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Migration modelling

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European Commission

Practical guidelines migration modelling

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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

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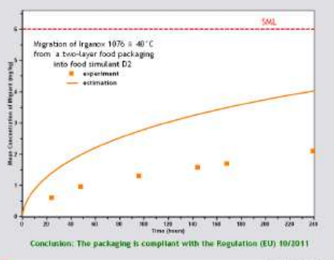
2015

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



EUR 27529 EN

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Regulation (EC) No 10/2012

Compliance test

- Verification method
- Screening method
  - Overall migration
  - Residual content
  - Migration modelling
  - Food simulant substitutes

No underestimation of modelled specific migration (section 2.2.3 of Annex V)

FCM not yet in contact

Art. 18.3

Compliant?

no

yes

OK

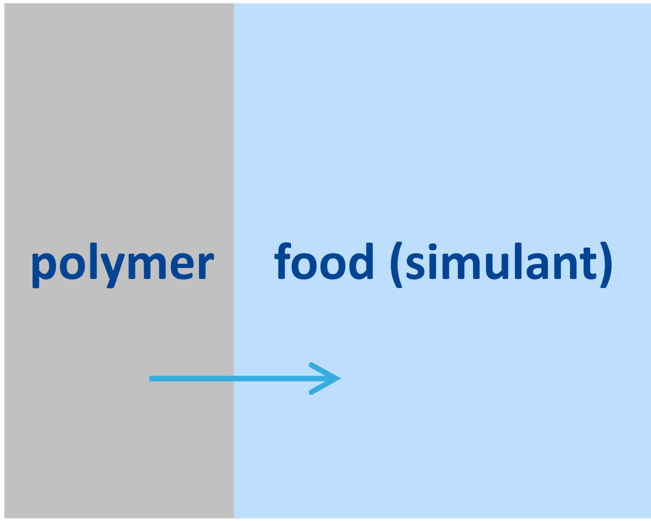
Migration

- Diffusion
- Convection
- Evaporation
- Reaction
- Partitioning

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

Diffusion is a good simplification for most food contact materials

Monolayer – one dimensional



Fick's second law of diffusion

$$\frac{\partial c_P}{\partial t} = D_P \frac{\partial^2 c_P}{\partial x^2}$$

At equilibrium (t=∞)

$$K_{P,F} = \frac{c_{P,\infty}}{c_{F,\infty}} \frac{\rho_P}{\rho_F}$$

Boundary conditions

- Constant thickness of polymer film
- Polymer film in contact with finite volume of food (similant) and contact area
- Migrant homogeneously distributed in polymer at t=0
- Neglecting mass transfer resistance at food (simulant) side
- Migrant homogeneously distributed in food (simulant) at t>0
- No interaction between polymer and food (simulant)
  - ✓ no swelling of polymer
- Diffusion coefficient of migrant in polymer is constant
  - ✓ in place and time
- No migrant in food (simulant) at t=0
- The amount of migrant in polymer + food (simulant) is constant

$$m_{F,\infty} + m_{P,\infty} = m_{P,0}$$

Mass transfer equation

- **Analytical solution**

$$\frac{m_{F,t}}{A}=c_{P,0}\rho_P d_P\left(\frac{\alpha}{1+\alpha}\right)\left[1-\sum_{n=1}^{\infty}\frac{2\alpha(1+\alpha)}{1+\alpha+\alpha^2 q_n^2}\exp\left(-q_n^2\frac{D_P}{d_P^2}t\right)\right]$$

$$\alpha=\frac{1}{K_{P,F}}\frac{V_F}{V_P}=\frac{c_{F,\infty}}{c_{P,\infty}}\frac{\rho_F}{\rho_P}\frac{V_F}{V_P}=\frac{m_{F,\infty}}{m_{P,\infty}}$$

$$\tan q_n=-\alpha\, q_n$$

- **Maximum concentration in polymer**

$$MIC=SML\frac{V_F\rho_F}{A}\left\{\rho_P d_P\left(\frac{\alpha}{1+\alpha}\right)\left[1-\sum_{n=1}^{\infty}\frac{2\alpha(1+\alpha)}{1+\alpha+\alpha^2 q_n^2}\exp\left(-q_n^2\frac{D_P}{d_P^2}t\right)\right]\right\}^{-1}$$

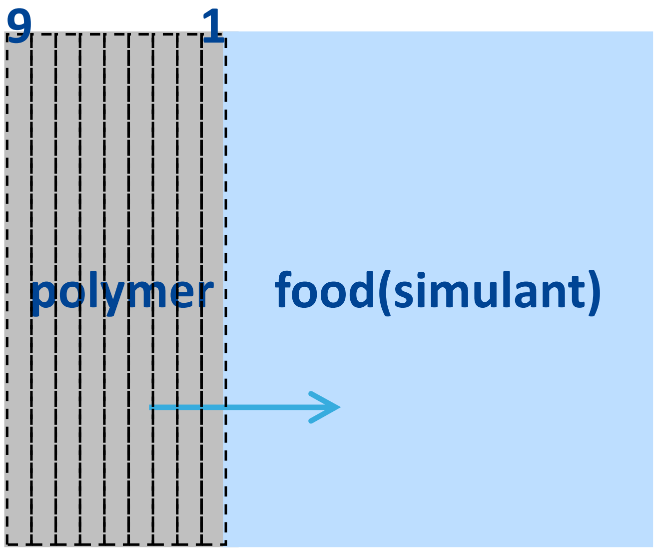
Disadvantages of analytical solution

- **Only monolayer**
- **Only mean concentrations in polymer and food (simulant)**
- **No successive contact cycles possible**
  - ✓ **Repeated use articles**

Alternative

- **Numerical solutions**
  - ✓ **e.g. finite element or finite differences algorithms**
  - ✓ **Analytical solution serves as reference for validation**

Multi-layer – one dimensional



Fick's second law of diffusion

$$\frac{\partial c_P}{\partial t} = D_P \frac{\partial^2 c_P}{\partial x^2}$$ **For each layer**

At equilibrium (t=∞)

$$K_{P_n,F} = \frac{c_{P_n,\infty}}{C_{F,\infty}} \frac{\rho_{P_n}}{\rho_F}$$

$$K_{P_{n+1},P_n} = \frac{c_{P_{n+1},\infty}}{c_{P_n,\infty}} \frac{\rho_{P_{n+1}}}{\rho_{P_n}}$$

Estimation of diffusion coefficient

Different approaches

- **Arrhenius**

$$D_P = D_0 \exp\left(\frac{-E_A}{RT}\right)$$

- **Estimation (Piringer)**

Reference activation energy

$$D_P^* = \exp\left(A_P^* - 0.1351 M_r^{2/3} + 0.003 M_r - \frac{10454R}{RT}\right)$$ **(m s⁻²)**

$$A_P^* = A_P'^* - \frac{\tau}{T}$$

Polymer specific temperature constant

Polymer specific constant

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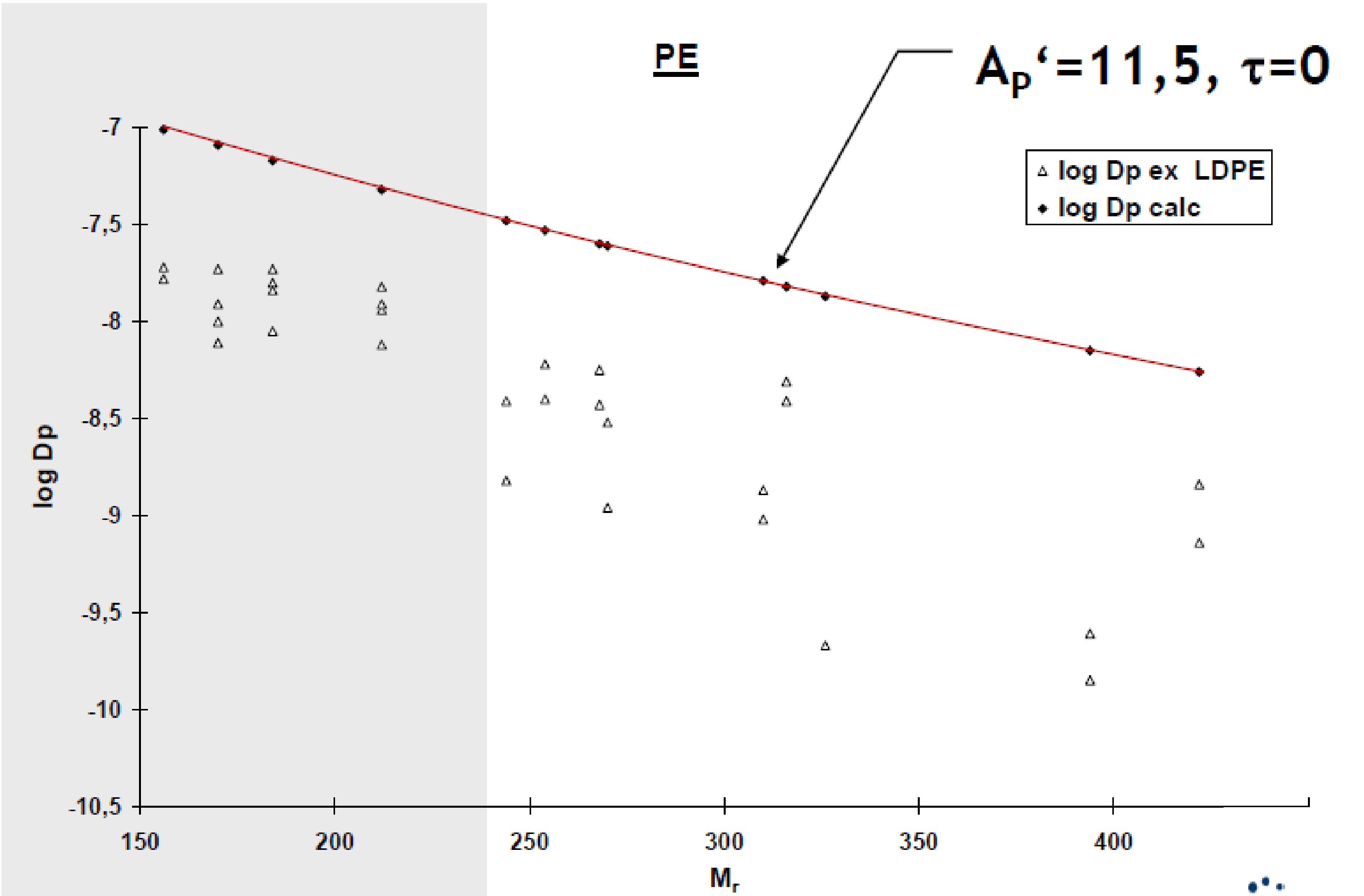
Estimation of A_P' for each T



R. Brandsch, 2010

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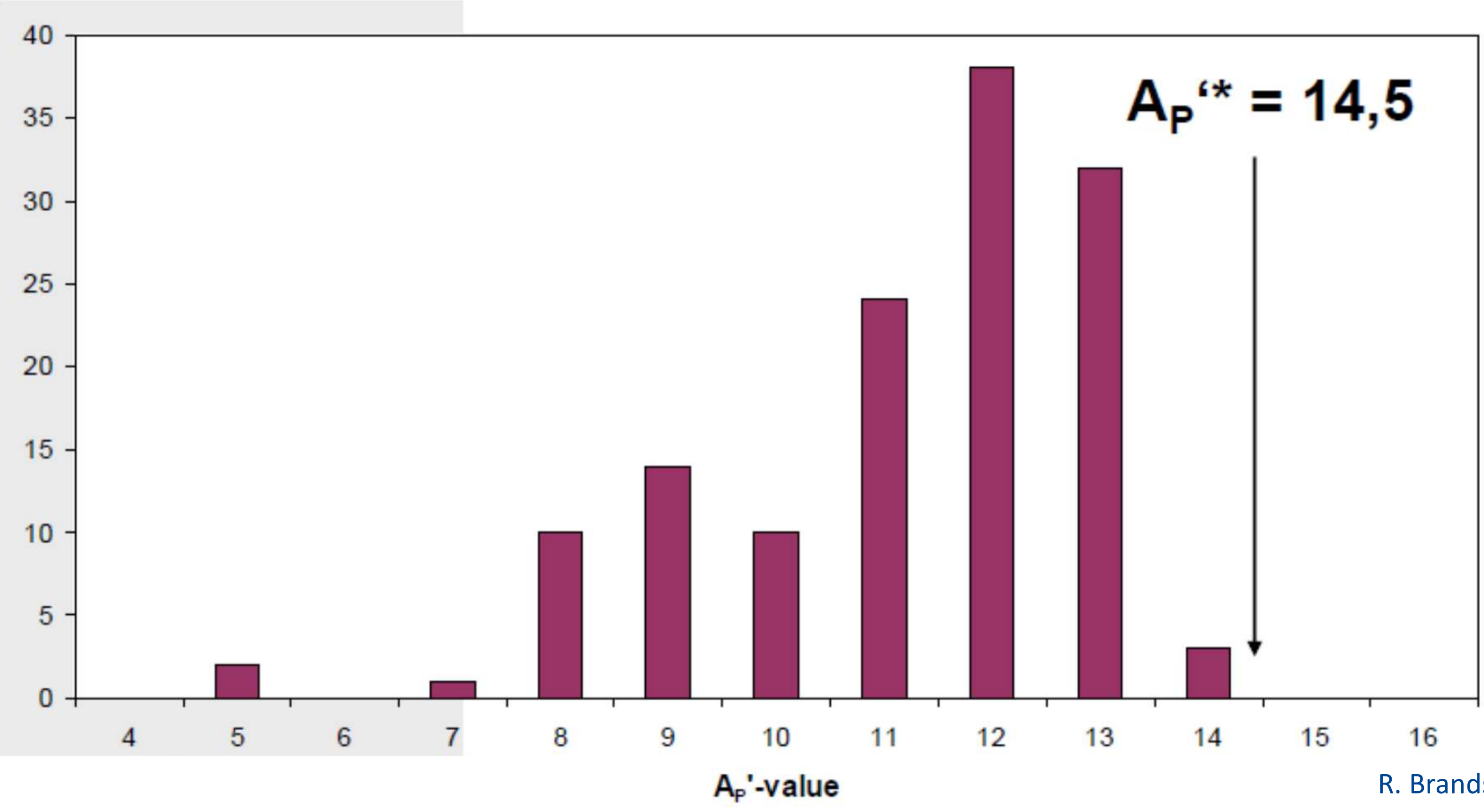
Estimation of $A_p'^*$



R. Brandsch, 2010

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Applicability for polyolefins

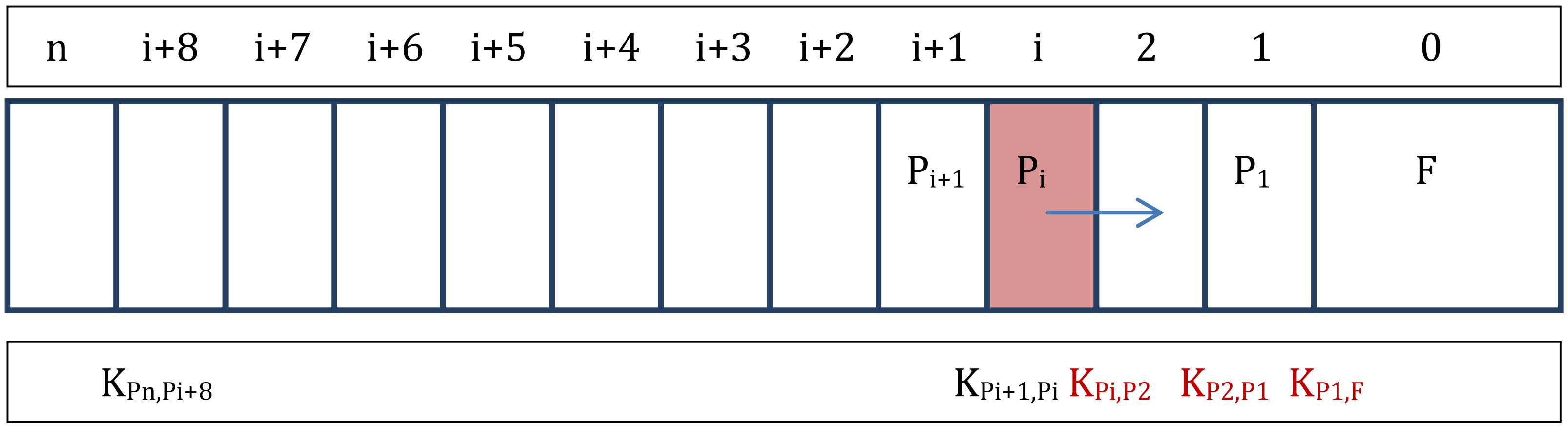
$c_{P,0} < 1\%$

$K_{P,F}$ = 1 for high solubility of migrant in food.

$K_{P,F}$ = 1000 for low solubility of migrant in food.

Polymer	T (° C)	M_r (g/mol)	A_P'*	τ (K)
LDPE	≤80	30 - 2000	11.5	0
LLDPE	≤100	30 - 2000		
HDPE	≤90	30 - 2000	14.5	1577
PP (homo)	≤120	30 - 2000	13.1	1577
PP (random)	≤120	30 - 2000		
PP (rubber)	≤100	30 - 2000	11.5	0

Multi-layer: worst case scenario



- **Forced specific migration of migrant in one layer (i) to food.**
- **K in black is 0.001**
- **K in red is 1**

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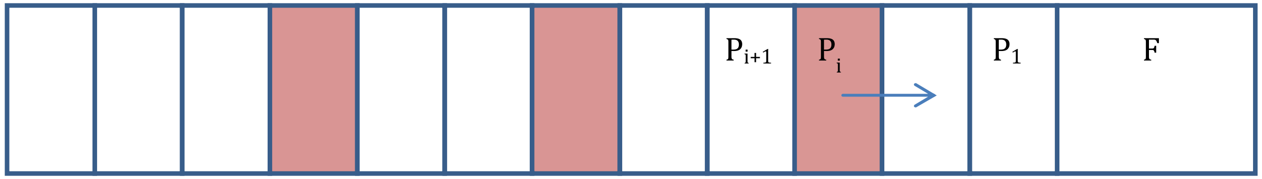
Multi-layer: worst case scenario's

Scenario 1: only migration from P_i to food

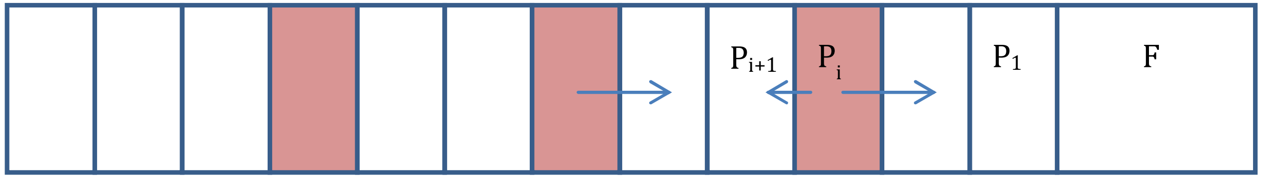
n i+8 i+7 j i+5 i+4 x i+2 i+1 i 2 1 0



$K_{Pn,Pi+8}$ $K_{Pj+1,Pj}$ $K_{Pj,Pj-1}$ $K_{Px+1,Px}$ $K_{Px,Px-1}$ $K_{Pi+1,Pi}$ $K_{Pi,P2}$ $K_{P2,P1}$ $K_{P1,F}$

Scenario 2: migration from P_x and P_i to food

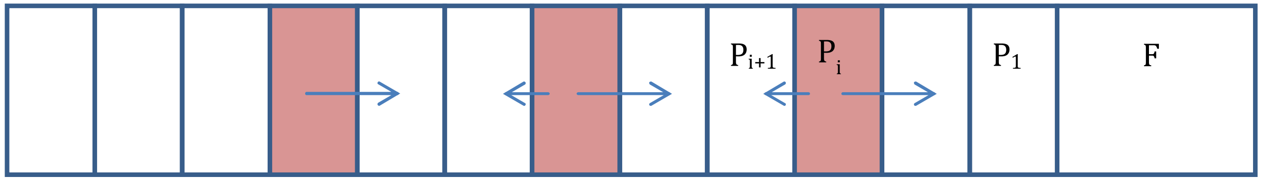
n i+8 i+7 j i+5 i+4 x i+2 i+1 i 2 1 0



$K_{Pn,Pi+8}$ $K_{Pj+1,Pj}$ $K_{Px+1,Px}$ $K_{Px,Px-1}$ ⟵ ⟶ $K_{Pi+1,Pi}$ $K_{Pi,P2}$ $K_{P2,P1}$ $K_{P1,F}$

Scenario 3: migration from P_j, P_x and P_i to food

n i+8 i+7 j i+5 i+4 x i+2 i+1 i 2 1 0



$K_{Pn,Pi+8}$ $K_{Pj+1,Pj}$ $K_{Pj,Pj-1}$ ⟵ ⟶ $K_{Px+1,Px}$ $K_{Px,Px-1}$ ⟵⟶ $K_{Pi+1,Pi}$ $K_{Pi,P2}$ $K_{P2,P1}$ $K_{P1,F}$

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Substances eligible for migration modelling

- All organic, non-gaseous substances with a well-defined molecular mass, soluble in the polymeric matrix
- All organic substances known to deliberately bloom out from some polymeric materials, e.g. antistatic or antifogging agents incorporated in polyolefines, at levels where blooming does not occur
- All specific substances in a mixture, typically derived from natural sources like fats and oils, rosins, waxes, starch, proteins, cellulose, cotton, with a well defined molecular mass below 2000 g/mol

Substances not eligible for migration modelling

- All organic substances known to deliberately bloom out from some polymeric materials, e.g. antistatic or antifogging agents incorporated in polyolefines, at levels where blooming occurs
- All organic mixtures with undefined molecular mass, typically derived from natural sources like fats and oils, rosins, waxes, starch, proteins, cellulose, cotton
- All inorganic substances, metals, metal oxides, metal salts, etc.

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Crucial information needed for migration modelling

- Polymer identity
- Potential substances that can migrate
  - e.g. additives, residual amounts of monomers
- Initial concentrations
- “worst-case” intended use
  - type of food
  - maximum temperature
  - maximum packaging time
  - Intended highest surface-to-volume ratio

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