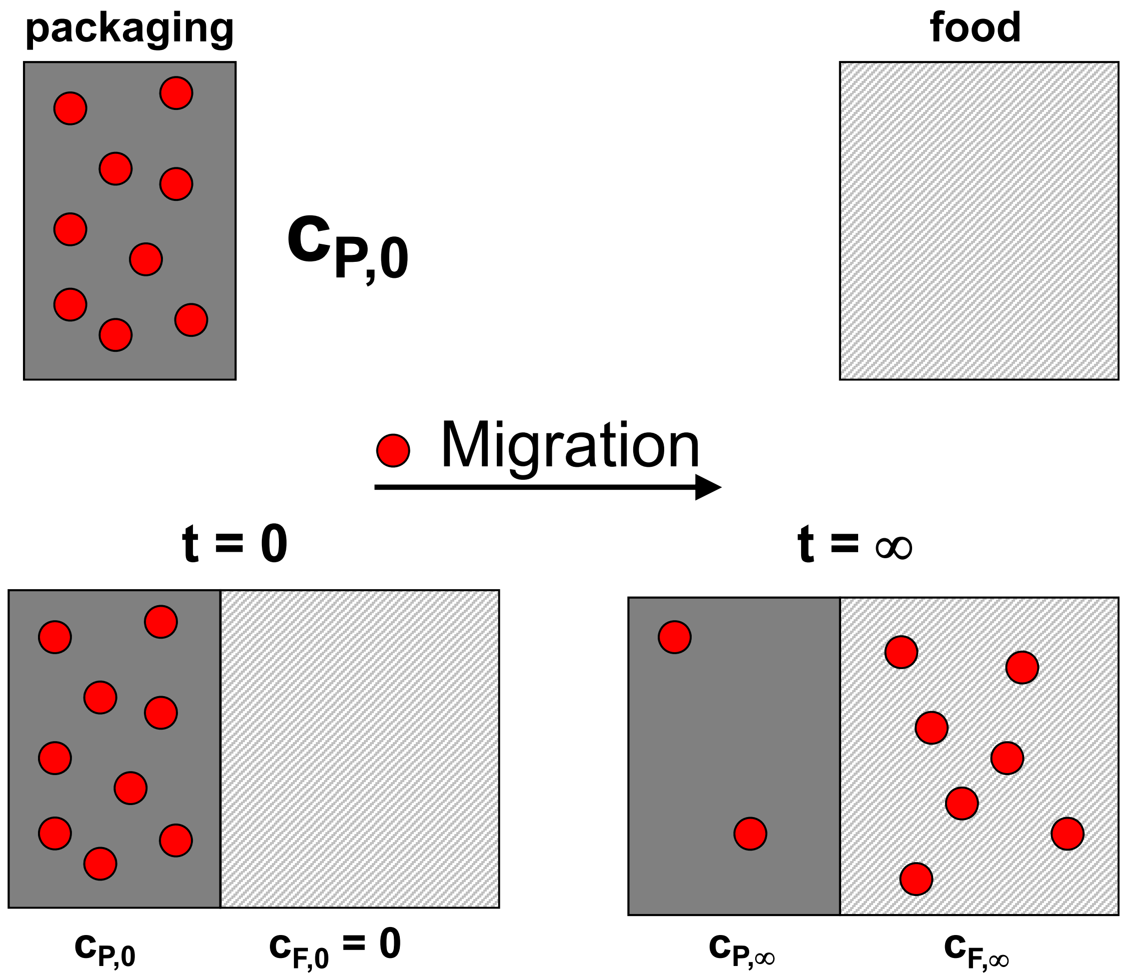
Partitioning



Partition coefficient (in closed systems)

► **equilibrium related - "<u>how much</u>"**

平衡状態で　どれくらいの量が？移動するか？

$$K_{P,F} = \frac{c_{P,\infty}}{c_{M,\infty}} \approx \frac{S_P}{S_M}$$

K	**- Partition coefficient**	**K**	**分配係数**
c	**- concentration [mg/l]**	**C**	**濃度**
P	**- packaging**		
F	**- filled good**		

► Functional Barrier

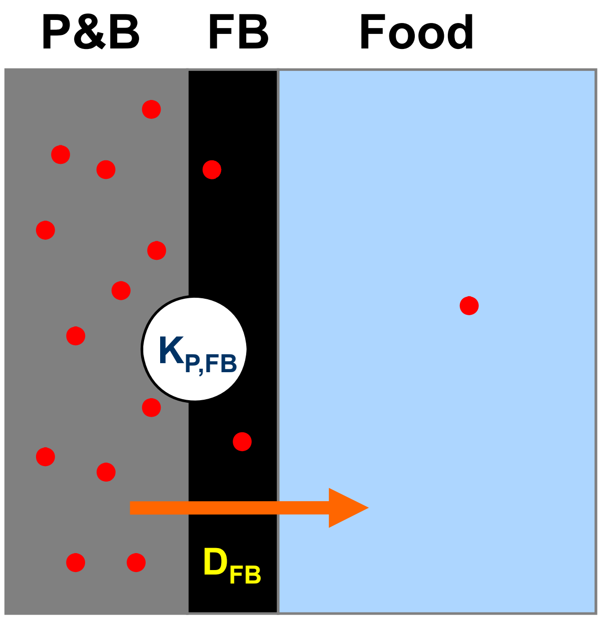
Functional barrier

» absolute barrier　　機能性バリア
glass and metals may ensure complete blockage of migration.　ガラスや金属は移行を完全に阻止できます。

» functional barriers
plastics materials can act as an effective barrier which reduces the migration of specific substance below a SML or a limit of detection

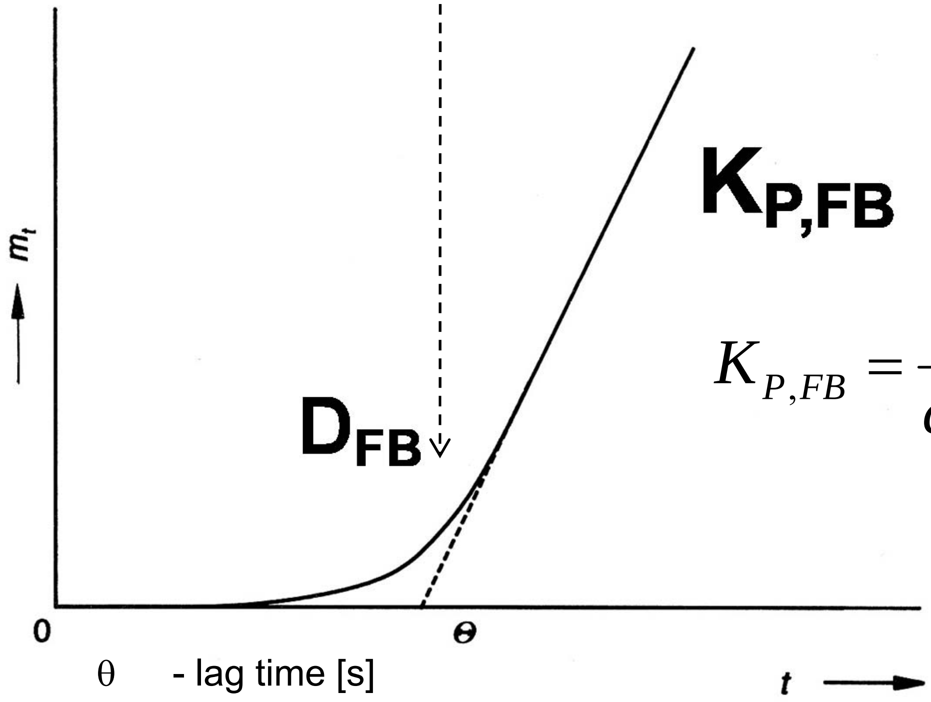
=> efficiency depends on:
- material type
- material thickness
- size of molecule
- time & temperature

Functional barriere



● e.g. mineral oil

$$\theta = \frac{1}{6} \cdot \frac{d_P^2}{D_{FB}}$$



$$K_{P,FB} = \frac{c_{P,\infty}}{c_{FB,\infty}}$$

θ - lag time [s]
d - thickness
D - diffusion coefficient [cm²/s]
K - partition coefficient

► Experimental determination of diffusion coefficients (D_P) and partition coefficients ($K_{P,F}$)

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Certified Reference Materials for the specific migration testing of plastics for food packaging

食品包装用ポリマーの特定移行量テスト用　認証標準物質

PROJECT G6RD-CT-2000-00411

PARTNERS :

Fraunhofer Gesellschaft	D	(IVV)
Pira International	UK	(PIRA)
MAFF-CSL	UK	(CSL)
FABES Forschungs-GmbH	D	(FABES)
BIT-FCA	B/EU	(FCA)

Migration testing 溶出試験

- **migration cell**

  溶出試験セル

Polymer matrix : HDPE

HDPE

type 1: ρ = 0,948

d = 1043 µm

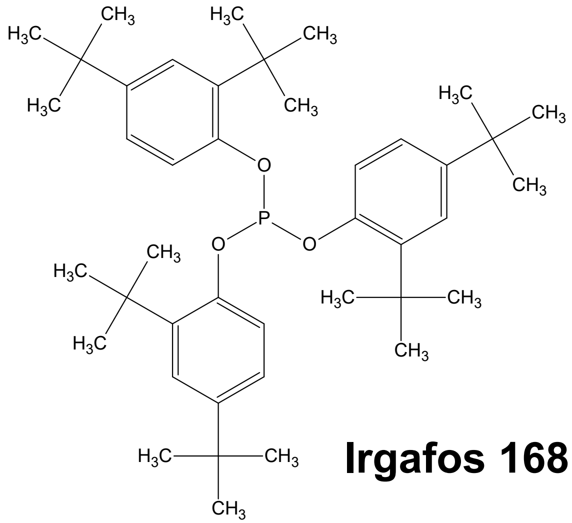
migrants: Irganox 1076 (antioxidant)
Irgafos 168 (antioxidant)

type 2: ρ = 0,933

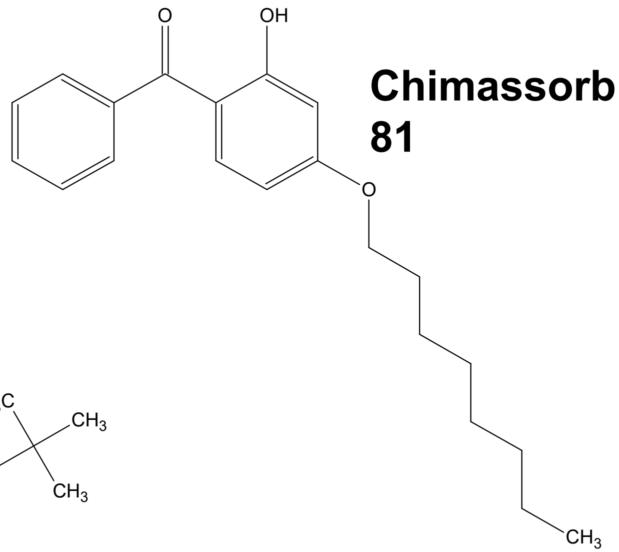
d = 356 µm

migrants: Chimassorb 81 (UV-absorber)
Uvitex OB (optical brightener)

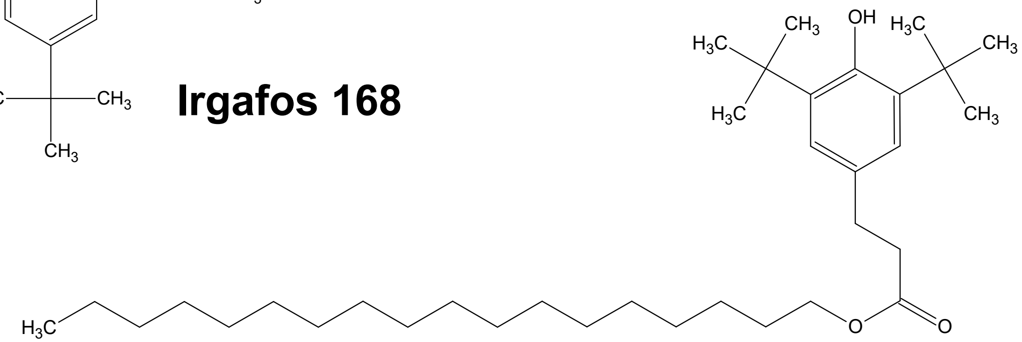
Structure of migrants



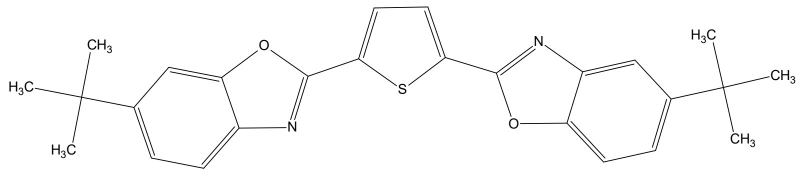
Irgafos 168



Chimassorb 81



Irganox 1076

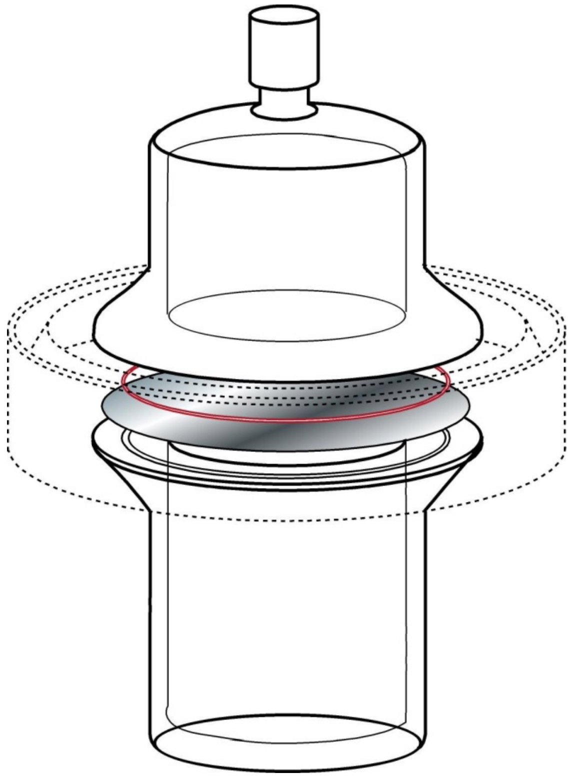


Uvitex OB

Experimental considerations

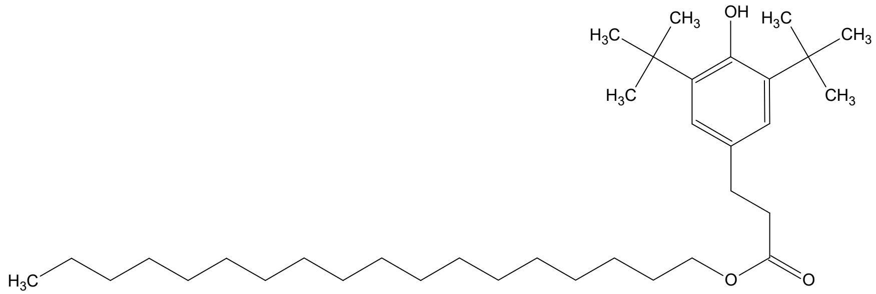
migration cell (one sided)

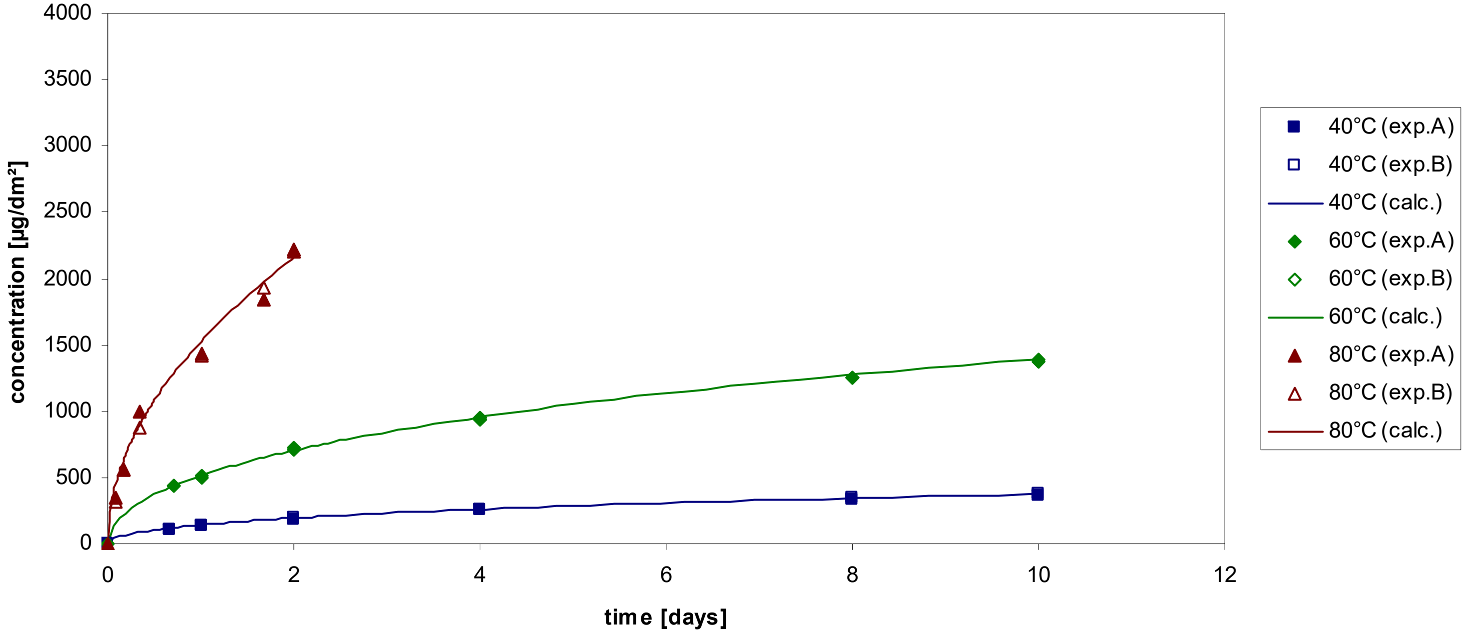
area, A = 48 cm²
volume, V = 10 ml



Modelling of Irganox 1076 migration

$c_{P,0}$ = 850 ppm (8404 µg/dm²)





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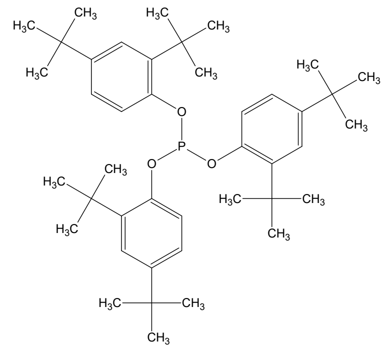
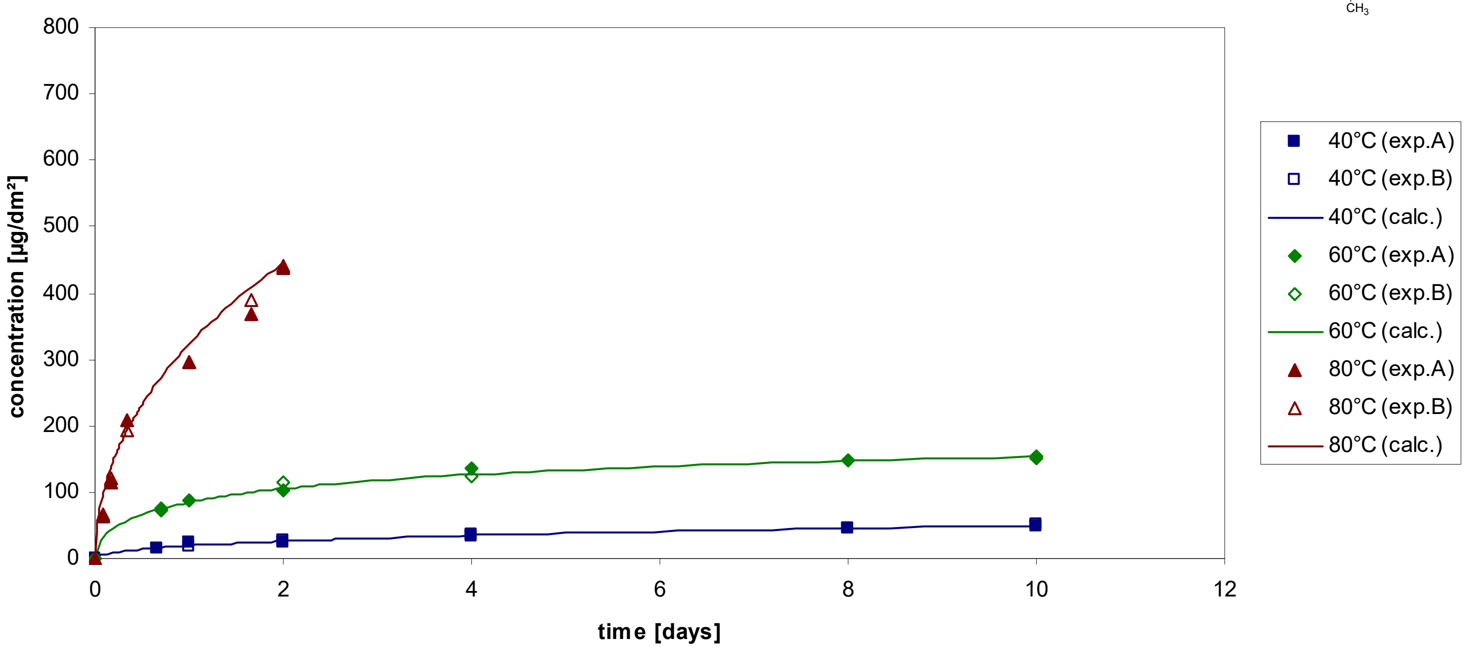
Modelling of Irgafos 168 migration

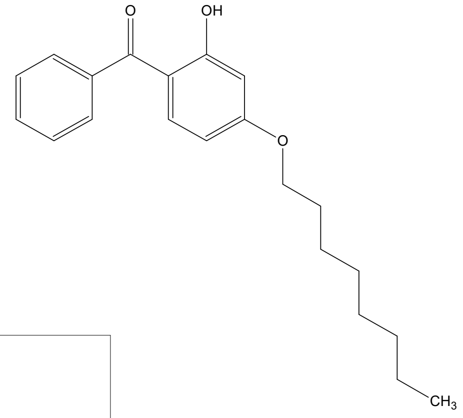
$c_{P,0}$ = 517 ppm (5112 µg/dm²)

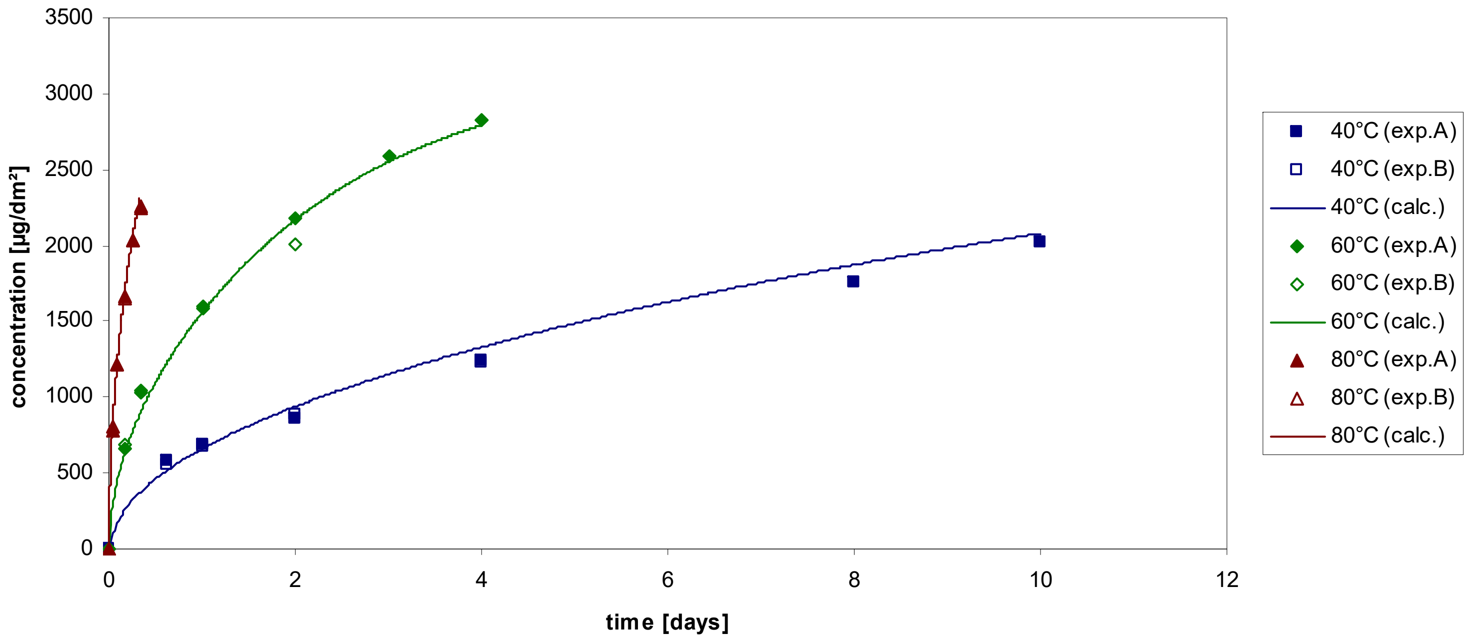




Modelling of Chimassorb 81 migration

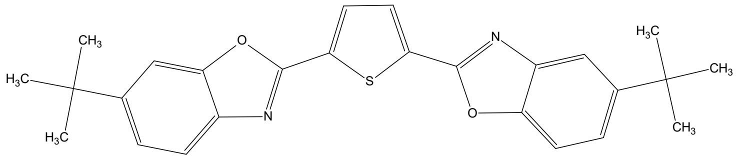
$c_{P,0}$ = 935 ppm (3106 µg/dm²)

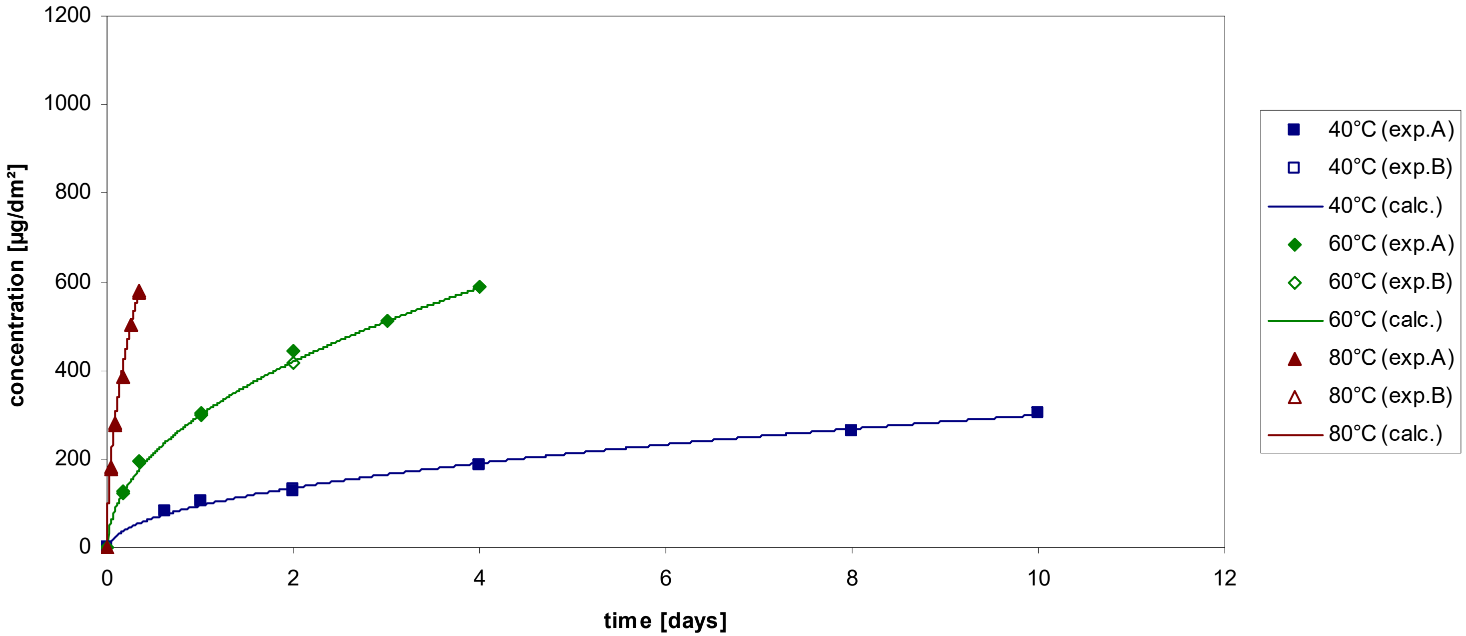




Modelling of Uvitex OB migration

$c_{P,0}$ = 471 ppm (1564 µg/dm²)





Mass transfer constants

Fitting procedure by variation of the diffusion coefficient, D_P and the partition coefficient, $K_{P,F}$ gives for the best fit:

Migrant	Diff.coef			Part.coeff		
	40℃	60℃	80℃	40℃	60℃	80℃
Irganox 1076	3,9E-11	4,3E-10	3,3E-09	15,0	3,0	0,1
Irgafos 168	2,1E-12	7,2E-11	4,5E-10	80,0	50,0	3,0
Chmiassorb 81	5,0E-10	2,7E-09	1,9E-08	0,1	0,1	0,1
Uvitex OB	4,5E-11	4,5E-10	4,7E-09	1,0	1,0	0,1

► Estimation of diffusion coefficients (D_P) and partition coefficients ($K_{P,F}$)

拡散係数(D_P) and 分配係数($K_{P,F}$)の推定

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Estimation of diffusion coefficients

» Diffusion coefficients (D_P)

Arrhenius	$D_P=f(D_0,E_A,T)$
Piringer	$D_P=f(A_P',tau,M_r,T)$
Interpolation T_g	$D_P=f(A_P',tau,M_r,T, T_g,)$
Brandsch	$D_P=f(T_g,M_P,T_{m,}M_M,T)$

D_P - diffusion coefficient
D_0 - pre-exponential factor (Arrhenius)
E_A - activation energy (Arrhenius)
T - temperature [K]
A_P' - polymer specific constant (Piringer)
tau - polymer specific temperature constant (Piringer)

M_M - molecular weight of migrant [g/mol]
M_P - molecular weight of polymer [g/mol]
M_r - relative molecular weight
T_g, - glass temperature of polymer [K]
T_m, - melting point of migrant [K]

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Estimation of diffusion coefficients based on A_P-values

(Piringer equation) ***A_P値による拡散係数の推定***

$$D_P = D_0 \exp\left(A_P - 0.1351 \cdot M_r^{2/3} + 0.003 \cdot M_r - \frac{R \cdot 10454}{R \cdot T} \right)$$

D_P	- Diffusion coefficient ($D_0 = 10^4$ cm²/s)	拡散係数
$A_P = A_P' - \tau/T$	- ***material*** specific constant (τ - material specific temperature constant)	物質特定係数 **物質特定温度係数**
M_r	- relative molar mass of ***migrant*** in Dalton	移行物質の相対分子量
T	- ***temperature*** in K	絶対温度**K**
$\mathbf{E_A}$	- reference ***activation energy*** (= R·10454 = ***86,9 kJ***, R = 8,314 J/K·mol)	**基準活性化エネルギー**

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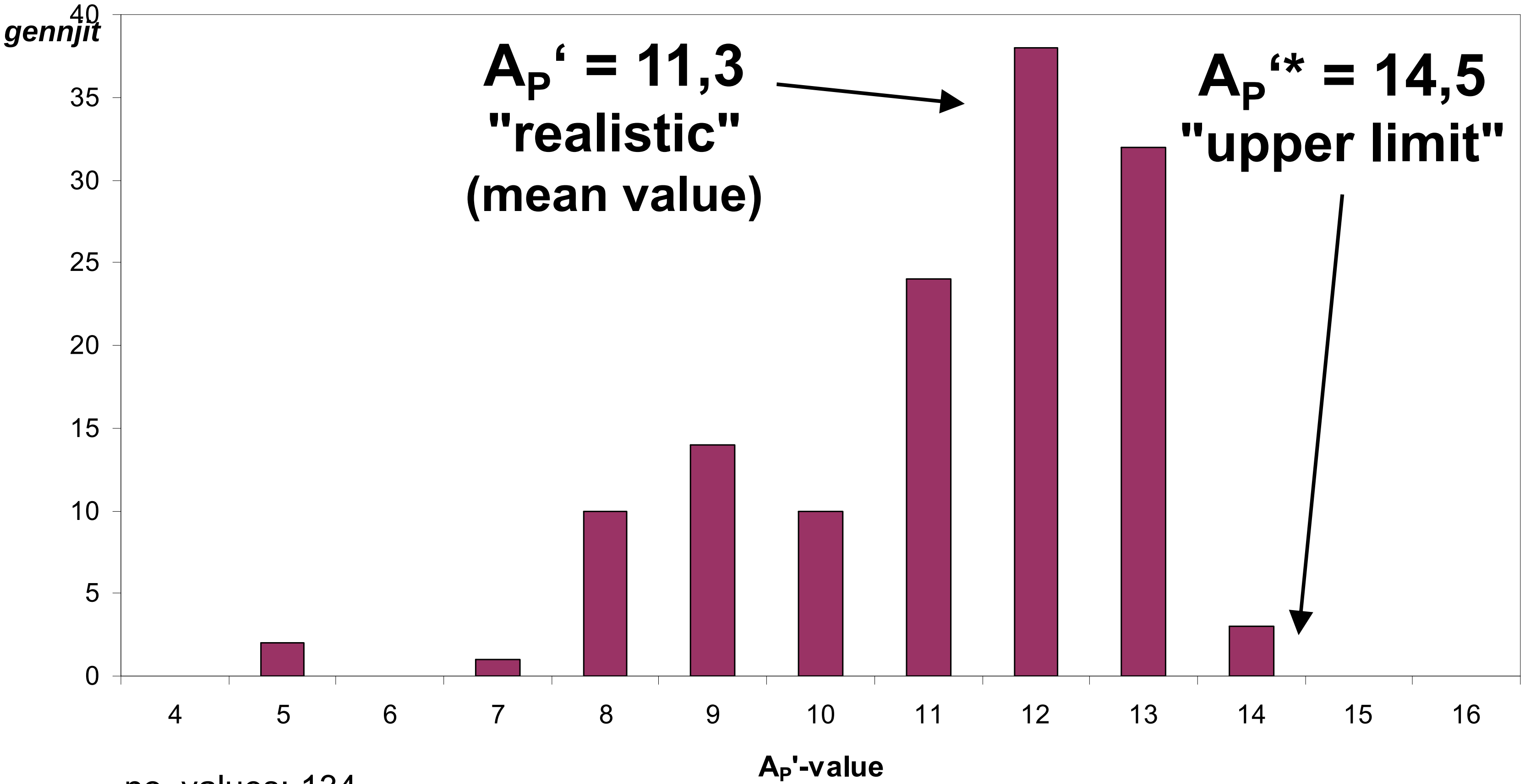
Upper limit A_P-value (HDPE) / mean A_P-values*

A_Pの上限値と平均値 (現実的なA_P 値)



no. values: 134
mean value A_P' = 11,29
standard deviation = 1,76
confidence interval (95%) = 7,85 - 14,74 (= MW ± 1,96*STABW)

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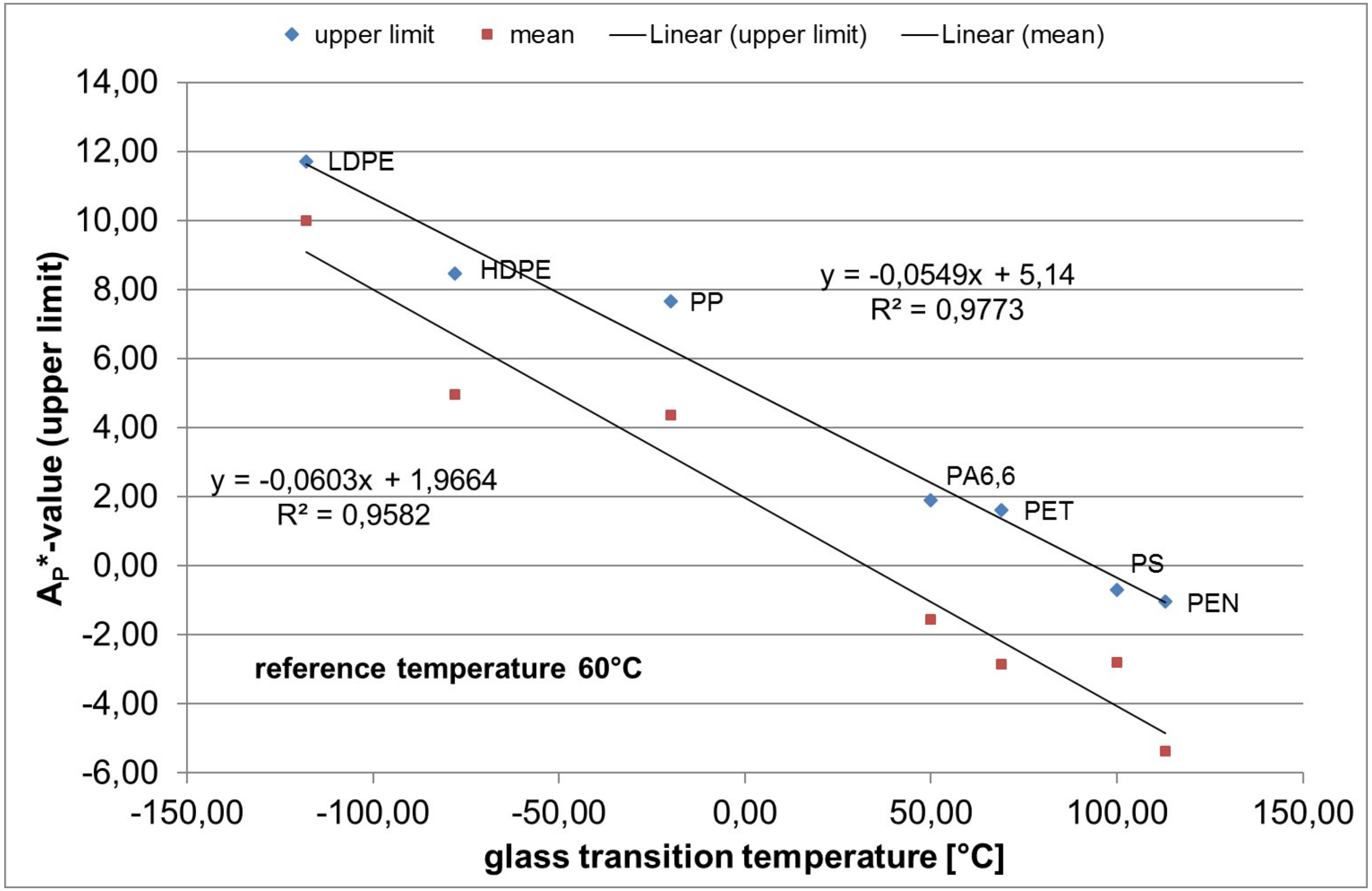
Estimation of Diffusion Coefficients based on T_g



ガラス転移点温度　Tg

Estimation of partition coefficients *分配係数の推定*

» Partition coefficients ($K_{P,M}$) 分配係数

worst case	$K=1$, ($V_P << V_M$)
solubility	$K=S_P/S_M$
Brandsch	$K=f(S_M)$ $K=f(P_{O/W})$

} SML5/6は2種類の設定が可能

$K_{P,M}$	- partition coefficient	分配係数
V_P	- volume of polymer	ポリマーの体積
V_W	- volume of medium	媒体体積
S_W	- solubility of migrant in contact medium	接触溶媒中の移行物質の溶解度
S_P	- solubility of migrant in polymer	ポリマー中の移行物質の溶解度
S_M	- solubility of migrant in contact medium	接触溶媒中の移行物質の溶解度
$P_{O/W}$	- octanol/water partition coefficient of migrant	移行物質のO/W分配係数

Estimation of Partition Coefficients *分配係数の推定*

<u>According to Guideline on migration modelling</u>: 移行モデルのガイドラインによれば

- if the migrant is soluble in the food or food simulant
  移行物質が食品または食品媒体に溶けるならば
  - e.g. water soluble migrant in aqueous food or simulant
  - e.g. fat soluble migrant in fatty food or simulant

  K = 1 („worst case" because $V_P << V_F$) 最悪ケースを想定

- if the migrant is not soluble in the food or food simulant (e.g. aqueous foods)
  移行物質が食品または食品媒体に不溶であれば
  - e.g. water soluble migrant in fatty food or simulant
  - e.g. fat soluble migrant in aqueous food or simulant

  K = 1000

- real partition coefficients between packaging and food are in the range of; K = 10 ~100 **実際の包装と食品間の分配係数はK=10~100**

Correlation between Partition Coefficients Polymer/Food Simulant, $K_{P,F}$, and Octanol/Water, Log P_{OW} – a New Approach in support of Migration Modeling and Compliance Testing

Asako Ozaki[1,2], Anita Gruner[2], Angela Störmer[2], Rainer Brandsch[3] and Roland Franz[2#]

ポリマー/模擬食品の分配係数$K_{P,F}$とオクタノール/水のLogP_{OW}との間の相関

移行モデル化支援の新しい方法と整合試験

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資料名：Deutsche Lebensmittel-Rundschau 巻：106 号：4 ページ：203-208
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Estimation of Partition Coefficients based on P_{ow}

オクタノール/水のLogP_{OW} を基礎とする分配定数の推定

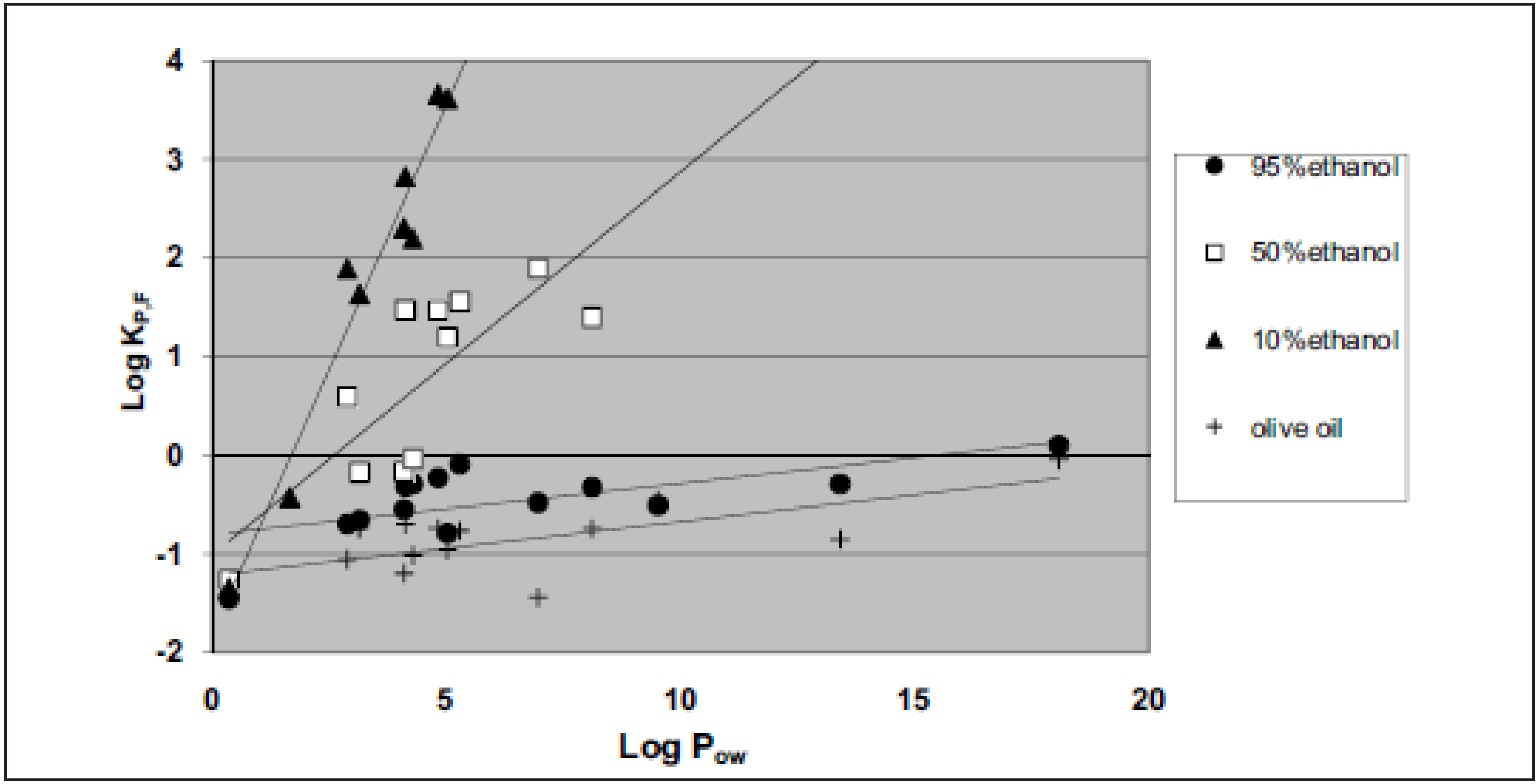

Fig. 3 Correlation between log P_{OW} and log $K_{P,F}$

Ethanol 10%	y = 1.07·x -1.82
Ethanol 50%	y = 0.389 ·x -1.02
Ethanol 95%	y = 0.052 ·x -0.807
Olive oil	y = 0.054 ·x -1.22

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► Migration Modeling with SML software

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Software Tools

► ***must solve the diffusion equation numerically (partial differential equation, PDE)***
拡散係数を計算(偏微分方程式)で解明する必要があります。

→ the analytical solution of the diffusion equations serves as reference for validation
拡散係数を測定分析データから求めることにより、バリデーションの基準とします。

→ validation required, i.e. experimental examples must be reproduced correctly
求める拡散方程式はバリデーションが要求されます。
例えば実験データは再現性が要求されます。

Numerical solution of the diffusion equation

» » numerical solution 計算による解決法のメリット

- for multilayer materials 多層膜に対応可能

- concentration profile available 濃度勾配プロファイル対応

- exchange cycles / repeated use can be simulated

リサイクルのシミュレーション対応可能

SML6 新機能 Repeated use cycle function

→ see standard textbooks for Numerical Mathematics

e.g. Finite Elements and Finite Differences algorithms

Migration modeling (Diffusion Law) *移行モデル（拡散法則）*

- **1. step** Solution of the diffusion equation (numerical mathematics)
  拡散係数の解明
- **2. step** Packaging geometry (contact area, food volume)
  包装品の形状を定義（接触エリア、食品体積）
- **3. step** Packaging structure (number of layers = n +1 for food)
  - specify polymer type (from database or user defined)
  包装品構造（層の数は食品層の１層を加えてn+1と定義）
- **4. step** Migrants of concern 移行物質に関して
  - specify substance(s) (from database or user defined)
  物質を特定する（データベースまたはユーザによる定義）

Migration modeling (Diffusion Law) *移行モデル（拡散法則）*

- » **5. step** Initial concentration for each migrant in each layer ($c_{P,0}$)
  - known from recipe/composition
  - from experiment by extraction study

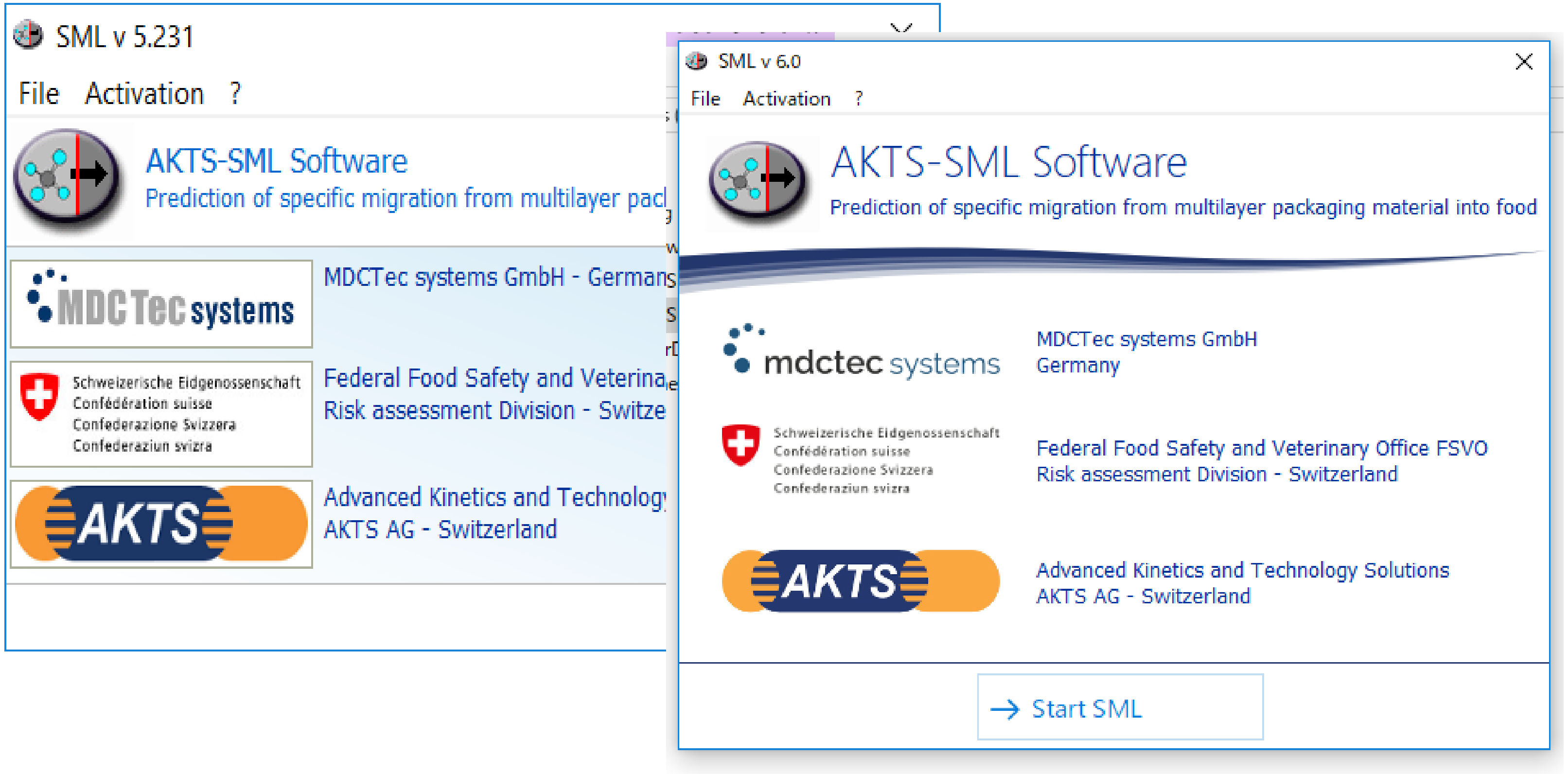
  それぞれの層におけるそれぞれの移行物質の初期濃度を設定
  - 構成物質/配合表から
  - 抽出研究による実験結果から
- » **6. step** Estimation procedure for mass transport parameters:
  - diffusion coefficient of migrant in each layer (D_P)
  - partition coefficient of migrant between layers ($K_{P,P}$ & $K_{P,M}$)

  物質移行パラメータによる推定手順
  - それぞれの層における移行物質の拡散定数（DP）
  - 層間における移行物質の分配定数（$K_{P,P}$ &$K_{P,M}$）
- » **7. step** Modelling calculation - estimation of migration for:
  - any time and temperature

  移行モデルによる計算
  - 時間と温度の諸条件による移行量（溶出量）の推定

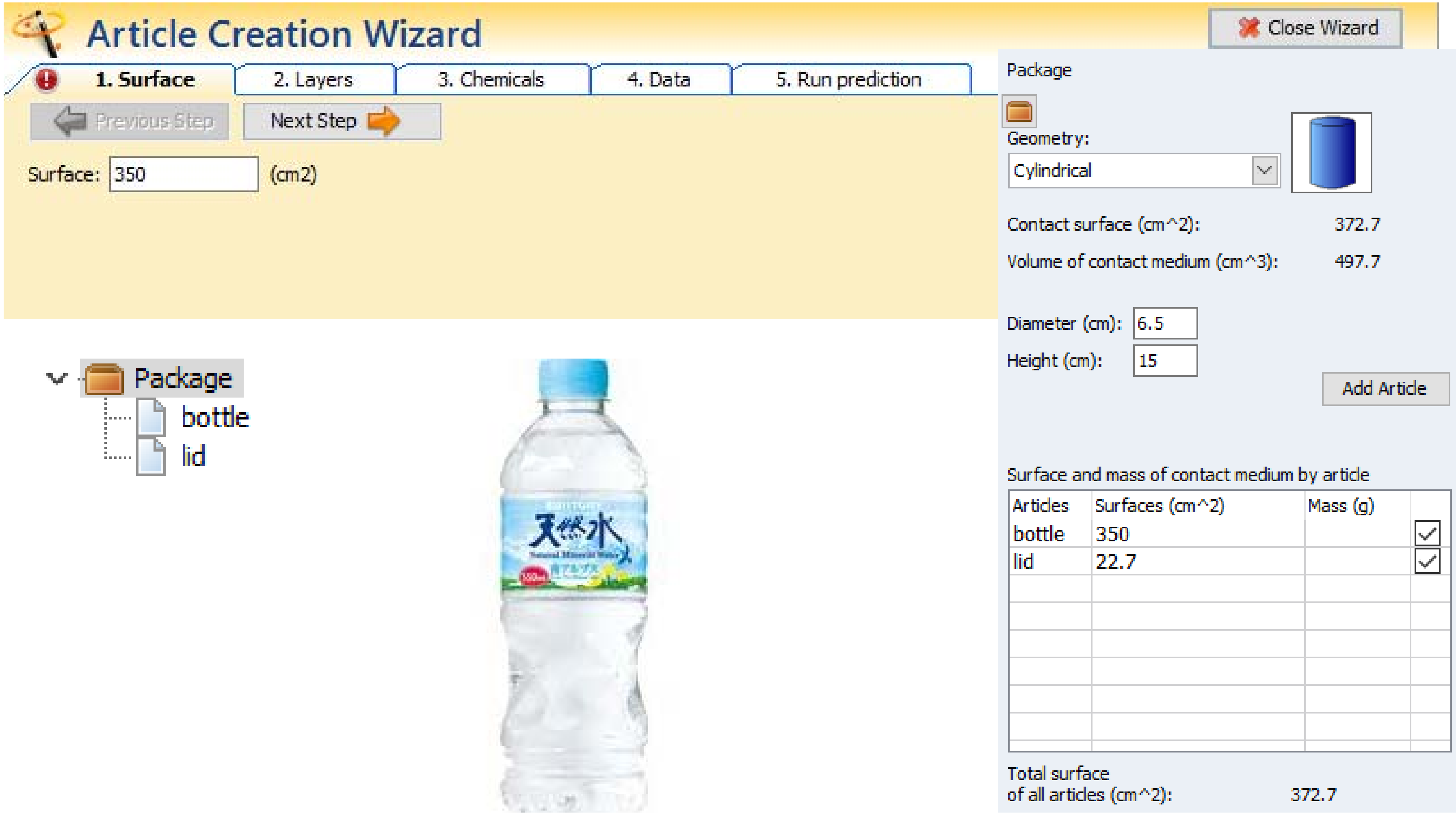
1. step Solution of the diffusion equation (numerical mathematics)

SML Software **SML5.231 ⇒ SML6.0**

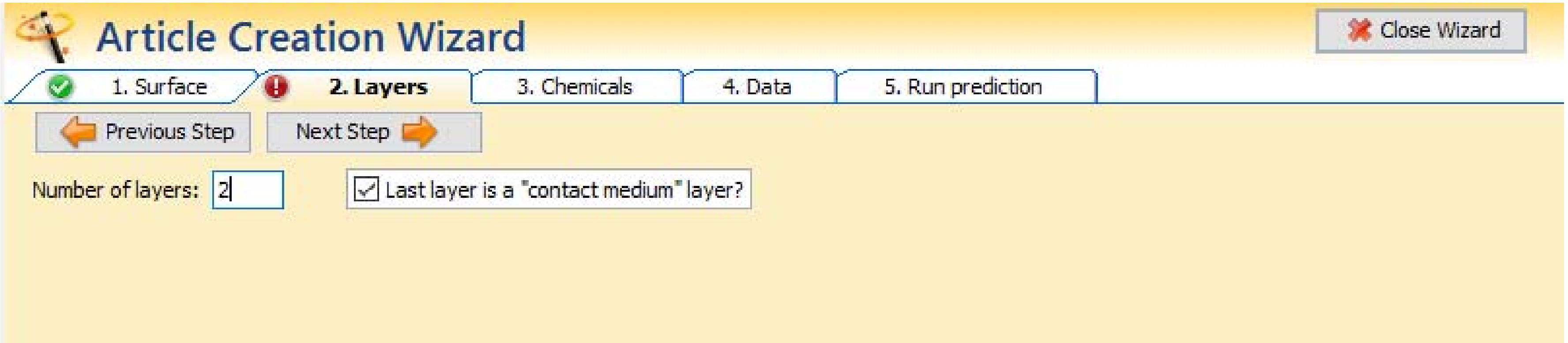


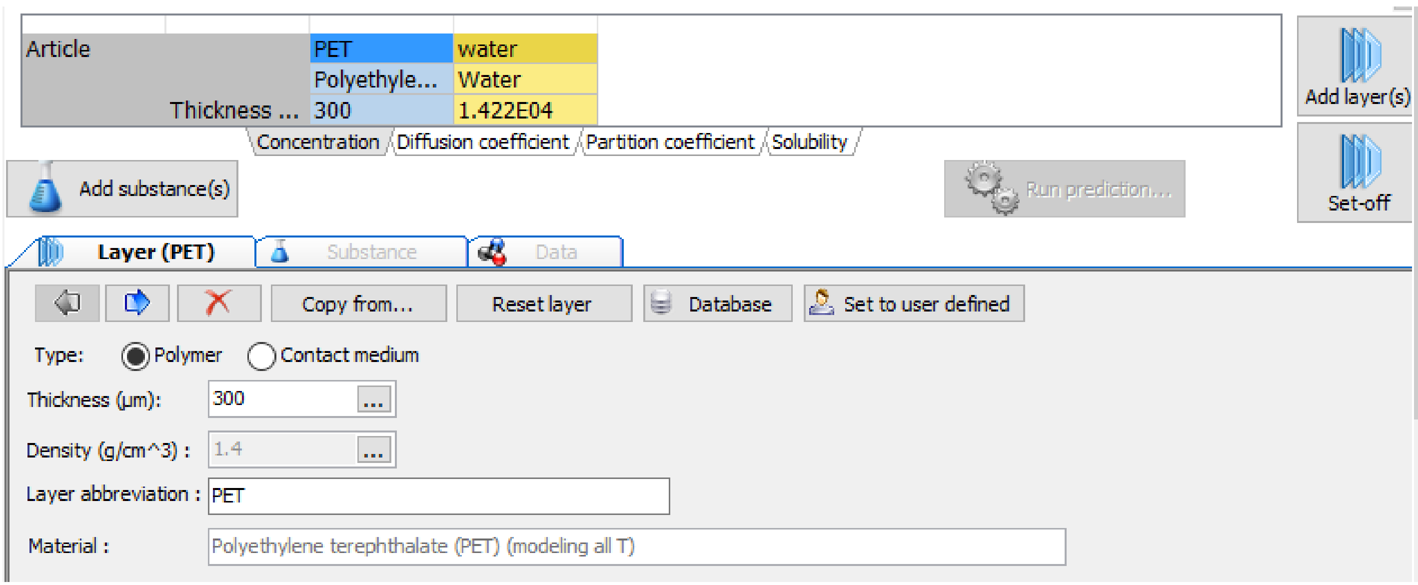
► **joint development AKTS & MDCTec**

2. step Packaging geometry (contact area, food volume)



3. step Packaging structure (number of layers = n +1 for food)
- specify polymer type (from database or user defined)





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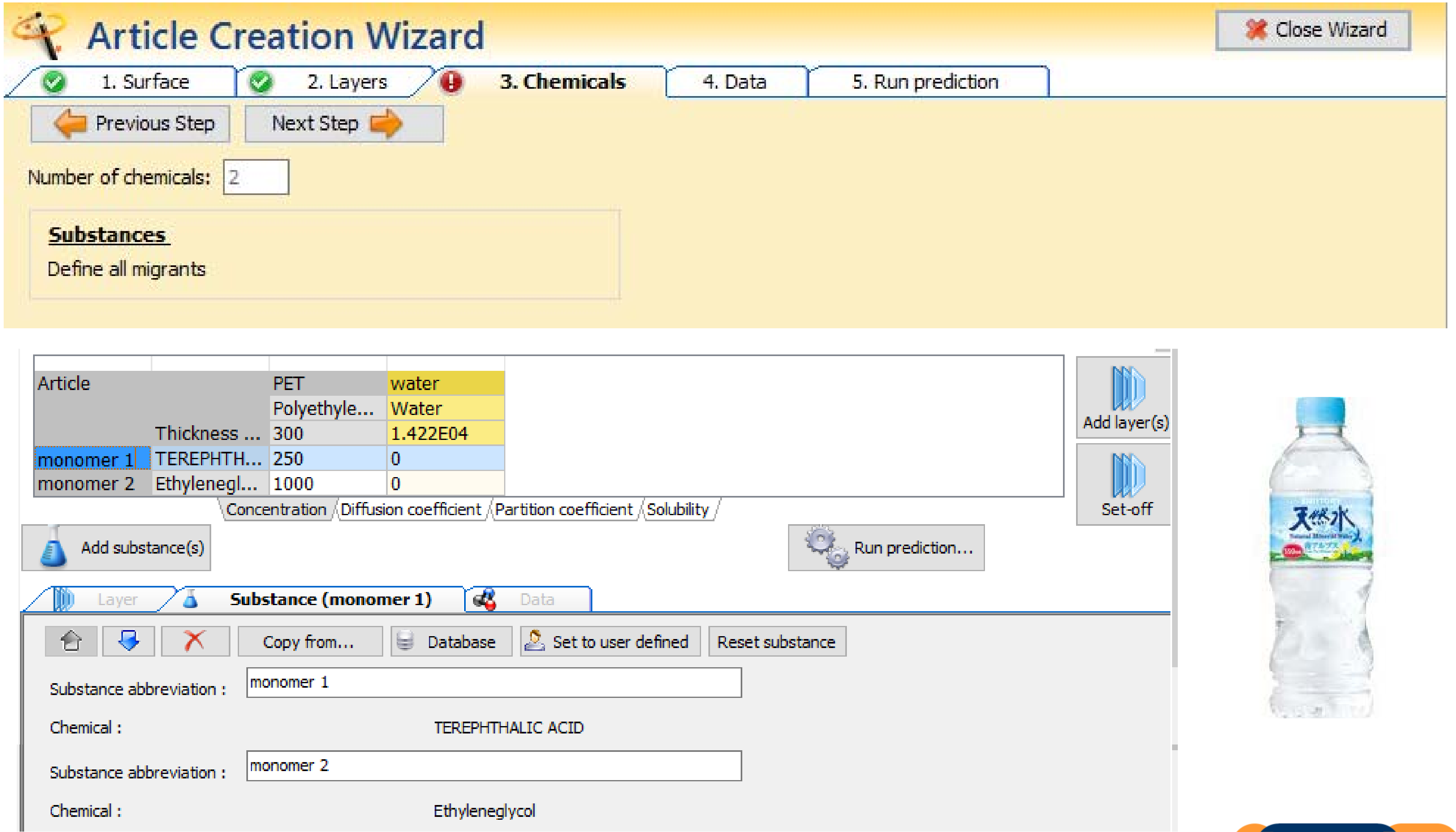
4. step Migrants of concern

- specify substance(s) (from database or user defined)



5. step Initial concentration for each migrant in each layer ($c_{P,0}$)

Article Creation Wizard

Close Wizard

1. Surface | 2. Layers | 3. Chemicals | **4. Data** | 5. Run prediction

Previous Step | Next Step

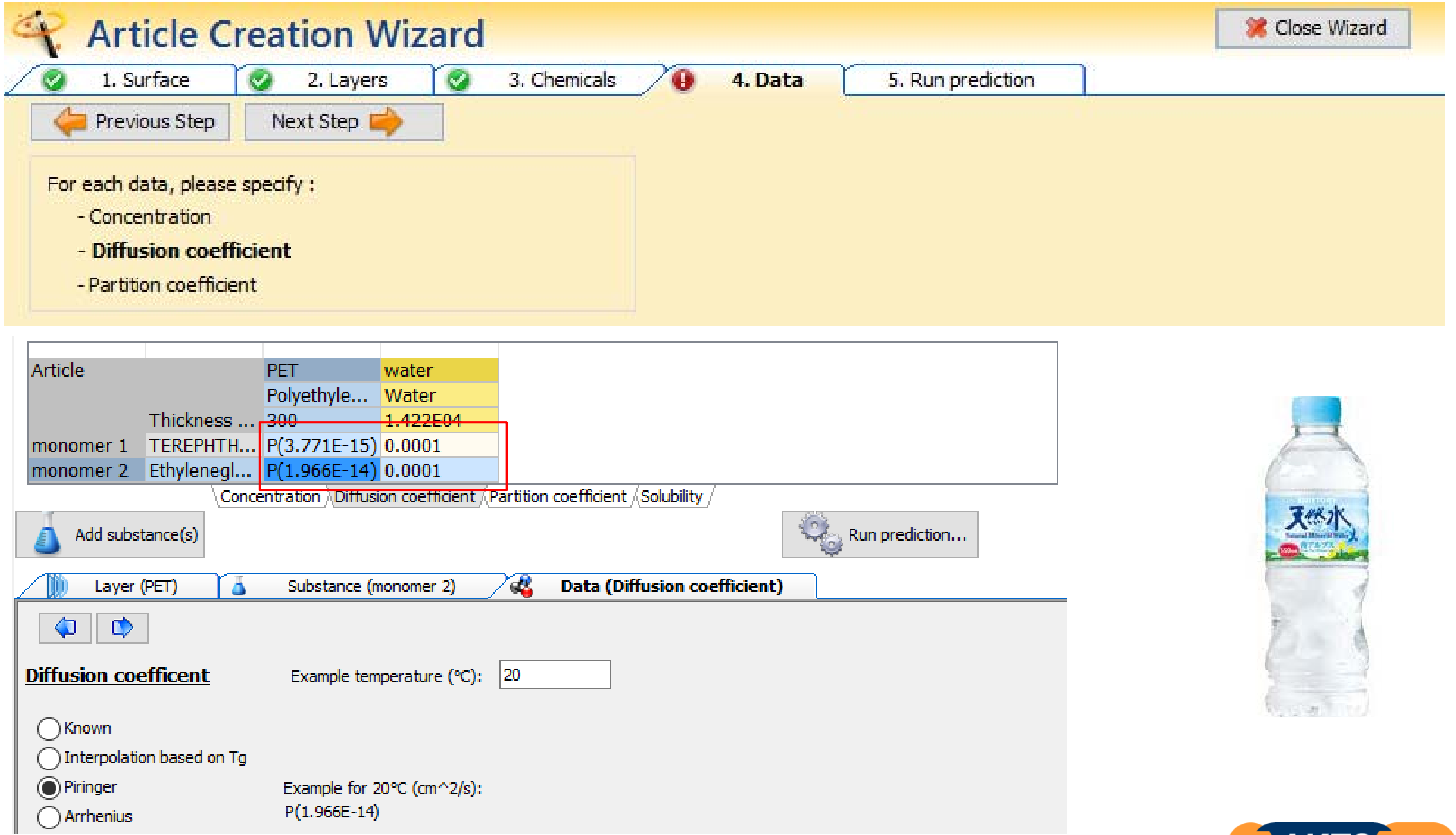
For each data, please specify :

- **Concentration**
- Diffusion coefficient
- Partition coefficient

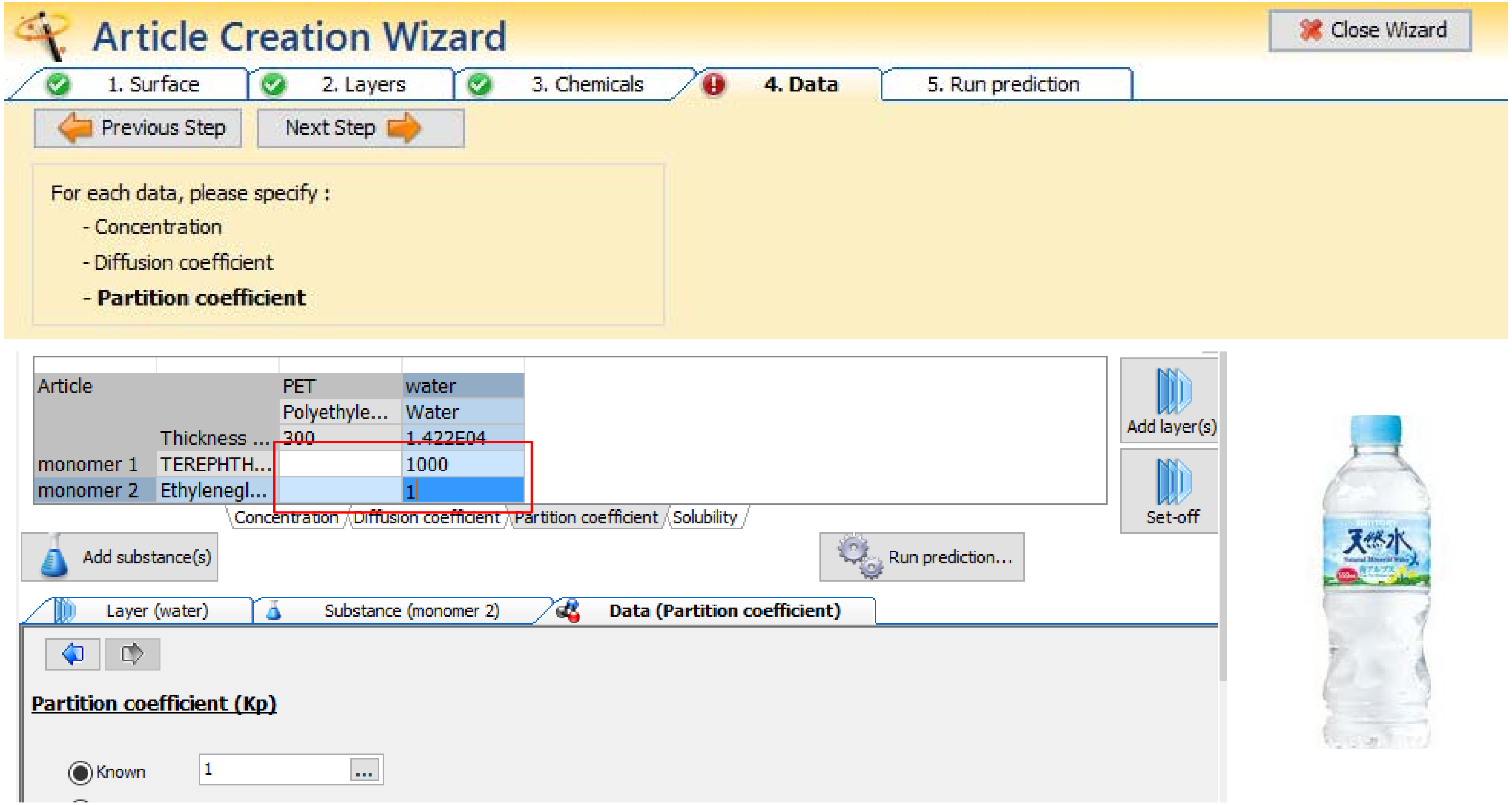
Article		PET	water
		Polyethyle...	Water
	Thickness ...	300	1.422E04
monomer 1	TEREPHTH...	250	0
monomer 2	Ethylenegl...	1000	0

Concentration | Diffusion coefficient | Partition coefficient | Solubility

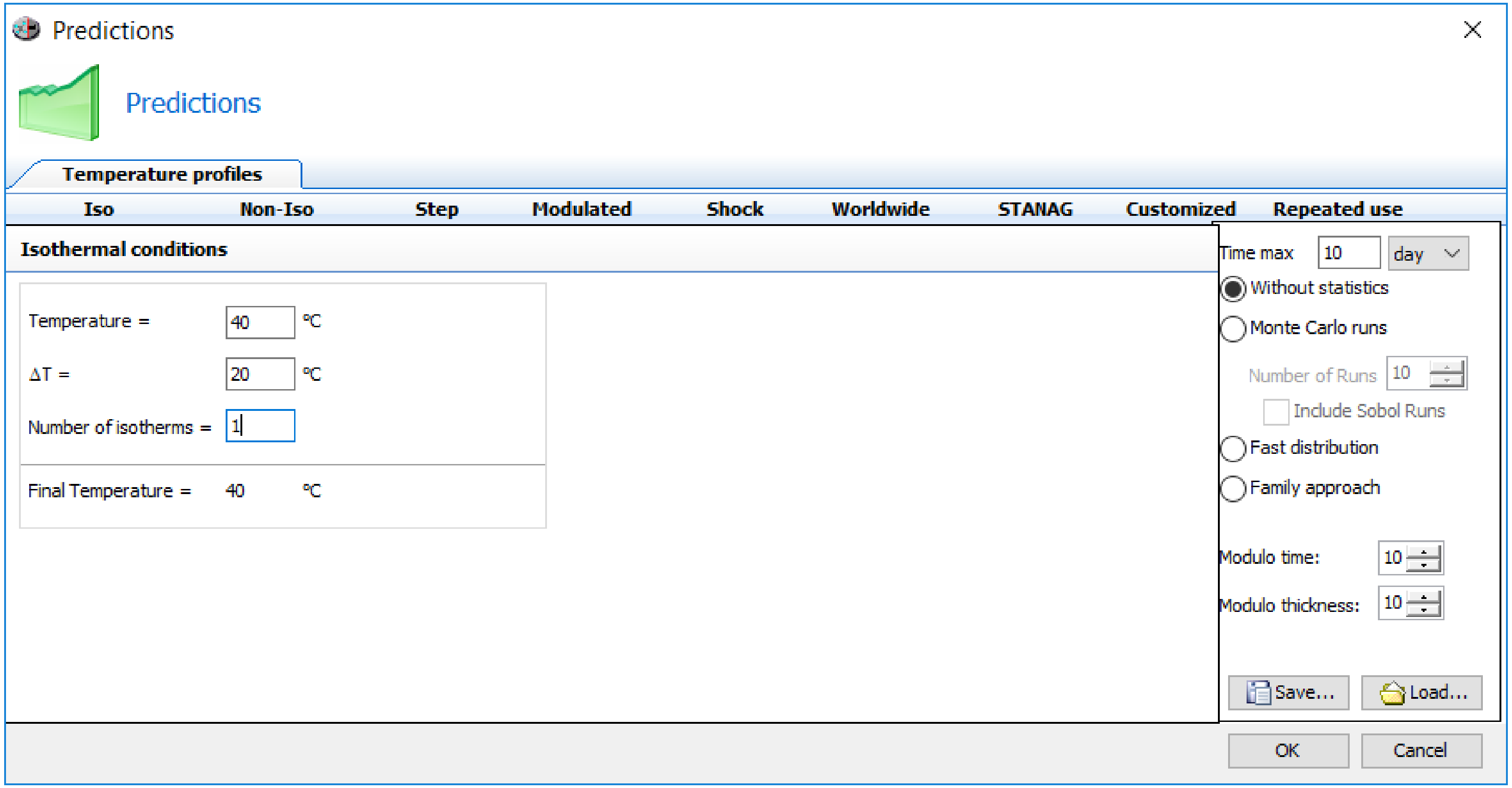
6. step Estimation procedure for mass transport parameters: - diffusion coefficient of migrant in each layer (D_P)



6. step Estimation procedure for mass transport parameters:
- partition coefficient of migrant between layers ($K_{P,F}$)



7. step Modelling calculation - estimation of migration for:
- any time and temperature

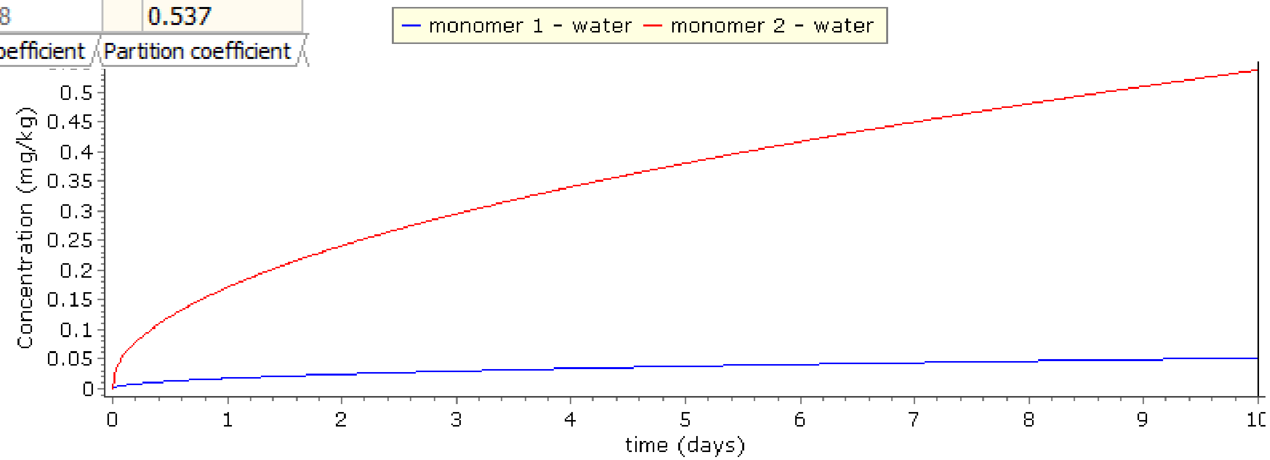


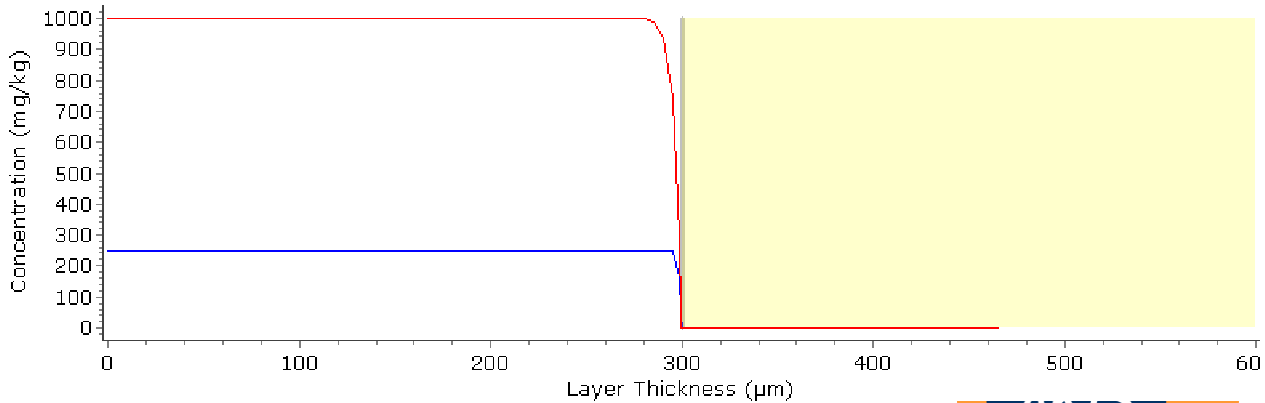
Simulation Result

Article		PET	water
		Polyethyle...	Water
	Thickness ...	300	1.422E04
monomer 1	TEREPHTH...	248.2	0.05185
monomer 2	Ethylenegl...	981.8	0.537

Concentration | Diffusion coefficient | Partition coefficient

- Package
  - bottle
    - Iso(40°C ,10d)
  - lid





SUMMARY

- simulation of migration from plastic food packaging to food or food simulants based on diffusion law
  拡散法則を基礎としたプラスチック食品包装から食品あるいは
  食品擬似物への移行シミュレーション

- SML software provides numerical solution of diffusion equation
  SML5/6ソフトウエアは拡散式により数値解析をします。

- simulation requires mass transfer coefficients:
  - diffusion coefficient
  - partition coefficient
  >> not available => use of estimation procedures
  シミュレーションには物質移動定数である
  拡散定数
- 分配定数
- これらの定数が得られないときは ⇒ いくつかの推定手順を使用します。

SUMMARY

- migration modeling result may be different from experimental result

  - due to overestimation ("upper limit" coefficients)
  - estimation procedure for coefficients are not precise enough
  - experimental migration does not follow law of diffusion

- 移行モデルによる結果は実験測定結果と異なるかもしれません。

  過剰な推定値を使用するため（upper_limit　上限値の定数）
  定数を推定する手順の精度が十分でないため
  実験による移行プロセスが拡散法則に従わない場合

Thank you for your attention !

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