➤ **Managing the safety of food contact materials** through preventive engineering approaches and innovation

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> Food inertia: a long history

The 1908 regulation: "...no food substance shall contain any harmful product, chemical..."

L'ART DE CONSERVER,

PENDANT PLUSIEURS ANNÉES,

TOUTES LES SUBSTANCES ANIMALES ET VÉGÉTALES;

Ouvrage soumis au Bureau consultatif des Arts et Manufactures, revêtu de son approbation, et publié sur l'invitation de S. Exc. le Ministre de l'intérieur.

PAR APPERT,

Propriétaire à Massy, Département de Seine et Oise, ancien Confiseur et Distillateur, élève de la bouche de la Maison ducal de Christian IV.

« J'ai pensé que votre découverte méritait un témoignage particulier de la bienveillance du Gouvernement ».

Lettre de S. Exc. le Ministre de l'intérieur.

A PARIS,

CHEZ PATRIS ET C^e IMPRIMEURS-LIBRAIRES, QUAI NAPOLÉON, AU COIN DE LA RUE DE LA COLOMBE, N° 4.

1810.

8^{me} ANNÉE. — N° 49

JUILLET 1910

LA CONSERVE ALIMENTAIRE

Bulletin mensuel de Vulgarisation Théorique et Pratique de Fabrication

PARAISANT LE 15 DE CHAQUE MOIS

Rédigé par un groupe de Fabricants-Industriels et de Chefs d'Emplois de cette Industrie

Nicolas APPERT
(1740-1841)

École Nationale D'INDUSTRIE ALIMENTAIRE Nicolas Appert

COMITÉ DE DIRECTION
Bourse du Commerce
— Paris —

L'idée de la création de cette école dont nous avons été les plus fervents propagandistes vient d'être mise définitivement au point par un groupe de praticiens, de chimistes et d'agronomes distingués qui vont en assurer le fonctionnement.

L'enseignement sera tout à la fois théorique et pratique.

Dans la voie pratique, le Comité de Direction se propose, non pas d'organiser une usine de fabrication de conserves et de produits alimentaires divers, destinée à concurrencer l'industrie libre, mais de créer des laboratoires d'essais et d'enseignement que dirigera un praticien qualifié et où chaque fabricant pourra venir se documenter et concourir aux progrès de la science alimentaire.

Les essais théoriques seront dirigés par un technologue éminent, M. CAULOUIS, chef de laboratoire à l'Institut Pasteur.

Une très large place sera réservée, dans l'enseignement à la question des machines, appareils et ustensiles employés par l'industrie alimentaire. Un ingénieur diplômé, M. RAYMOND MONOT, des usines de Diétrich, est chargé d'organiser cette partie du programme.

M. MORÉAL DE BRÉVANS, le distingué sous-directeur du laboratoire municipal, a bien voulu se charger de l'enseignement si important de la chimie appliquée à l'alimentation.

Enfin M. Ed. JACQUET, ingénieur-agronome, administrateur de l'école, occupera la chaire de professeur d'« Alimentation Commerciale ».

Ajoutons que notre bulletin transformé en revue bi-mensuelle à laquelle collaboreront désormais les personnalités ci-dessus, devient le Bulletin Officiel de l'École.

En un mot et suivant l'exemple d'autres pays, une Université nouvelle et bien moderne vient de naître en France, celle de l'Industrie Alimentaire. Cette industrie quitte ainsi, définitivement, le domaine empirique pour rentrer dans celui des sciences exactes, où elle avait

200

LA CONSERVE ALIMENTAIRE

sa place déjà marquée par les exigences et le progrès sans cesse grandissants de la vie contemporaine.

Pour le Comité de Direction :
Aug. CORTHAY.

Causerie Professionnelle par Nicolas APPERT

Mé lions-nous des Conserves Étrangères

Nous donnons ci-dessous la traduction d'un extrait du passage que M. Hamel consacre à la législation et l'inspection des conserves alimentaires au Canada, dans le traité qu'il publie en ce moment. (Modern practice of canning meats) :

« Comparés avec les règlements qui régissent l'inspection des conserves alimentaires aux États-Unis et en Europe, ceux du Canada sont encore à l'état embryonnaire.

Pour protéger les fabricants Canadiens contre la concurrence des États-Unis, il était nécessaire de créer une législation, au moins sur le papier.

« Je ne parle pas ici de l'inspection des viandes fraîches qui est soumise à un groupe de savants et de vétérinaires de valeur.

« Mais l'acheteur éclairé de conserves alimentaires quelles qu'elles soient, viandes, poissons, fruits ou légumes est loin d'avoir obtenu la même sécurité.

« Le règlement en date de 1908 qui régit l'inspection des conserves alimentaires nous dit :

Aucune substance alimentaire ne doit contenir de produit nuisible, produits chimiques, colorants ou antiseptiques, et plus loin on nous dit : Il sera fourni aux Inspecteurs par les soins du Ministère de l'Agriculture les noms des antiseptiques et colorants inoffensifs dont l'emploi est permis. L'addition de tout autre empêchera le produit de recevoir l'étiquette constatant l'inspection.

« Nous comprenons bien que les chimistes du Ministère sont là pour condamner tout produit alimentaire où l'analyse révélerait la présence d'un produit chimique dangereux, mais pour ceux qui sont au courant des discussions en cours entre les hygiénistes les plus distingués du monde entier au sujet de la plus ou moins grande nocivité de tel ou tel antiseptique, la satisfaction est maigre.

« Je répète que le fabricant de conserves en boîtes n'a pas besoin d'antiseptiques pour assurer la conservation indéfinie de ses produits. La stérilisation lui suffit.

« Pourquoi donc ne pas faire comprendre au monde entier que les mots « CANADA APPROVED » de l'étiquette signifient absence entière de substances nuisibles, aussi bien dans les conserves que dans les viandes fraîches.

« Que si quelques antiseptiques sont considérés comme inoffensifs par le Ministère de l'Agriculture, pourquoi ne pas faire connaître au public comme aux fabricants le nom de ce qui est permis et de ce qui est prohibé ?

« Le règlement de 1908 ne prend nullement en considération la qualité de la soudure employée, pas plus que celle de l'acide, et il semble que sur ce point les japonais sont bien en avance sur nous lorsqu'ils donnent les commandes pour leur armée.

« Pour en finir, il semble que des instructions plus complètes auraient été pour le plus grand intérêt du fabricant lui-même, en donnant au public consommateur une garantie parfaite de sécurité. La consommation en aurait été accrue en regagnant la confiance des consommateurs qui sont peu confiants dans les conserves, généralement sans raisons, d'ailleurs. »

G. T. HAMEL, ingénieur.

L'auteur faisant une œuvre purement technique et non de polémique est évidemment très modéré. Mais pour qui lit entre les lignes et pour nous qui savons combien sont rares parmi le personnel de l'inspection les gens compétents, toutes les places étant prises par les politiciens, nous ne nous sentons pas rassurés.

➤ Assessing migration and exposure to chemicals

Recent history.

<https://nepis.epa.gov/Exe/ZyPURL.cgi?Dockey=P100BCMB.TXT>

1990

Food Additives and Contaminants, January 2005; 22(1): 73–90

Taylor & Francis
Taylor & Francis Group

Evaluation of migration models that might be used in support of regulations for food-contact plastics

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2005

> Is migration modeling a trusted science?

EU REGULATION 10/2011/EC on plastics

“We have reviewed the proposed recycling process as well as the information you obtained from surrogate testing and migration modeling, which were submitted to demonstrate the capability of the proposed recycling process to remove potential contaminants from PCR-PET. Based on our review of these data, we have determined that the proposed recycling process, as described in the subject submission,”

<https://www.fda.gov/Food/IngredientsPackagingLabeling/PackagingFCS/RecycledPlastics/default.htm>

18 As migration testing is complex, costly and time consuming it should be admissible that compliance can be demonstrated also by calculations, including modelling, other analysis, and scientific evidence or reasoning if these render results which are at least as severe as the migration

Workshop "Predicting the safety of food contact articles" - New science and digital opportunities
4 October 2018, Zurich, Switzerland
<https://www.foodpackagingforum.org/events/predicting-the-safety-of-food-contact-articles-new-science-and-digital-opportunities>

CHEMICAL INNOVATIONS

FOR Plastics in a Circular Economy

➤ **Circularity**
by design
by recycling
by alternative feedstocks

EFSA has issued upward of 140 positive scientific opinions on the safety of processes to recycle plastics for use in food contact material.

ONLY recycled PET is authorized in EU.

500 M€ have been invested in plants capable of converting recycled plastic materials into materials suitable for packaging and food contact applications

In 2014, more than 50% of the recycled PET in Europe was used in food contact applications.

The lack of harmonisation amongst Member States generates legal uncertainty and unnecessary burden for the industry using recycled materials.

It also sets up obstacles for the Circular Economy

Recycling plastics for food contact

REGULATION 282/2008/EC

Polyolefins are rubber polymers which can be easily contaminated by high molecular weight contaminants after use.

Misuse issues (post-use contaminations) of Polyethylene terephthalate (**PET**) can be easily handled : glassy polymer, it is mainly contaminated by small contaminants which can be removed by a devolatilization step above T_g

Foodgrade HDPE milk bottles

1. Filling and use of HDPE milk bottles
2. Recollection
3. Sorting

Suitable for Food Contact?

Recycling

Paper and board contains large amount of residues from printing inks: aromatic (carcinogenic) and aliphatic **mineral oils** can be transferred without contact and lead to cross-contamination between materials

J. of Chromatography A. 2013;1293:107-19.

Recycling of PET vs other materials

Recycled PET for food contact is authorized (282/2008/EC)
 Recycled polyolefins are authorized only in Germany
 Recycled paper and boards is source of recurring crises in EU.

➤ What is migration modeling and how to use it?

$Fo = \frac{D_P t}{l_P^2}$ = dimensionless time; D_P : diffusion coefficient; $K_{i,F/P} = \frac{C_{i,F}^{eq}}{C_{i,P}^{eq}}$: partition coefficient

monolayer

with barrier to diffusion

multilayer

➤ Is migration modeling a trusted science?

<http://publications.jrc.ec.europa.eu/repository/handle/JRC98028>

<https://publications.europa.eu/en/publication-detail/-/publication/e0845ae1-1b60-11e7-aeb3-01aa75ed71a1>

➤ The principles of migration modeling = Tier modeling

- *conservatism*. modeling overestimates real migration.
- *reliability*. mass transfer pathways and substances obey to well-described mechanisms
- *consistency*. $D_{i,P}$ and $K_{i,F/P}$ are enough known with enough conservatism.
- *parsimony*. sophisticated and refined scenarios should be considered only when simplified ones fail.
- *proportionality*. non-compliance cannot be demonstrated by calculation.

➤ Migration pathways where modeling is applied

Preventive approaches

From preventive approaching to integrated engineering

Safety concepts

[Regulation EC 2023/2006](#) - Good Manufacturing Practice for materials and articles intended to come in contact with food

**+ Voluntary approaches
& local ordinances**

Our recommendations

➤ CHAINED STEPS: where is the critical step?

Risk of contamination by a photoinitiator in UV-curing printing ink

➤ CHAINED STEPS

UV-curing printing ink

➤ ASSESSING THE SEVERITY OF A SINGLE STEP

CASE OF "SETOFF" STEP

Full methodology described in *AIChE J.* 2013, 59(4), 1183-1212

comparison with step i alone

$$\text{Severity}(\hat{C}_F(\text{step } i)) = f\left(\max(C_{F_M}|_{1 \rightarrow 2 \rightarrow \dots \rightarrow M} - C_{F_M}|_{1 \rightarrow 2 \rightarrow \dots \rightarrow M/i}, C_{F_i}|_i)\right)$$

comparison with step i removed

➤ COMPARING THE SEVERITY OF SEVERAL STEPS, PACKAGING DESIGNS, SUBSTANCES...

Critical step (severity scale)

Unacceptable when *severity* > 100

$$severity = 100 \times \frac{C_F}{SML}$$

Concurrent design (criticality scale)

$$criticality = \sum_{all\ components} \sum_{all\ substances} \sum_{all\ modalities} pr(modality) \times severity$$

Critical substance

➤ Failure Mode Effects and Criticality Analysis

Collaborative research project SAFEFOODPACK DESIGN

FMECA « milk for infants stored in a brick »					
Phase	Formulation	Design	Process	Informations	Mechanisms
	 Formulation	 design	 Process	 Informations	 Described mechanisms
Inventaire	<ul style="list-style-type: none"> monomers (plastics, adhesives) catalysts antioxidants lubricants biocides (cardboard, ink) mineral oil (cardboard) solvents photoinitiators other residus (NIAS) 	<p>two components:</p> <ul style="list-style-type: none"> brick body (4 materials, 5 layers) cap (two materials incl. the sealing system) <p>six materials</p> <ul style="list-style-type: none"> LDPE, PP (cap) aluminum foil cardboard (origin) « ink » « adhesives » 	<ul style="list-style-type: none"> production, storage, assembly of materials assembly and storage of components printing (printing technology, curing/drying...) storage of empty packaging aseptic packaging filling (temperature, pretreatment...) storage and retailing of the bricks filled with milk conditions of use or storage by the consumer/end-user: chilled, ambient, oven heating? Consumption-type (bottle feed with direct contact between the mouth and the neck...) 	<ul style="list-style-type: none"> identity and nature of materials in assemblies formulation of materials (substances specifically regulated or not) test conditions used to evaluate the risk of contamination conditions of preparation, packaging filling, storage, consumption of packaged food communication of revisions and modifications in la formulation, design, process and in the final use 	<ul style="list-style-type: none"> diffusion across layers set-off cross-contamination between materials and with the storage ambience effects of poor drying and curing on printing inks
	<p>Highly concentrated</p> <ul style="list-style-type: none"> antioxidants, lubricants, biocides mineral oils, photoinitiators monomers, catalysts, solvents other residues 	<p>Barrier material</p> <ul style="list-style-type: none"> aluminum foil <p>Materials acting as reservoir of low molecular weight contaminants</p> <ul style="list-style-type: none"> ink adhesive <p>Materials acting as reservoir of high molecular weight of contaminants</p> <ul style="list-style-type: none"> PP, LDPE paper and board 	<p>steps associated to long-time contact</p> <ul style="list-style-type: none"> storage of materials storage of components storage of finished products <p>steps associated to high temperatures</p> <ul style="list-style-type: none"> aseptic filling oven heating <p>steps which may lead to cross-contamination</p> <ul style="list-style-type: none"> storage printing assembling / laminating 	<ul style="list-style-type: none"> non-documented or missing information accessible information documented information, which follow each component and materials verifiable and auditable information frequency of update of information : regular, when a change occur, only when the design is modified,... 	<ul style="list-style-type: none"> mass transfer, which can be evaluated rapidly from calculations: from, trough LDPE, PP layers mass transfer, which can be tested experimentally in a simple manner : set-off mass transfer, which require a depth expertise: cross-contamination, aging

Hierarchisation

Contamination without contact

*Cross-contamination=Main of NIAS and new
(old) routes of contamination*

old routes but new issues

➤ CONTAMINATION THROUGH THE GAS PHASE

TENAX packed within a 50 µm thick BOPP bag and exposed to a cardboard material formulated with 15 surrogates

SURROGATES (i)
Decane (C10)
Tetradecane (C14)
Hexadecane (C16)
Octadecane (C18)
Eicosane (C20)
Tetracosane (C24)
Octacosane (C28)
Dibutyl phthalate (DBP)
Bis(2-ethylhexyl) phthalate (DEHP)
Benzylbutyl phthalate (BBP)
Benzophenone
4-methyl benzophenone (MBP4)
Isopropyl-9H-thioxanthen-9-one
Anthracene
Naphthalene

$$\frac{m_{i,F}^{(t)}}{m_{i,P}^0} = \frac{V_F}{m_{i,P}^0} \int_0^t C_{i,F}^{(t)} d\tau$$

Experimental results
at 60°C, $i=1\dots15$

Detailed modeling
with FMECAengine

$\widehat{C}_F(T, t, i)$
 $i = 1..15$ solutes
at any
temperature

Simplified modeling
Solute independent

$\widetilde{C}_F(T, t, M)$
simplified
at any
temperature

➤ CONTAMINATION THROUGH THE GAS PHASE

TENAX packed within a 50 μm thick BOPP bag and exposed to a cardboard material formulated with 15 surrogates

> PARTITION COEFFICIENTS WITH AIR

>> **FMECAKairP acetophenone**

LOAD_CHEMSPIDER extraction of ChemSpiderID=7132 ('acetophenone') completed in 10.26 s
LOAD_CHEMISPIDER: updated cache
7132.mat 21-sept.-2015 21:37:19 77.6 kBytes C:\Data\Olivier\INRA\Codes\MS\cache.ChemSpider
CHEMSPIDER reuses cached data for 'acetophenone' (date=21-sept.-2015 21:37:19)
ans =
9.1995e-06

>> **FMECAKairP ethylbenzene**

LOAD_CHEMSPIDER extraction of ChemSpiderID=7219 ('ethylbenzene') completed in 11.9 s
LOAD_CHEMISPIDER: updated cache
7219.mat 21-sept.-2015 21:42:34 107.1 kBytes C:\Data\Olivier\INRA\Codes\MS\cache.ChemSpider
CHEMSPIDER reuses cached data for 'ethylbenzene' (date=21-sept.-2015 21:42:34)
ans =
2.2485e-04

>> **FMECAKairP 'benzoic acid'**

LOAD_CHEMSPIDER extraction of ChemSpiderID=238 ('benzoic acid') completed in 5.746 s
LOAD_CHEMISPIDER: updated cache
238.mat 21-sept.-2015 21:45:01 41.2 kBytes C:\Data\Olivier\INRA\Codes\MS\cache.ChemSpider
CHEMSPIDER reuses cached data for 'benzoic acid' (date=21-sept.-2015 21:45:01)
ans =
1.3674e-08

Cross-contamination in biotechnological applications

STEP 1
STUDY
"LOADING"

Cross-contamination in biotechnological applications

Storage before use of over-
packaging A (0 – 1 year)

Redistribution of contaminant
within the over-packaging

OUR SCOPE

Storage of over-packaging A and
bag B (t_1 : 0 – 3 years)

Cross-transfer between over-
packaging and bag

Use of bag B with a liquid F
(t_2 : 0 – 1 year)

Cross-transfer between bag and
liquid in use

STEP 2
STUDY
"MIGRATION"

Nguyen P-M, Dorey S, Vitrac O. The Ubiquitous Issue of Cross-Mass Transfer: Applications to Single-Use Systems. *Molecules*. 2019;24:3467.

Cross-contamination in biotechnological applications

a) Migrant distributions and concentration profiles

b) Concentration kinetics of migrants s_A and s_B in A and B
Step 1: storage Step 2: contact

c) Concentration kinetics of migrants s_A and s_B in F

TRANSPORT

diffusion coefficients D
and their activation E_a

Worst-case
approaches (arbitrary)

For compliance testing
(Piringer's equation)

Food Additives and Contaminants. 2005;**22**:73-90.

Group contribution
methods (fitting)

Decision tree

Journal of Applied Polymer Science. 2006;**101**:2167-86.

Theory from first
principles
(statistical physics)

European Polymer Journal. 1998;**34**:797-803.

Full atomistic
simulation
or coarse-grained
(no assumptions)

for $D \geq 10^{-14} \text{ m}^2 \cdot \text{s}^{-1}$

Journal of Chemical Physics. 2010;**132**:194902.

THERMODYNAMICS

chemical affinity
(Flory-type isotherms)

$$K_{F/P} = 1 \text{ or } 10^{-3}$$

JRC Scientific and Technical Reports EUR 27529 EN.
Ispra (Italy): European Commission; 2015.

UNIQUAC, UNIFAC, Flory—Huggins

Prausnitz, Lichtenthaler & de Azevedo. *Molecular Thermodynamics of Fluid-Phase Equilibria*: Pearson Education; 1998.

Self-association
theory

Kontogeorgis & Folas. *Thermodynamic Models for Industrial Applications: From Classical and Advanced Mixing Rules to Association Theories*: Wiley; 2009.

Industrial & Engineering Chemistry Research. 2010;**49**:7263-80.

> Diffusivities in polymers

Molecular dynamics: 0.5 ns NVT @ 298K

• 10 He

• 10 CH₄

$$D \approx \frac{1}{6} \frac{\partial}{\partial t} \left\langle \left(x_{CM}(t) - x_{CM}(0) \right)^2 \right\rangle$$

Free-volume theory

➤ Free-volume theory

$$D(\xi, T, T_g) = D_0(\xi) \exp\left(-\frac{E^*(\xi)}{RT}\right) \exp\left(-\frac{\tilde{V}_1^*(\xi)}{V_1} \frac{\alpha_{lin}(T, T_g) + \beta_{lin}}{\alpha_{lin}(T_g)}\right)$$

Solute effects (any solute) (orange box) and *FV effects (any polymer)* (green box).

$$\approx D_0(\xi) \exp\left(-\frac{E^*(\xi)}{RT}\right) \exp\left[-\frac{\tilde{V}_1^*(\xi)}{0.24(u + vT_g)} \left(2 + \frac{K_\alpha}{r(T - T_g) + K_\beta}\right)\right]$$

$$D(\text{blobs}) = 3^{-\alpha} f(\text{blob}) f(\text{blob})$$

➤ Diffusivities of homologous solutes

$$\textcircled{1} - \textcircled{2} - \dots - \textcircled{n} \quad M = n \cdot M_{\text{blob}}$$

$$\frac{D_{\text{lin}}(M, T)}{D_{\text{lin}}(M_{\text{blob}}, T)} \propto \left(\frac{M}{M_{\text{blob}}} \right)^{-\alpha_{\text{lin}}(T, T_g)}$$

➤ Universal scaling including for non-documented polymers

$$\frac{D_{lin}(M,T)}{D_{lin}(M_{blob},T)} \propto \left(\frac{M}{M_{blob}} \right)^{-\alpha_{lin}(T,T_g)}$$

$$\alpha_{lin}(T,T_g) = 1 + \frac{K_\alpha}{r(T-T_g) + K_\beta}$$

with $r = \begin{cases} 1 & \text{when } T \geq T_g \\ \frac{\alpha_g}{\alpha_c} & T < T_g \end{cases}$

$$D(\xi,T,T_g) = D_0 \exp\left(-\frac{E^*}{RT}\right) \exp\left(-\tilde{V}_1^* \frac{\alpha_{lin}(T,T_g) + 1}{0.24}\right)$$

parameter	water	toluene
D_0 (m ² ·s ⁻¹)	$2.94 \cdot 10^{-6}$	$1.87 \cdot 10^{-8}$
E^* (kJ·mol ⁻¹)	26.5 ± 2	0
$\tilde{V}_1^*$ (cm ³ ·g ⁻¹)	19.3	84.48
r when $T \leq T_g$	0.34 ± 0.03	0.7 (dry)/0.28 (swollen)

Diffusivities of water in amorphous glassy and rubber PET inferred from the scaling of n -alkanes (α_{lin}^{T,T_g}) in PET above T_g .

➤ The conventional description of migration

The level of contamination depends essentially on the fatty character of the food in contact

50 × more chemical affinity for P

50 × more chemical affinity for F

$K_{i,F/P} =$

1/50

50

$$K_{i,F/P} = \frac{C_{i,F}^{eq}}{C_{i,P}^{eq}} = \frac{1}{1 - \text{crystallinity}} \frac{\gamma_{i,P}^v}{\gamma_{i,F}^v}$$

➤ Calculating chemical potentials from an explicit representation of polymer entanglements, liquid structures

0: system state without solute

1: system state with one solute

- **Free energy perturbation:** $\exp\left(-\frac{F_1-F_0}{k_B T}\right) = \left\langle \exp\left(-\frac{U_1-U_0}{k_B T}\right) \right\rangle$
- **based on Jarsynski's equality:** $\exp\left(-\frac{F_1-F_0}{k_B T}\right) = \left\langle \exp\left(-\frac{W_{fast}}{k_B T}\right) \right\rangle$
- **Thermodynamic integration** to extended ensembles: $\frac{\partial}{\partial \lambda} F = \left\langle \frac{\partial}{\partial \lambda} U \right\rangle_\lambda$
- **Replica exchange methods** = variant of above but without reaction coordinates (Metropolis algorithm to select likely configurations)
- **Possible biases:** only thermally accessible configurations contribute to exponential averaging

$$K_{i,F/P} = \frac{C_{i,F}^{eq}}{C_{i,P}^{eq}} = \frac{1}{1 - \text{crystallinity}} \frac{\gamma_{i,P}^v}{\gamma_{i,F}^v}$$

➤ Flory theory of amorphous states at equilibrium: implicit representation of polymers

$$\frac{\mu_{i,k}^{excess}}{k_B T} = \ln \gamma_{i,k}^v = \left(1 - \frac{1}{r_k}\right) \phi_k + \chi_{i,k}^T \phi_k^2 \approx \left(1 - \frac{1}{r_k}\right) + \chi_{i,k}^T \text{ when } \phi_k \rightarrow 0$$

*lattice approximation
(incompressible)*

random coil in
absence of
volume
exclusion

same
configuration
with excluding
volumes

*off-lattice approximation
(incompressible, atomistic scale)*

$$2k_B T \chi_{i,k}^T = \langle h_{i+k} \rangle_T + \langle h_{k+i} \rangle_T - \langle h_{k+k} \rangle_T - \langle h_{i+i} \rangle_T$$

with $\langle h_{A+B} \rangle_T = \langle Z_{A+B} \epsilon_{A+B} \rangle_T \approx \langle Z_{A+B} \rangle \langle \epsilon_{A+B} \rangle_T$

Pair contact energy: $\langle \epsilon_{A+B} \rangle_T$

Number of neighbors: $\langle Z_{A+B} \rangle$

scaling: $r_k = \frac{\overline{V_k}}{\overline{V_i}}$

➤ Partition coefficients water-EVA for polar solutes

➤ Molecular modeling challenged the choice of food simulants

Ind. Eng. Chem. Res. 2010, 49(16), 7263-7280.
Food Additives and Contaminants, 2009, 26(12), 1556-1573.

	Date of case	Last change	Reference	Country
6.	08/09/2005		2005.631	ITALY

RASFF Portal

food contact materials
migration of isopropyl thioxanthone (250 $\mu\text{g/l}$) from packaging of milk for babies from Spain

➤ Tailored calculations for IAS and NIAS

Partition coefficient calculator

temperature: 40

Solute in the list:

Food Simulant:

Polymer 1: Plasticizer concentration: Plasticizer A, Plasticizer B, no plasticizer

Polymer 2: Plasticizer concentration: Plasticizer A, Plasticizer B, no plasticizer

crystallinity:

browse values estimate

Industrial & Engineering Chemistry Research 2009, 48 (11), 5285-5301.
 International Journal of Chemical Reactor Engineering 2010, 8.
 Industrial & Engineering Chemistry Research 2010, 49 (16), 7263-7280.
 Industrial & Engineering Chemistry Research 2017, 56 (3), 774-787.

Conclusions & Perspectives

PARIS SMART CITY 2050
Vincent Callebaut Architectures, 2015

➤ Future of modeling = safe-by-design + ecodesign

Think
BIG
with modeling

FV: hole-free volume theory of diffusion
(r =rigid and f =flexible solutes)

FH: Flory Huggins
approximation of chemical affinities and temperature effects
(2=binary and 3=ternary mixtures,
 b = formulation for block polymers)

Our research

Rapid prototyping

Minimized waste, migration risk, optimized shelf-life, optimized process and supply chain
Computer-aided engineering (mechanical resistance) and manufacturing (extrusion-blowing)
Additional validation (e.g., consumer acceptance)
Global environmental footprint
Safe-by-design and eco-design approaches
3D printing, augmented-reality

applications

*Feasible solutions
(Optimal or Pareto-optimal)*

Collaborations

FDA (WEAC, Boston, MA, USA)
 IRSN (Fontenay-les-Roses, France)

INRA
 SCIENCE & IMPACT

> Let's foresight modeling support public decision

$$\text{ignorance} = \frac{IT}{\text{WHAT ABOUT IT}}$$

- Online lectures
- Common modules
1. What is food packaging
 - 1.1 Panorama of food packaging
 - 1.2 Packaging materials and shaping process
 - 1.3 Basic legal framework
 2. Properties of food packaging materials
 - 2.1 Thermal, mechanical and barrier properties
 3. Packaging and food preservation
 - 3.1 Common physical chemical factors affecting food stability
 - 3.2 Food packaging and shelf life

author: undef

part 1/1	references	extra	casestudies	howto	solutions
Session 4. Mass transfer in food packaging - Unit 4.2. Migration modeling in monomaterials					

4.3 Modelling for multi-materials, multi-steps process

Migration modeling for multi-materials, multi-steps process, reusable materials - SPECIALIZED TRAINING MODULES

author: undef

part 1/1	references	extra	casestudies	howto	solutions
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- MY LECTURES AT MSU (MI,USA):
http://www.fshn.msu.edu/events/event/Vitrac_diffusion
https://mediaspace.msu.edu/media/dr.+olivier+vitrac+presentsa+diffusion+coefficients+of+organic+solute+in+polymersa/1_zz20dgt9
 PARTITIONING
https://mediaspace.msu.edu/media/Dr.+Olivier+Vitrac+presentsA+An+atomistic+Flory-Huggins+formulation+for+the+tailored+prediction+of+activity+and+partition+coefficients/1_uzi6h91k
 SAFETY MANAGEMENT:
https://mediaspace.msu.edu/media/WorkshopA+Prediction+of+the+migrationA+beyond+conventional+estimates*/1_won1m7aw