L'emballage alimentaire comme objet d'étude : de la substance à l'homme et l'environnement.

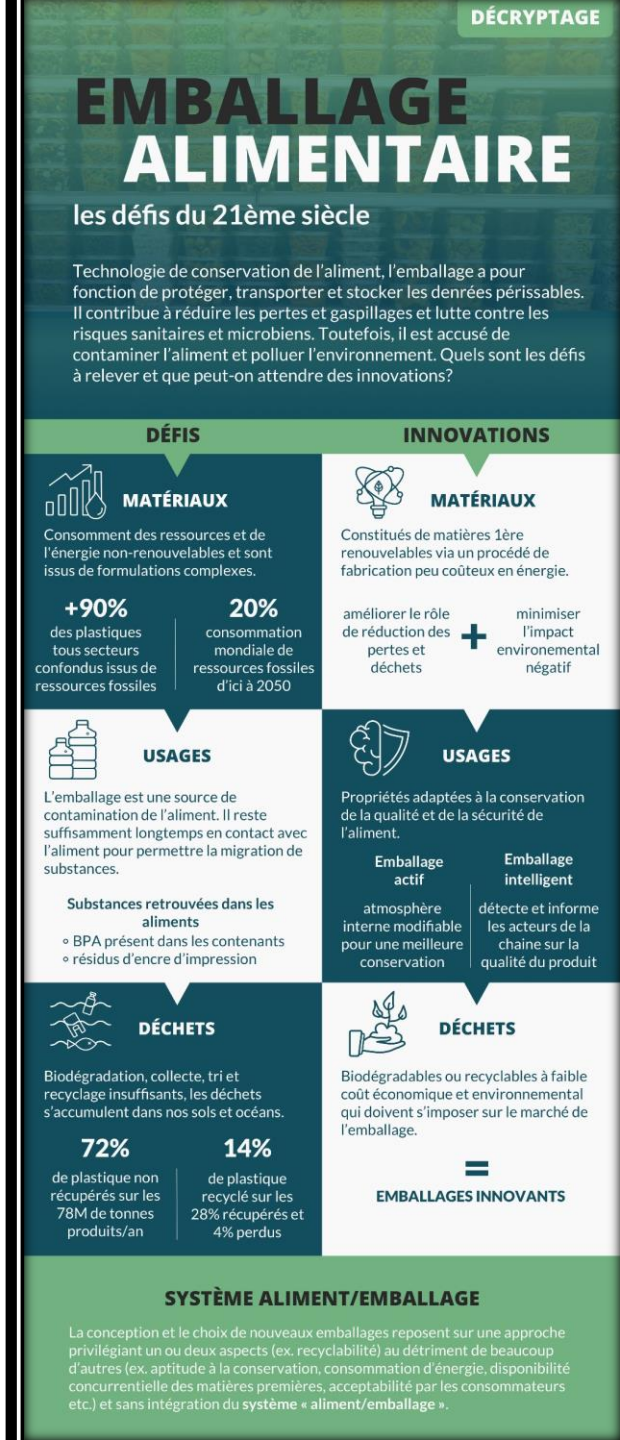
Olivier Vitrac, olivier.vitrac@agroparistech.fr

University of Paris-Saclay, INRAe, AgroParisTech

UMR 0782 SayFood "*Food Processing and Engineering of Paris-Saclay*"

UMT SafeMat "*Safe Food Contact Materials*" between AgroParisTech/INRAe and LNE

1 rue des Olympiades, 91300 Massy, France

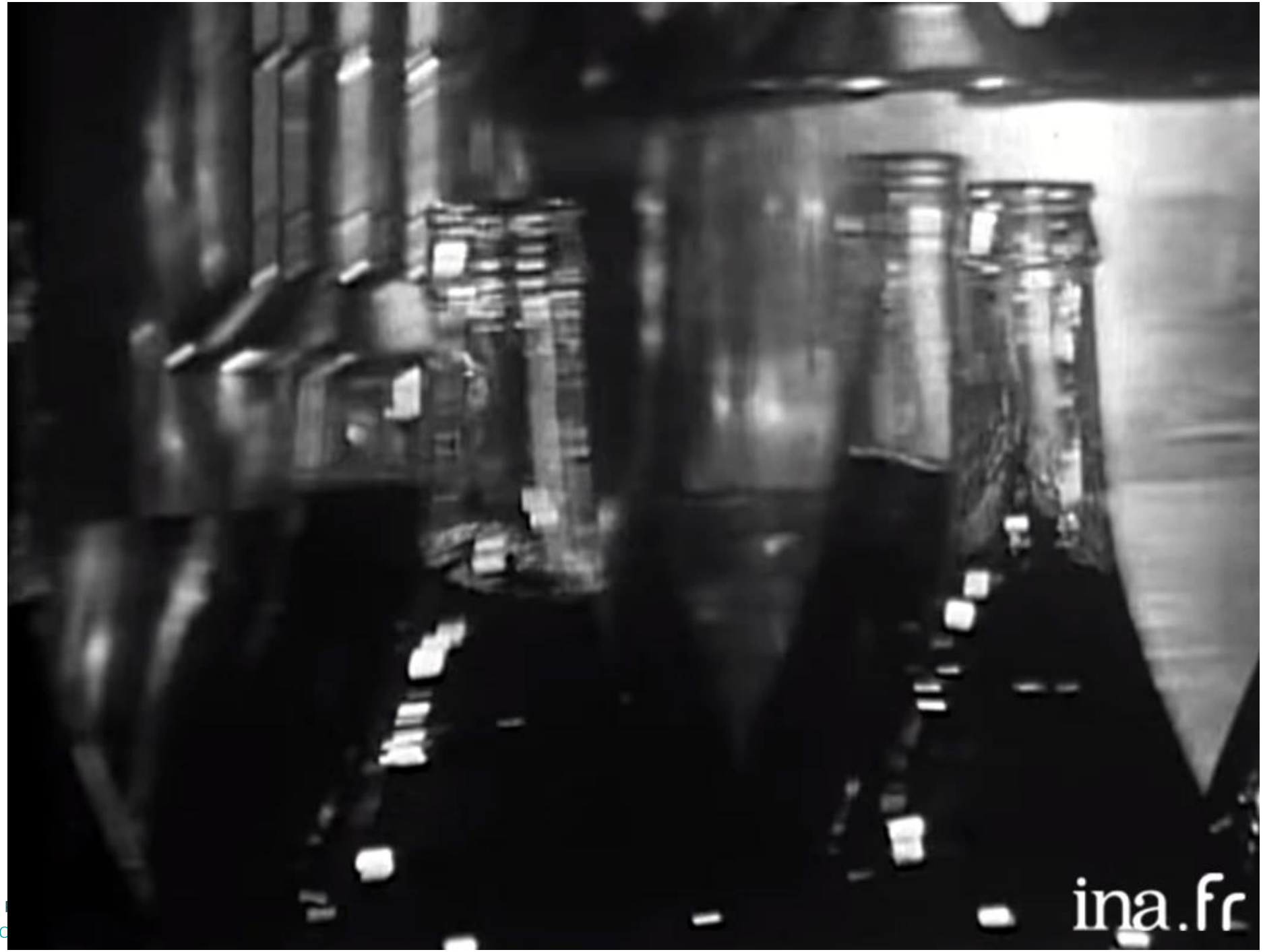


1964

La malbouffe et les additifs, progrès ou danger pour le futur ?

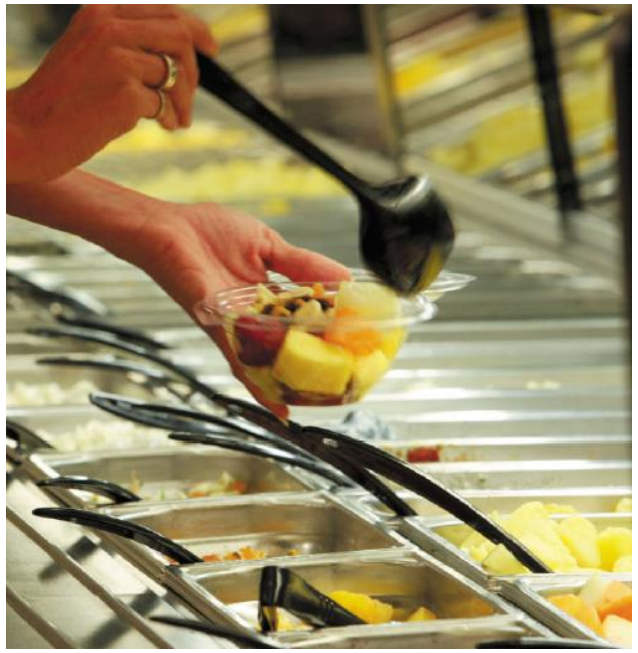
Archive INA

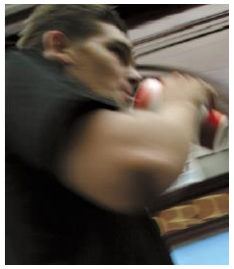
https://www.youtube.com/watch?v=aZcNza1xHSk




JUST
WATER
• Paper-based carton • Plant-based cap •
100% Spring Water
330mL


JUST
WATER
100% Spring Water
500mL
JUST
WATER
Infused
Spring Water
500mL
JUST
WATER
Infused
Spring Water
500mL





INRAE

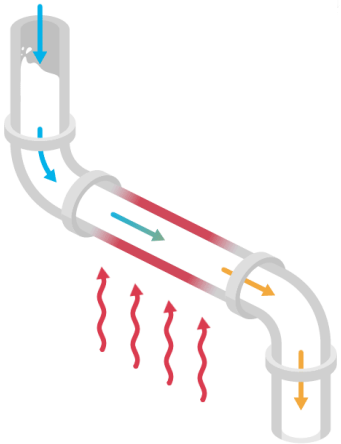
Turn into constructive controversy

"Truth in science can be defined as the working hypothesis best suited to open the way to the next better one." – Konrad Lorenz, Austria

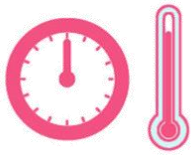
1950

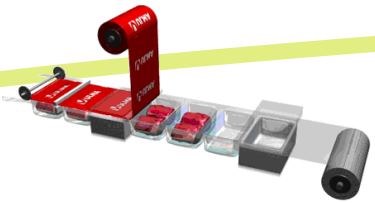
1980

1990

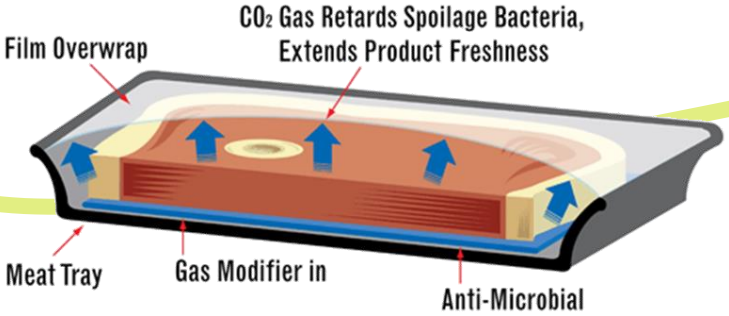


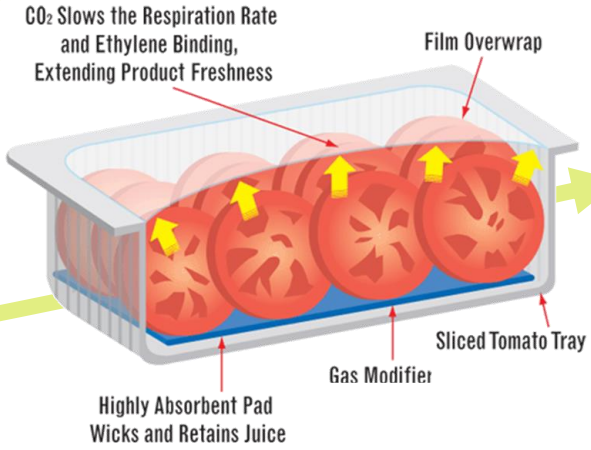
Ultra High Temperature

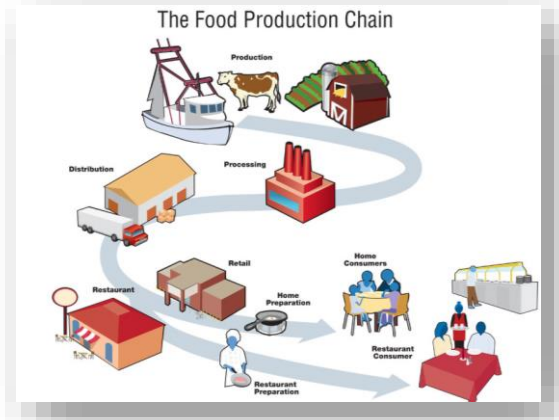




2000







L'emballage bienveillant, actif, intelligent, utile

L'emballage encombrant, inutile, dangereux

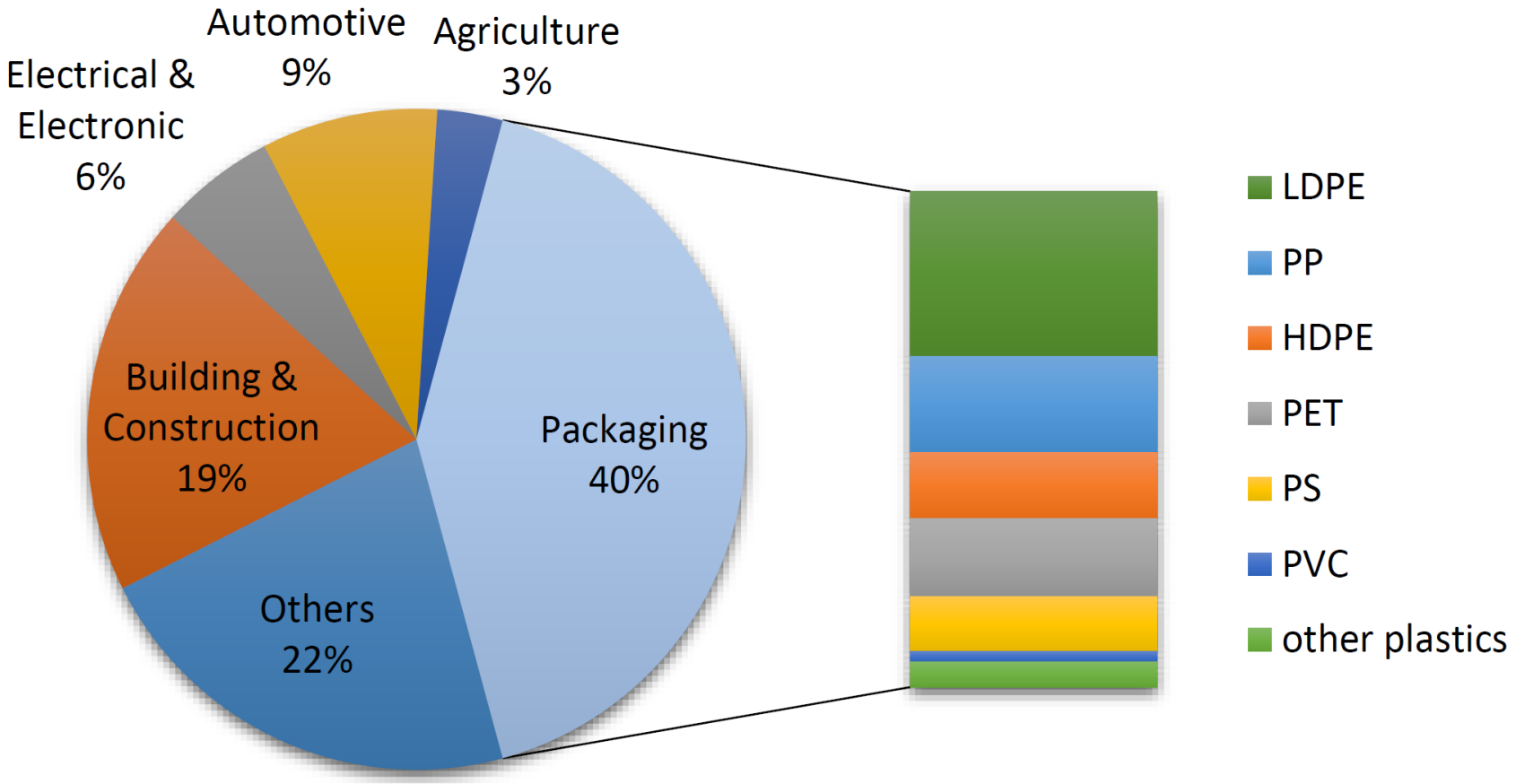
Environmental impacts

From known to unforeseen consequences

Packaging have been used for long before thinking about the consequences

Main applications of plastics

Recycling 2018, 3, 1; doi:10.3390/recycling3010001



LDPE (low-density polyethene),
PP (polypropene),
HDPE (high-density polyethene)
PET (polyethylene terephthalate),
PVC (polyvinyl chloride),
PS (polystyrene),
PA (polyamide)

Google

plastic contaminacion ecuador galapagos

Tous | Images | Actualités | Vidéos | Maps | Plus | Paramètres | Outils | Éléments enregistrés | SafeSearch

Prohiben fundas plásticas en Galápagos – Mi…
mingasporelmar.org

Basura: los números rojos de Ecuador | Pla…
planv.com.ec

Residuos de todo el planeta también llegan a G…
eluniverso.com

De dónde proviene el plástico que amenaza la vi…
es.aleteia.org

ONU-Medio Ambiente y Ecuador llaman a comb…
manabinoticias.com

Hasta Galápagos llega basura plástica de As…
elcomercio.com

Combatir la contaminación por plástico pi…
efeverde.com

Ecuador prohíbe uso de bolsas de plástico en isl…
bloglemu.blogspot.com

En 2025 habrá un kilo de plástico por cada tres d…
elcomercio.com

Hasta Galápagos llega basura plástica de Asia, E…
elcomercio.com

Los habitantes de las icónicas islas G…

La Playatón 2015 congrega a varias empresas al…

ONU Medio Ambiente y Ecuador llaman a comb…

Turismo, Ambiente y Transporte Aéreo » Blog Ar…

En Galápagos se hundió una embarcación turística…

Google microplastics

Tous | Images | Actualités | Vidéos | Maps | Plus | Paramètres | Outils | Éléments enregistrés | SafeSearch

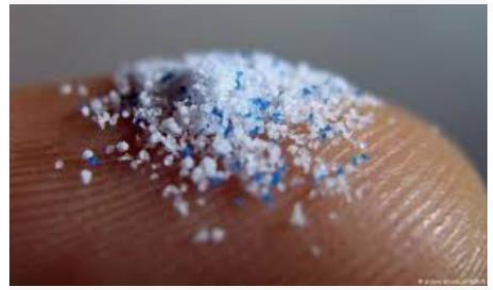
ocean microplastics | bottled water | hawaii | microplastic pollution | stealth microplastics | plastic pollution | noaa | microbeads | marine debris | particles

Are You Seasoning Your Food With Microplasti...
youtube.com

What are microplastics?
oceanservice.noaa.gov

Microplastics: Small plastics, big problem...
eco-business.com

Japan passes bill to reduce microplastics in ord...
globalcosmeticsnews.com



MICROPLASTICS IN COSMETICS: CNR ISMA...
ismac.cnr.it

Diving Deeper: Microplastics
oceanservice.noaa.gov

Microbe Mishap: Microplastic Polluti...
oceanbites.org

Microplastics make marine...
phys.org

Microplastics: A Macro Concern - Seacoast S...
seacoastsciencecenter.org

What are Microplastics? How ar...
azocleantech.com

A lot to digest: are nanoplastics bad f...
irishtimes.com

Microplastiques dans la Méditerranée

PLANÈTE · POLLUTIONS

Partage

« Le plastique est omniprésent dans les fleuves » français

La goélette scientifique Tara a sillonné neuf cours d'eau européens pour y étudier la pollution aux microplastiques. Le chercheur Jean-François Ghiglione évoque les premières conclusions de la mission.

Propos recueillis par Martine Valo · Publié le 23 novembre 2019 à 11h40 - Mis à jour le 24 novembre 2019 à 21h10

Lecture 5 min.

Article réservé aux abonnés

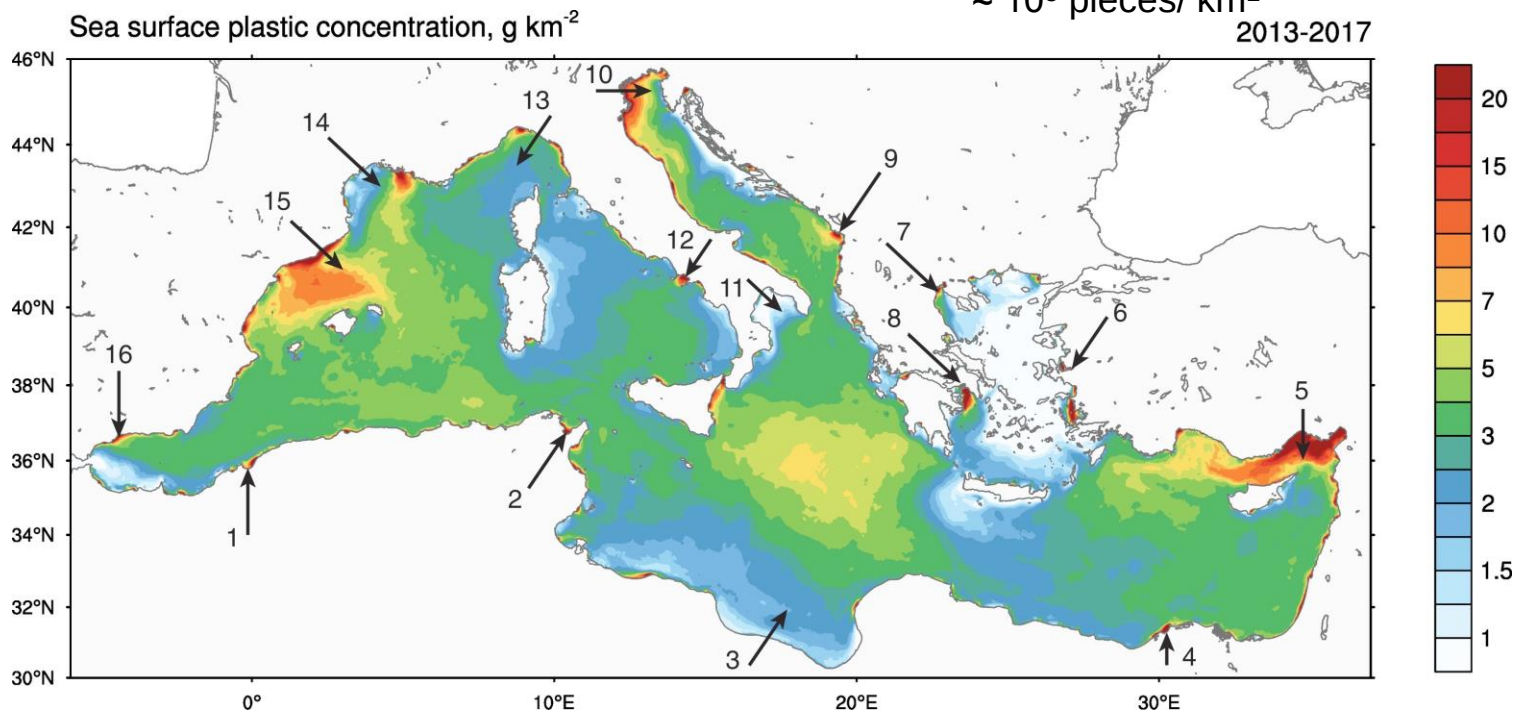
PUBLIC

MP primaire: entrant directement dans l'océan (abrasives, pré-production de granulés, fibres de circuits de lavage de textiles, ...)

MP secondaire: fabriqué in situ par dégradation mécanique, chimique, thermique, biologique

Taille (cm)	
≥ 1	Macroplastique
≥ 0,5 à 1	Mésoplastique
≤ 0,5	Microplastique
≤ 0,01	Nanoplastique

≈ 10^5 pièces/ km^2

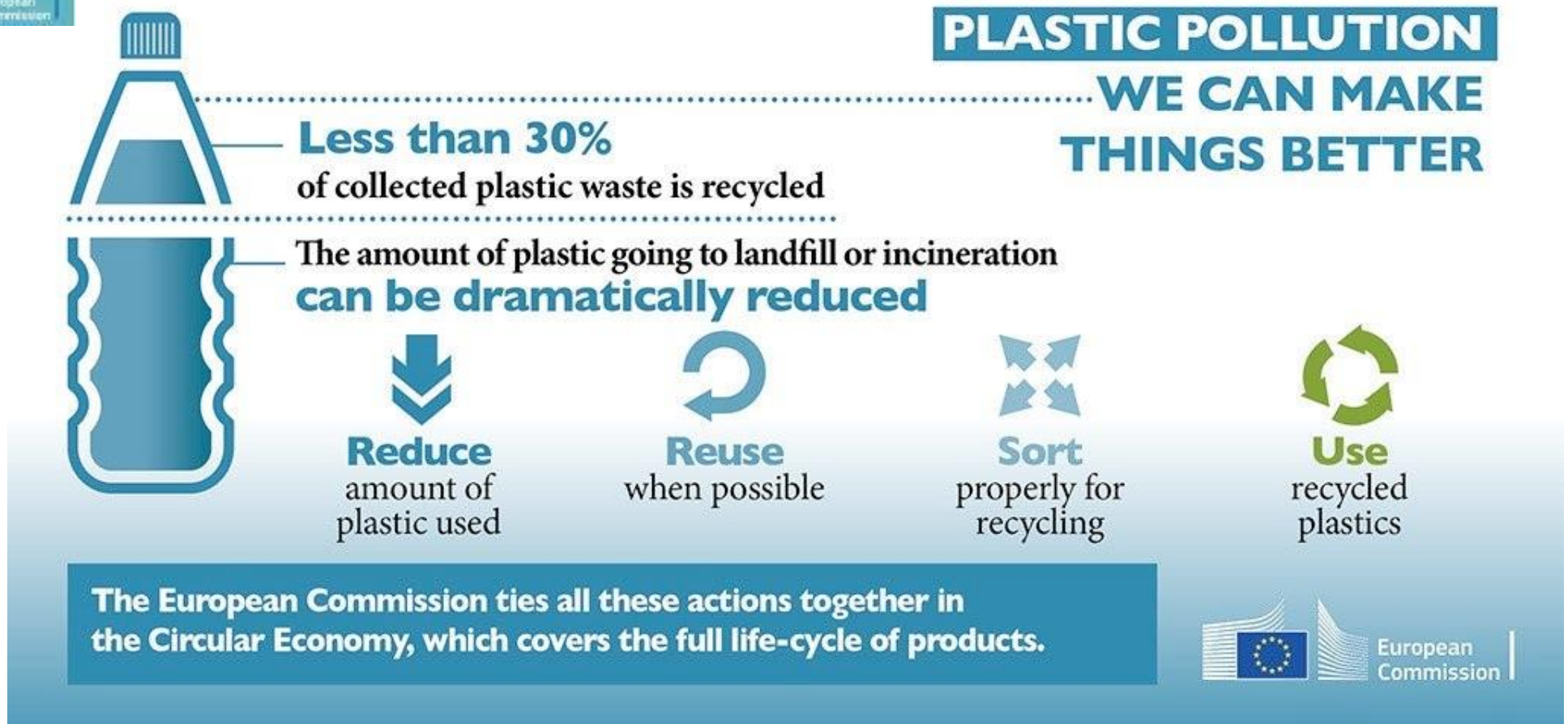


Cincinelli et al, Trends Ana Chem, 2019
Liubartseva et al, Mar Pollut Bull, 2018

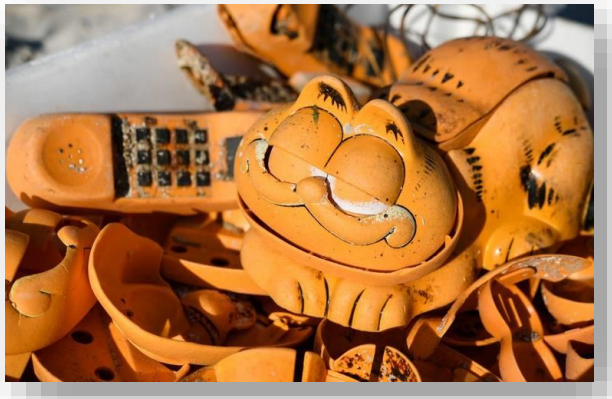
European Strategy for Circular Economy

The overall goal is to reach by 2040:

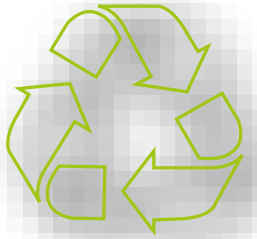
- 90 % of collection by 2029
- and 50 % plastics waste recycling.

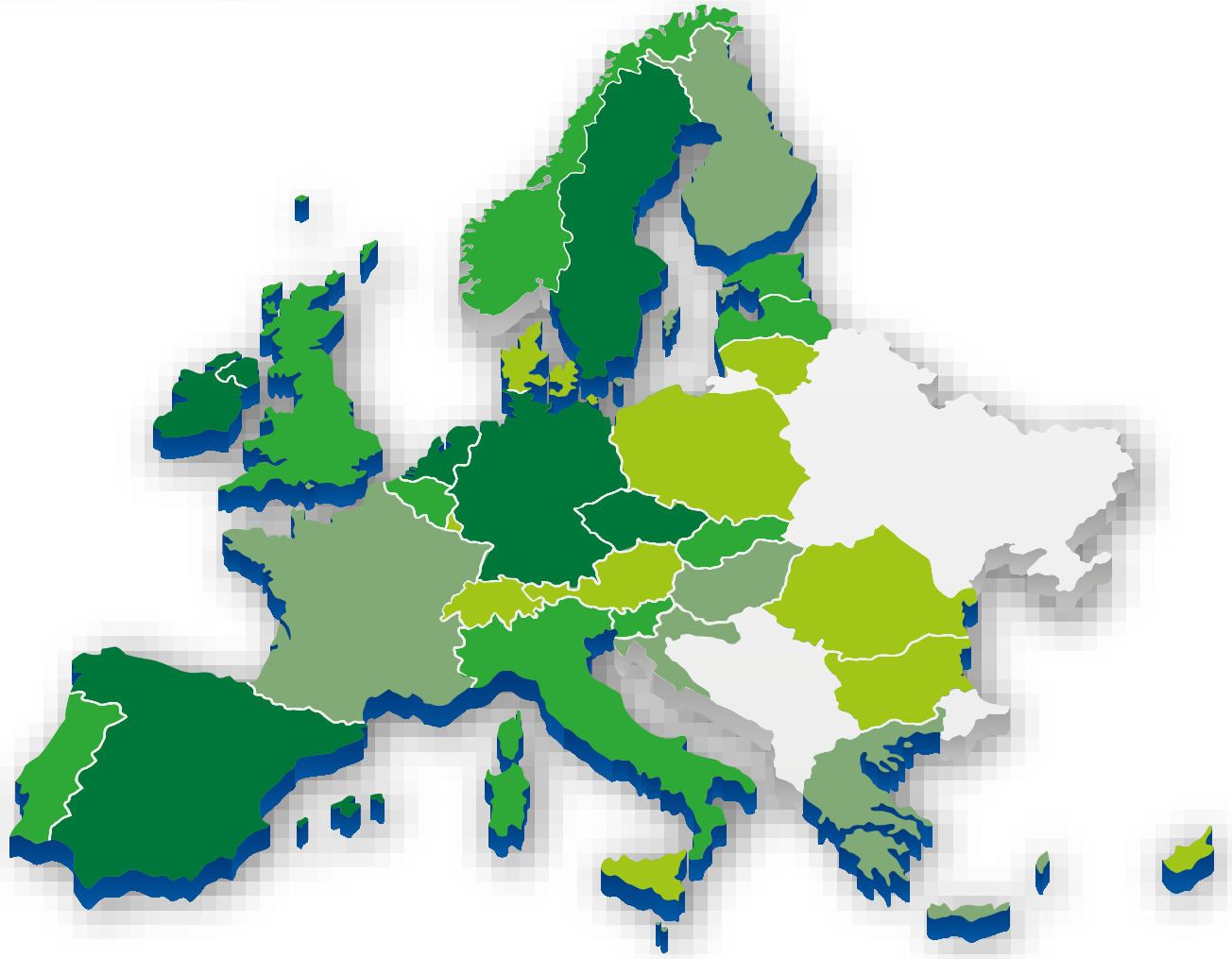


France – peut mieux faire…



Plastic **PACKAGING** recycling rates across Europe





More than	45%
From	40 to 45%
From	30 to 40%
Less than	30%

PLANÈTE · POLLUTIONS

Partage

Le gouvernement temporise sur la consigne des bouteilles plastiques

Après le rejet de la mesure au Sénat, fin septembre, l'exécutif a choisi de privilégier des « expérimentations » pour une mise en place à l'horizon 2023.

Le Monde avec AFP · Publié aujourd'hui à 08h36

Lecture 1 min.

PUBLICITÉ

A world without plastics?

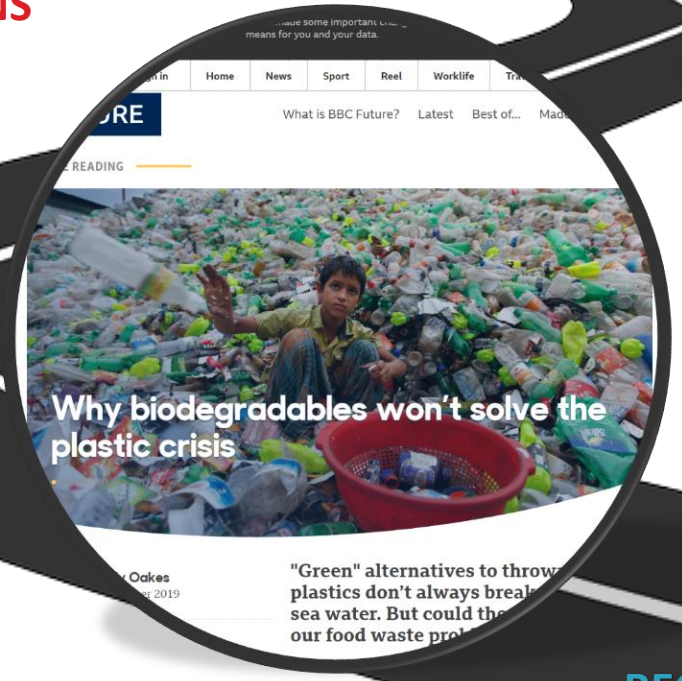
REUSED, EDIBLE PLASTICS
(new supply food supply chains)

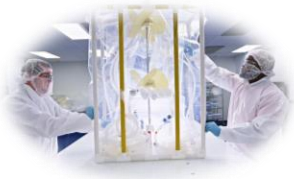
NO PLASTICS
(new organizations)

FULL COLLECT
(new usages)

ENFORCED REGULATIONS
China, EU, US

5 China Market Entry Tips... After 7 Years Analyzing Trade Policy, Legislation and Regulations

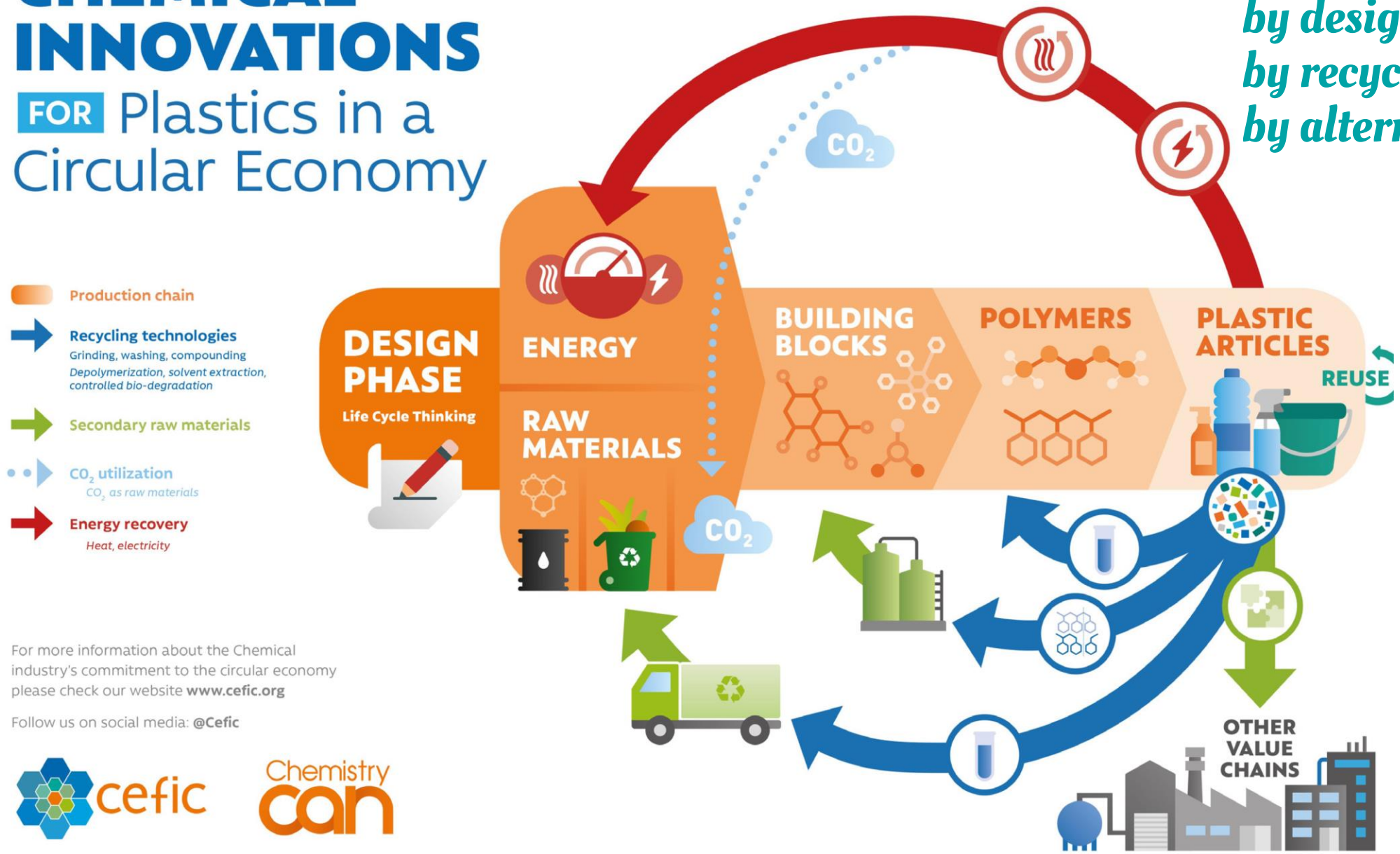




RECYCLED PLASTICS
+Food-contact

CHEMICAL INNOVATIONS FOR Plastics in a Circular Economy

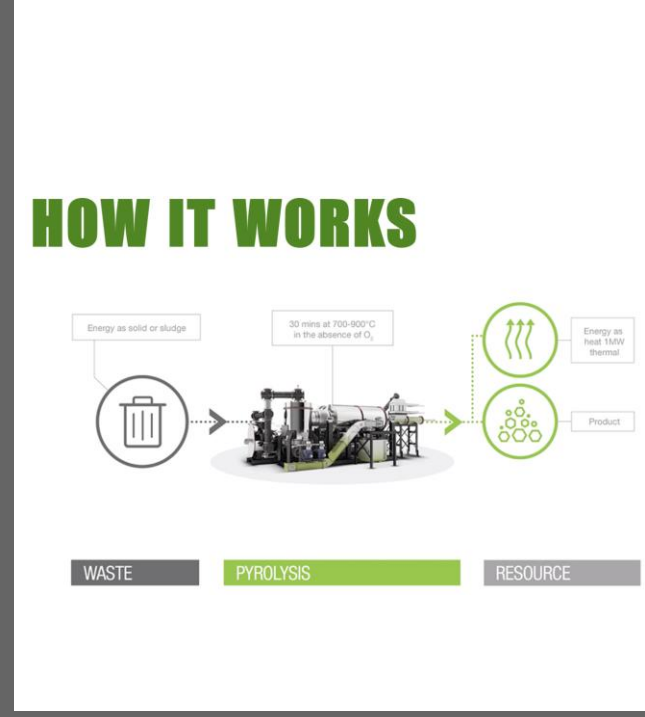
Circularity
by design
by recycling
by alternative feedstocks

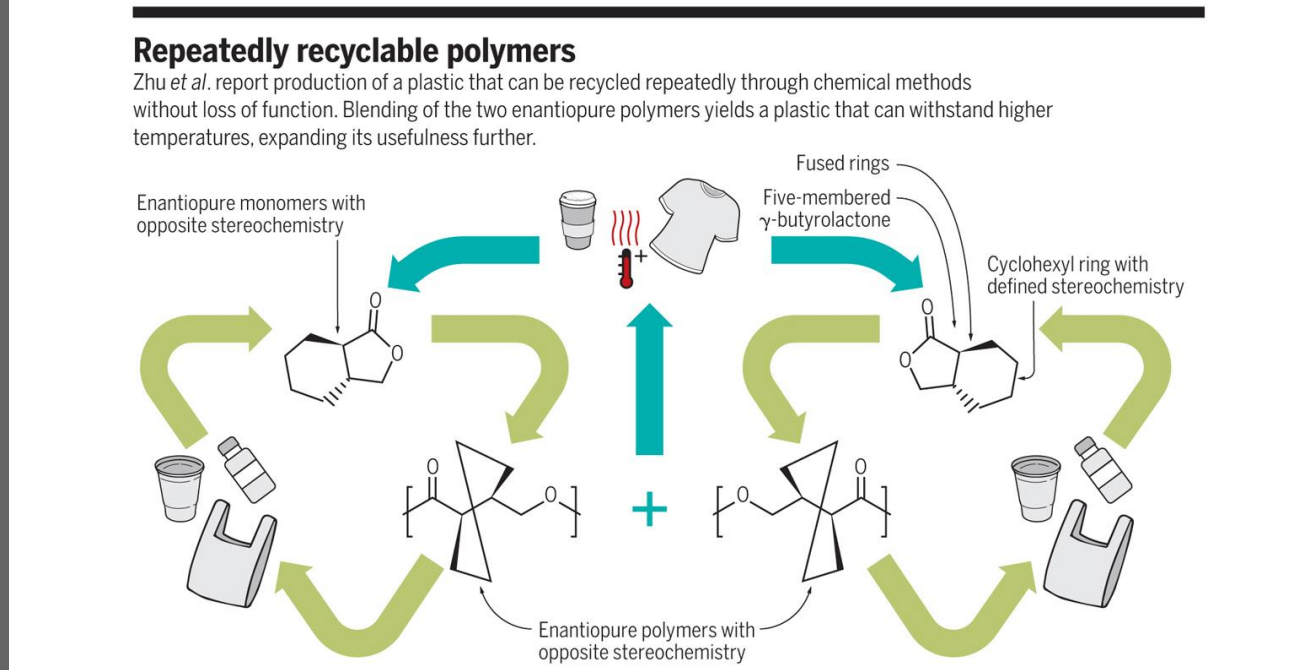


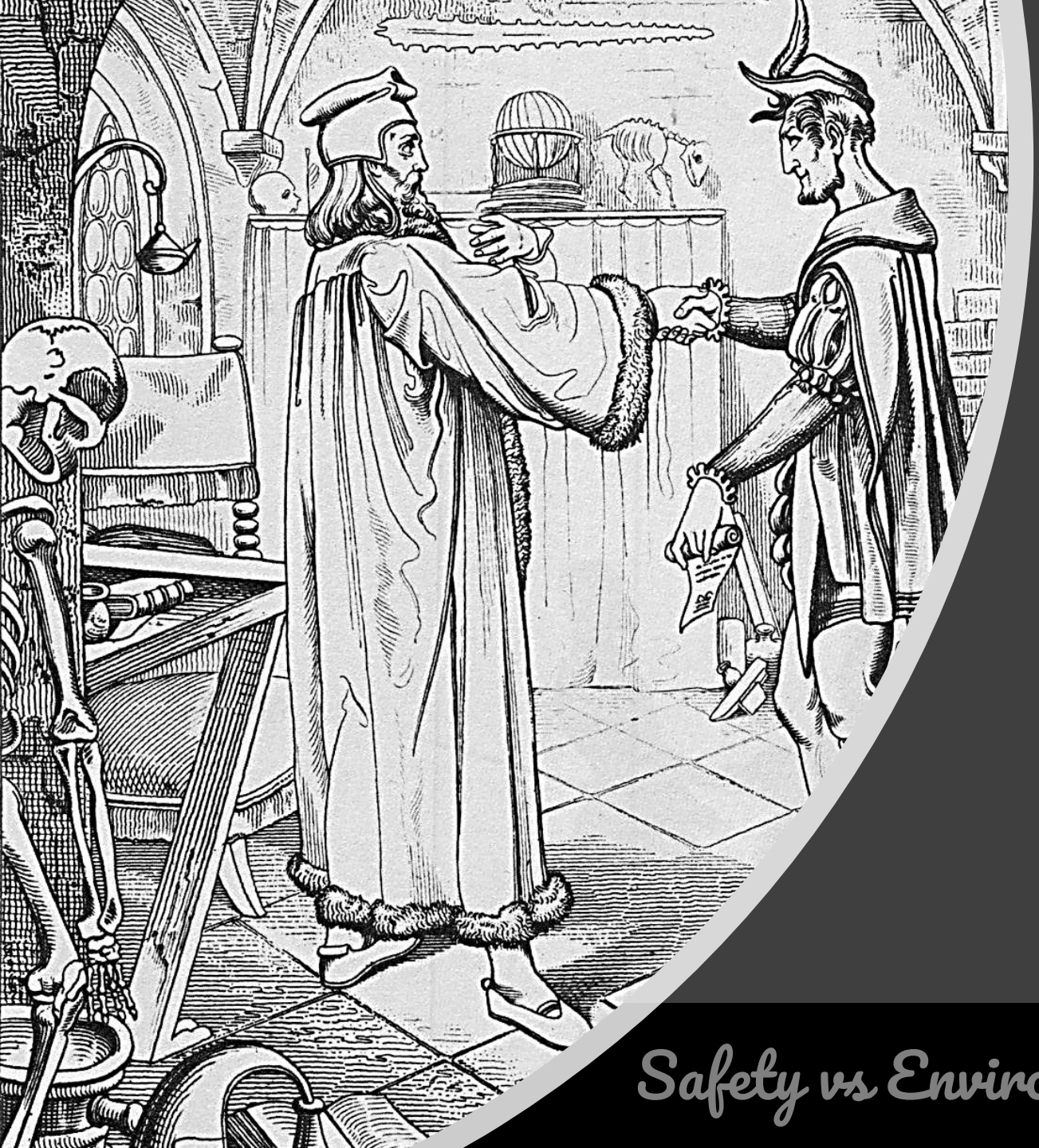
Source: Cefic

Current researches

- MATERIAL DESIGN
  - Longer lifetime
  - Decrease material usage
  - Improve sorting, separation, recyclability
  - Trigger biodegradability
- ARTICLE DESIGN
  - Design for dismantling
  - Decrease material usage
  - Digital design for reuse
  - Digital development of biobased
- RECYCLING
  - Mechanical
  - Chemical
  - Thermal and thermomechanical
  - Multimaterial, multilayer
- FEEDSTOCKS
  - Plastic waste based
  - Food waste based
  - CO/CO_2 based







« Ce grand homme à mon avis mérite d'être préféré à tous les autres… il a établi une doctrine fondée sur des raisons physiques et palpables sans se servir des énigmes inintelligibles qui font tourner la tête plutôt que d'instruire »

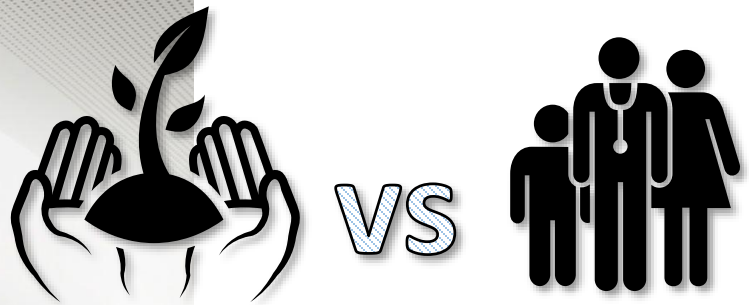
François-Marie-Pompée Colonna – Abrégé de la doctrine de Paracelse et de ses Archidoxes - Paris, 1724.

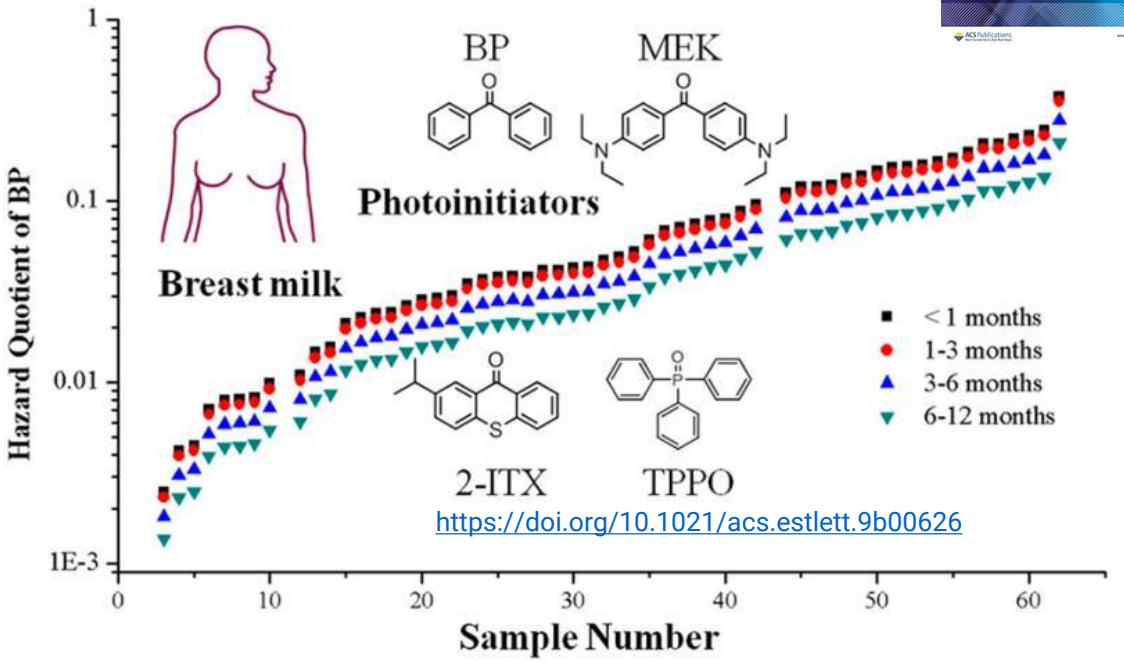
Chemicals risks and possible human impacts

Hazard Analysis

Risk Assessment, Risk Management

Safety vs Environnent: the impossible deal





https://doi.org/10.1021/acs.estlett.9b00626

Hazard Analysis *vs* Risk assessment

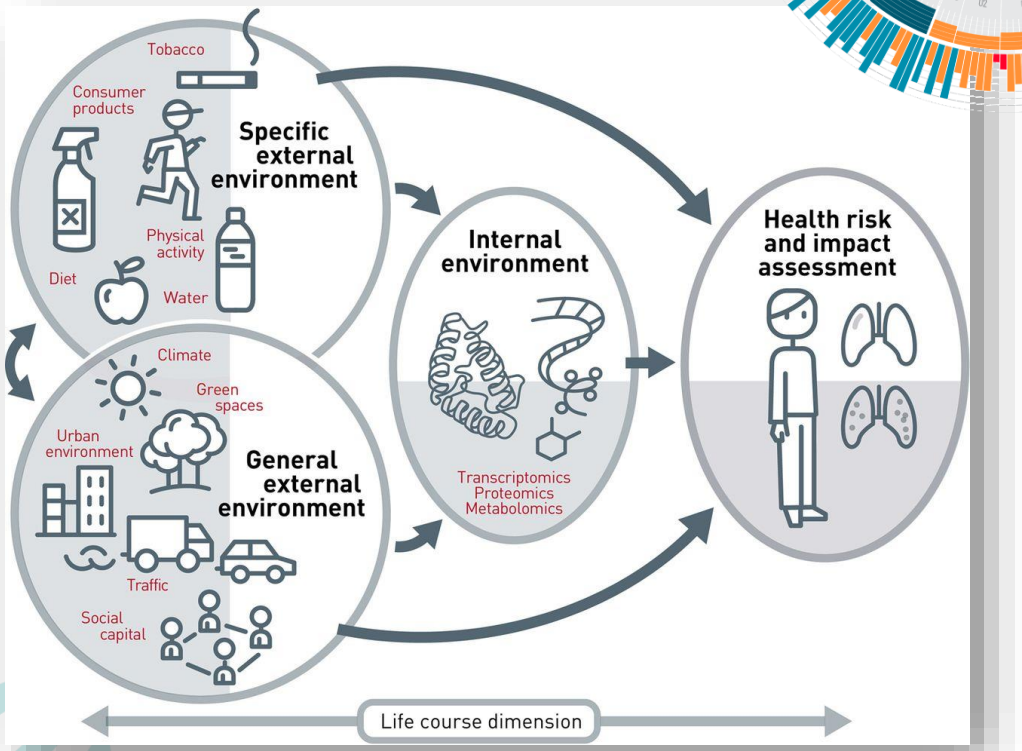
Hazard = health

Risk = occurrence

The cascade of risk assessment and management

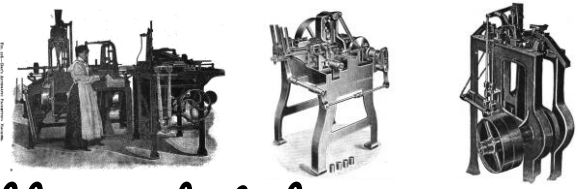
Chronic exposure

Human exposome



			Risk Tradeoff
		Risk balancing	Conflicts *cognitive, evaluative, normative*
	Scientific risk assessment	Conflict: *evaluative*	
Routine	Conflict: *cognitive*	Targets: BfR, anses, ISTITUTO SUPERIORE DI SANITÀ, FOOD STANDARDS AGENCY, efsa European Food Safety Authority	Targets:DG SANCO, industry stakeholders 
Target: *industry*	Target: *professional associations*		
Discourse: *internal*	Discourse: *cognitive*	Discourse: *reflective*	Discourse: *participatory*
Outcome: simple	***Outcome: complex***	***Outcome: uncertain***	***Outcome: ambiguous***

Food inertia: a long history



Le règlement de 1908: « ...aucune substance alimentaire ne doit contenir de produit nuisible, produit chimiques... »

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 ducale 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 Cie Imprimeurs-Libraires, quai Napoléon, au coin de la rue de la Colombe, n° 4.

1810.

8me Année. — N° 19 — Juillet 1910

LA CONSERVE ALIMENTAIRE

Bulletin mensuel de Vulgarisation Théorique et Pratique de Fabrication

PARAISSANT LE 15 DE CHAQUE MOIS

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

Nicolas APPERT
(1750-1841)

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. Crolbois, 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'Ecole.

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

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

Méfions-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 Etats-Unis et en Europe, ceux du Canada sont encore à l'état embryonnaire.

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

« Je ne parle pas ici de l'inspection des viandes fraiches 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 susbstances nuisibles, aussi bien dans les conserves que dans les viandes fraiches.

« Que si quelques antiseptiques sont considérés comme inoffensifs par le Ministère de l'Agriculture, pourquoi ne pas faire connaitre 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. »

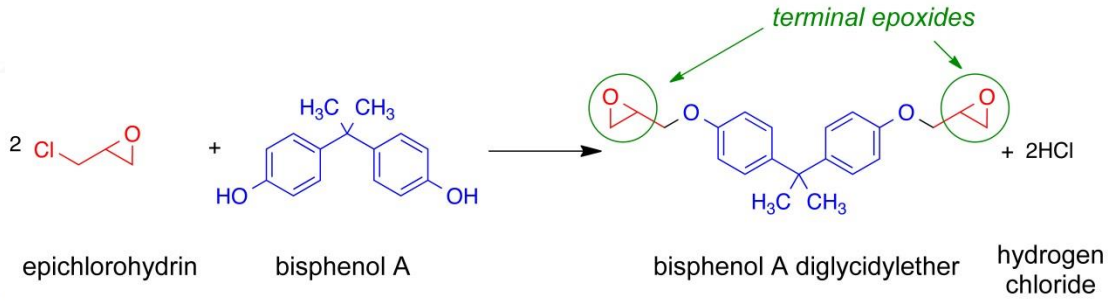
G. T. Hamel, ingénieur.

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 rassu-

Google Trends / Bisphenol A: (Worldwide)

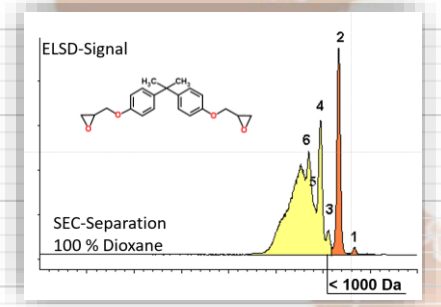
#	M +1	Substances (originated from the resin)
1	359	BADGE·H_2O
2	341	BADGE
3	643	BADGE(n=1)·H_2O
4	569	Cyclo-DiBADGE
5	625	BADGE(n=1)
6	927	BADGE(n=2)·H_2O
7	491	BADGE·tBuPh*
8	909	BADGE(n=2)
9	775	BADGE(n=1)·tBuPh
10	641	BADGE·2tBuPh
11	477	BADGE·H2O·BuEtOH**
12	403	BADGE·EG*** (+)
13	459	BADGE·BuEtOH
14	509	BADGE·H2O·tBuPh
15	577	BADGE·2BuEtOH
16	687	BADGE(n=1)·EG (+)
18	743	BADGE(n=1)·BuEtOH
19	609	BADGE·BuEtOH·tBuPh
20	971	BADGE(n=2)·EG (+)

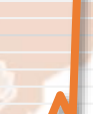
* tBuPh tert.-Butylphenol (chain stopper)
** BuEtOH Butoxyethanol
*** EG Ethyleneglycol
(+) Further confirmations are necessary

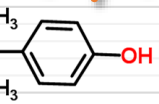


CANCO: Ensuring the safety of consumers: can **coatings** for direct food contact. Project QLAM-2001-00066.

Current Biology 2003, 13, 546







LOI no 2012-1442 du 24 décembre 2012

Current Biology 2018, 28,1

REGULATION 2018/213/EC

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Bisphenol A Exposure Causes Meiotic Aneuploidy in the Female Mouse

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Summary

Background: There is increasing concern that exposure to man-made substances that mimic endogenous hormones may adversely affect mammalian reproduction. Although a variety of reproductive complications have been ascribed to compounds with androgenic or estrogenic properties, little attention has been directed at the potential consequences of such exposures to the genetic quality of the gamete.
Results: A sudden, spontaneous increase in meiotic disturbances, including aneuploidy, in studies of oocytes from control female mice in our laboratory coincided with the accidental exposu… environmental source of bisphe… estrogenic compound widely us… polycarbonate plastics and epo… damaged caging material as the … as we were able to recapitulate … ties by intentionally damaging c… In subsequent studies of female … daily oral doses of BPA to direc… that low levels of BPA disrupt female meiosis. Our results demonstrated that the meiotic effects were dose dependent and could be induced by environmentally relevant doses of BPA.
Conclusions: Both the initial inadvertent exposure and subsequent experimental studies suggest that BPA is a potent meiotic aneugen. Specifically, in the female mouse, short-term, low-dose exposure during the final stages of oocyte growth is sufficient to elicit detectable meiotic effects. These results provide the first unequivocal link between mammalian meiotic aneuploidy and an accidental environmental exposure and suggest that the oocyte and its meiotic spindle will provide a sensitive assay system for the study of reproductive toxins.

Introduction

An estimated 10%–25% of fertilized human oocytes are aneuploid; thus, numerical chromosome abnormalities are the leading cause of miscarriage, congenital defects, and mental retardation [1]. Because almost all such aneuploidy derives from meiotic errors, considerable effort has been directed at identifying factors that increase meiotic nondisjunction. A number of potential risk factors, including irradiation (e.g., [2, 3]), smoking or drinking (e.g., [4, 5]), oral contraceptives and fertility drugs (e.g., [4, 6]), and environmental pollutants/pesticides (e.g., [7]), have been suggested. However, significant effects have been small and difficult to verify or disputed, making positive associations hard to establish. In part, this may reflect difficulties in detection. For example, the extraordinary effect of maternal age on aneuploidy may obscure less obvious associations. Further, previous studies may have focused on the "wrong" population; that is, most utilized liveborns, although virtually all aneuploidy terminates in miscarriage. Thus, the contribution of environmental insults to meiotic chromosome errors remains unknown.

We recently experienced an inadvertent environmental exposure in our mouse colony to 2,2-(4,4-dihydroxydiphenol)propane, or bisphenol A. Bisphenol A (BPA) is the monomer that is polymerized to manufacture polycarbonate plastic products and resins, such as those used to line cans containing food and beverages and those found in dental sealents. The exposure was accompanied by highly significant increases in meiotic …abnormalities, including nondisjunction; …l A was implicated as a potent disruptor …e ability to experimentally recreate the …allowed us to verify our initial observations …lose-response studies.

A Sudden Increase in Meiotic Abnormalities Is Correlated with Damage to Caging Materials

We recently reported meiotic studies of mouse mutants with defects in the alignment of the chromosomes on the first meiotic (MI) spindle [8]. This meiotic abnormality, which we have termed congression failure (Figure 1), is of particular relevance to humans because it is an age-related feature of human oocytes and has been postulated to be causally related to the well-known increase in aneuploidy associated with advancing maternal age [9].

In the course of meiotic studies of mouse oocytes conducted in 1998, we observed a sudden and dramatic change in congression failure levels. The first wave of follicles that initiate growth in the sexually immature ovary provides access to a large cohort of oocytes, and, typically, only 1%–2% of oocytes from control females exhibit congression failure at metaphase I [8]. However, in experiments conducted in August 1998, congression failure levels suddenly spiked, and approximately 40% of control oocytes exhibited this phenotype or more severe aberrations (Figures 1 and 2).

At the same time that these studies were being conducted, we were also using the animal facility to house

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2003

Current Biology
Report

CellPress

Replacement Bisphenols Adversely Affect Mouse Gametogenesis with Consequences for Subsequent Generations

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https://doi.org/10.1016/j.cub.2018.06.070

SUMMARY

20 years ago, accidental bisphenol A (BPA) exposure caused a sudden increase in chromosomally abnormal eggs from our control mice [1]. Subsequent rodent studies demonstrated developmental effects of exposure with repercussions on adult health and fertility (e.g., [2–9]; reviewed in [10–17]). Studies in monkeys, humans, fish, and worms suggest BPA effects extend across species (e.g., [18–30]; reviewed in [31–33]). Widespread use has resulted in ubiquitous enviro… and human BPA exposure. …sulted in "BPA-free" produc… turally similar bisphenols t… environmental and huma… [34–41]). We report here stu… changes mirroring our pre… and implicating exposure t… replacement) from damaged polysulfone cages. Like with BPA [1, 2, 5], our data show that exposure

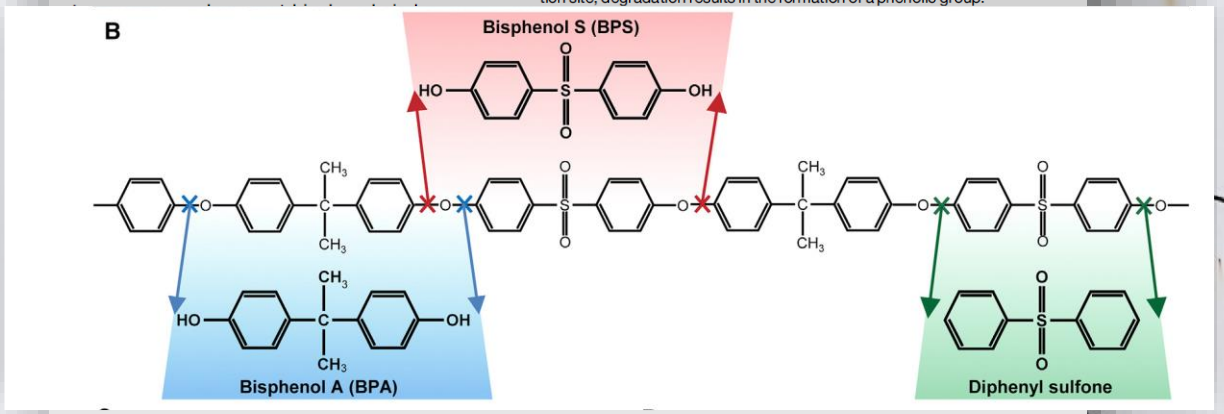
2018

Results and Discussion

In the course of meiotic studies in male and female mice, we observed variation in meiotic recombination (measured by the number of MLH1 foci in pachytene stage meiocytes), with levels in some controls reaching values characteristic of BPA-exposed animals [2, 5]. Although the change in pooled data was subtle, variation among litters was striking (Figure 1). Given our previous experience with BPA leaching from polycarbonate cages and water bottles [1], damaged materials were an obvious suspect. When white residue was evident on the surface of some polysulfone cages in our facility (Figure 2A), we suspected that exposure to chemicals leaching from the damaged polymer was eliciting …ts.

…ted Contaminant

…is comprised of BPA and diphenyl sulfone (Fig… , we suspected that these were the contaminants …iquid chromatography-tandem mass spectrometry …analysis of a methanol extraction of damaged ca… r, demonstrated the presence of both BPA and … 2C–2F). Because polymeric aromatic ethers, like …eric counterparts, cannot undergo nucleophilic substitution to generate an unsubstituted aromatic ring at the reaction site, degradation results in the formation of a phenolic group.



> 60% of ingested Chemicals are coming from Packaging (exposome)

Compliance (contaminations) of 70% of plastics tested by Modeling

Contaminations from non-plastic Materials not considered

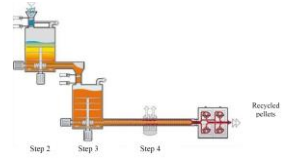
CIRCULAR ECONOMY vs SAFETY

Food Packaging Forum

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

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

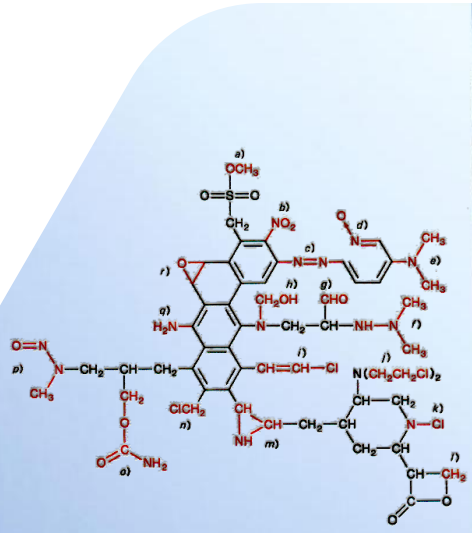
In 2014, more than 50% of the recycled PET in Europe was used in food contact applications.

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



Environ Sci Pollut Res (2009) 16:278–286
DOI 10.1007/s11356-009-0107-7

AREA 6 • PERSISTANT ORGANIC POLLUT

Endocrine disruptors in bot
estrogenic burden and migr

Martin Wagner · Jörg Oehlmann

Received: 6 November 2008 / Accepted: 18 December 2008

Abstract

Background, aim, and scope Food consumptio
important route of human exposure to endocrine-dis
chemicals. So far, this has been demonstrated by e
modeling or analytical identification of single substa
foodstuff (e.g., phthalates) and human body fluid
urine and blood). Since the research in this field is foc
few chemicals (and thus missing mixture effects), the
contamination of edibles with xenohormones is
unknown. The aim of this study was to assess the in
estrogenic burden of bottled mineral water as mod
stuff and to characterize the potential sources of th
genic contamination.

Materials, methods, and results In the present st
analyzed commercially available mineral water in an
system with the human estrogen receptor alpha and
estrogenic contamination in 60% of all samples
maximum activity equivalent to 75.2 ng/l of the nat
hormone 17β-estradiol. Furthermore, breeding of t
luskan model *Potamopyrgus antipodarum* in water
made of glass and plastic [polyethylene terepl
(PET)] resulted in an increased reproductive ou
snails cultured in PET bottles. This provides first e
that substances leaching from plastic food pa
materials act as functional estrogens in vivo.

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EDITORIAL

The perils of plastic

A 'round-robin' spam e-mail that is ci
servers worldwide claims that drinl
water that has been left in a warm c
breast cancer. Is this warning just an urban
it hold a grain of truth? The FDA, it seems,
the side of caution; earlier this year, the
revised its position on the safety of bisphen
chemical used in the manufacture of plastic
deemed safe for food-contact use, the FI
expressed "some concern" about the potentia
that BPA poses to fetuses, infants and youn

What exactly is BPA and why has its
alarm? First synthesized in 1905, BPA has s
a key component in the production of plas
ing polycarbonate and epoxy resins. Polyc
clear, heat-resistant, shatter-proof materia
that make it ideal for the manufacture of d
particularly those used by young children
Epoxy resins are also used by the food a
industry—they provide the protective co
inside many metal-based cans. Standard
tests supported the safety of BPA and the FI
it for food-contact use in the 1960s. Over
years, however, concern has mounted th
environmental exposure to BPA might dis
functioning of the endocrine system.

The term 'endocrine disruption' was coine
1990s. Endocrine disruptors comprise a div
industrial chemicals that exert numerous de
and functional effects on the endocrine syst
tiple biological pathways. Many of these cher
the effects of endogenous hormones, such
BPA and other endocrine-disrupting che
been implicated in obesity, neurological de
ductive dysfunction and cancer. In additio
octanoic acid (PFOA) and perfluorooctan
(PFOS)—common household chemicals fo
stick' and waterproof materials—have re
linked to thyroid disease.

The Endocrine Society has recognized t
problems associated with the widespread
trial chemicals. In June 2009, the society p
findings of a task force commissioned to
the mechanisms of action and potential he
endocrine disruptors (Diamanti-Kandara

cussed (Safe 2000, 2005; Sha
2005) due to the multifactoral
diseases, although evidence fo
to xenohormones and develop
tive disorders strengthens (Sha

WATER RESEARCH 46 (2012) 571–583

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Chemical compounds and toxicological assessments of drinking water stored in polyethylene terephthalate (PET) bottles: A source of controversy reviewed

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ABSTRACT

A declaration of conformity according to European regulation No. 10/2011 is required to ensure the safety of plastic materials in contact with foodstuffs. This regulation established a positive list of substances that are authorized for use in plastic materials. Some compounds are subject to restrictions and/or specifications according to their toxicological data. Despite this, the analysis of PET reveals some non-intentionally added substances (NIAS) produced by authorized initial reactants and additives.

Genotoxic and estrogenic activities in PET-bottled water have been reported. Chemical mixtures in bottled water have been suggested as the source of these toxicological effects. Furthermore, sample preparation techniques, such as solid-phase extraction (SPE), to extract estrogen-like compounds in bottled water are controversial. It has been suggested that inappropriate extraction methods and sample treatment may result in false-negative or positive responses when testing water extracts in bioassays. There is therefore a need to combine chemical analysis with bioassays to carry out hazard assessments.

Formaldehyde, acetaldehyde and antimony are clearly related to migration from PET into water. However, several studies have shown other theoretically unexpected substances in bottled water. The origin of these compounds has not been clearly established (PET container, cap-sealing resins, background contamination, water processing steps, NIAS, recycled PET, etc.).

Here, we surveyed toxicological studies on PET-bottled water and chemical compounds that may be present therein. Our literature review shows that contradictory results for PET-

List of abbreviations: AA, acetaldehyde; APEOs, polyethoxylated nonylphenols; BBP, benzylbutyl phthalate; BHET, bis(hydroxyethyl) terephthalate; BHT, butylated hydroxytoluene; BPA, bisphenol A; DBP, dibutyl phthalate; DiBP, di-iso-butyl phthalate; DEG, diethylene glycol; DEHP, di-2-(ethylhexyl) phthalate; DEHA, bis-2-ethylhexyl adipate; DEP, diethyl phthalate; DMSO, dimethyl sulfoxide; DMT, dimethylterephthalate; DOP, di-n-octyl phthalate; EEC, European economic community; EEQs, estradiol equivalents; GC–MS, gas chromatography–mass spectrometry; HDPE, high density polyethylene; HULYs, human blood lymphocytes; IPA, isophthalic acid; LDH, lactate dehydrogenase; MEG, ethylene glycol; NIAS, non-intentionally added substances; NP, 4-nonylphenol; OP, octylphenol; PA, polyamide; PC, polycarbonate; PhA, phthalic acid; PVC, polyvinylchloride; RPE, relative proliferative effects; Sb_2O_3, antimony trioxide; SEC–HPLC, size exclusion chromatography–high performance liquid chromatography; SML, specific migration limits; SPE, solid-phase extraction; SPME, solid-phase micro-extraction; SODIS, solar water disinfection; TPA, terephthalic acid; TDI, tolerable daily intake; TNPP, tris(nonylphenyl) phosphite; TOC, total organic carbon; YES, yeast estrogen screen.

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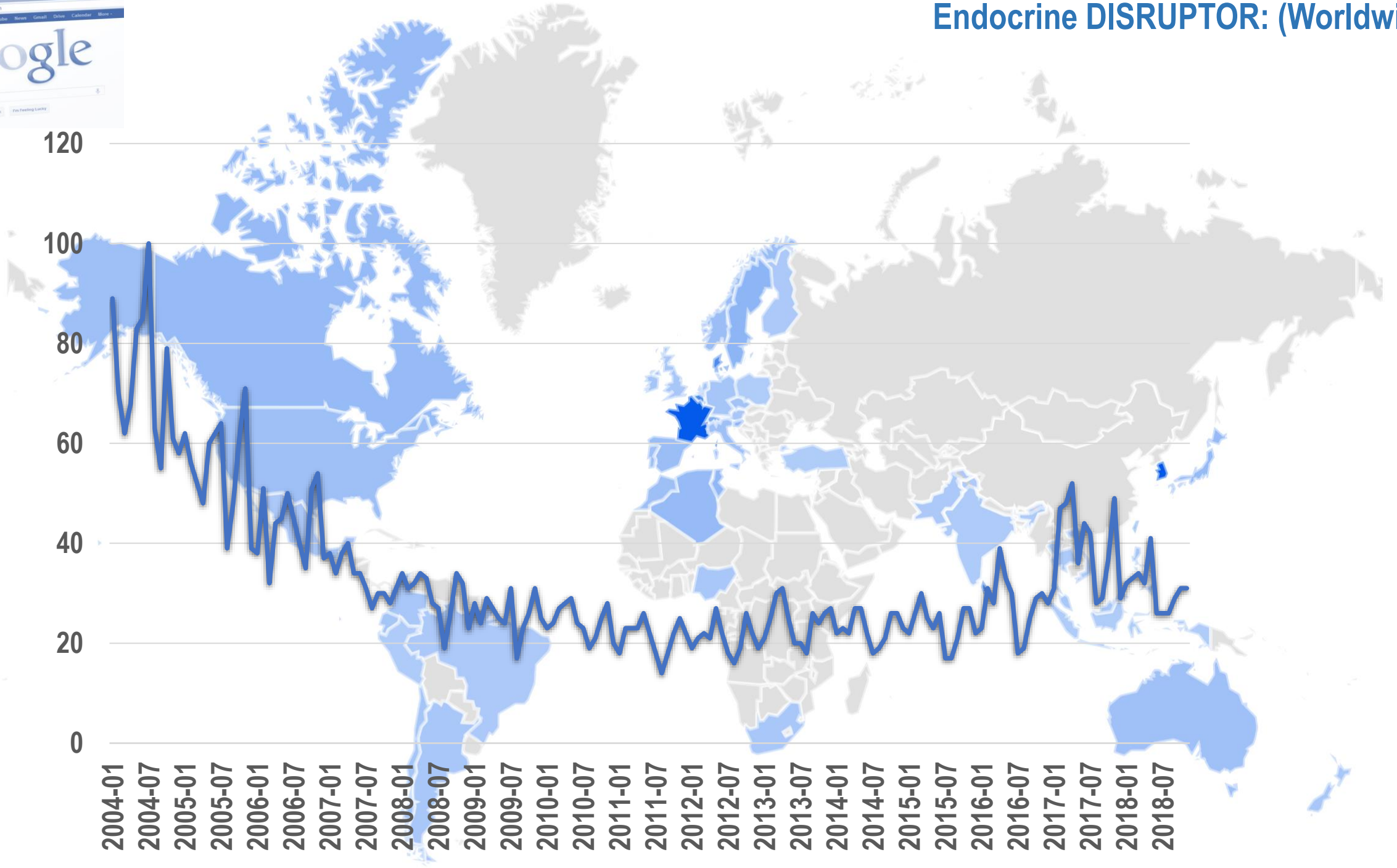
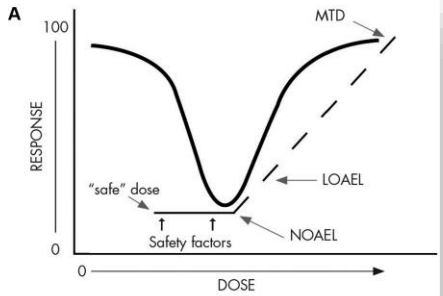
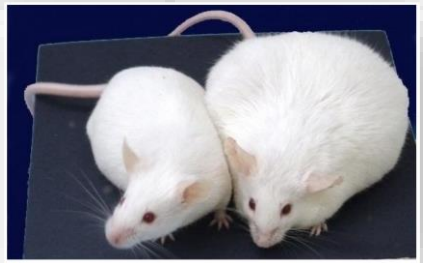
0043-1354/$ – see front matter
doi:10.1016/j.watres.2011.11.062

Endocrine DISRUPTOR: (Worldwide)







Hormones and Endocrine-Disrupting Chemicals: Low-Dose Effects and Nonmonotonic Dose Responses

Laura N. Vandenberg, Theo Colborn, Tyrone B. Hayes, Jerrold J. Heindel, David R. Jacobs, Jr., Duk-Hee Lee, Toshi Shioda, Ana M. Soto, Frederick S. vom Saal, Wade V. Welshons, R. Thomas Zoeller, and John Peterson Myers

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For decades, studies of endocrine-disrupting chemicals (EDCs) have challenged traditional concepts in toxicology, in particular the dogma of "the dose makes the poison," because EDCs can have effects at low doses that are not predicted by effects at higher doses. Here, we review two major concepts in EDC studies: low dose and nonmonotonicity. Low-dose effects were defined by the National Toxicology Program as those that occur in the range of human exposures or effects observed at doses below those used for traditional toxicological studies. We review the mechanistic data for low-dose effects and use a weight-of-evidence approach to analyze five examples from the EDC literature. Additionally, we explore nonmonotonic dose-response curves, defined as a nonlinear relationship between dose and effect where the slope of the curve changes sign somewhere within the range of doses examined. We provide a detailed discussion of the mechanisms responsible for generating these phenomena, plus hundreds of examples from the cell culture, animal, and epidemiology literature. We illustrate that nonmonotonic responses and low-dose effects are remarkably common in studies of natural hormones and EDCs. Whether low doses of EDCs influence certain human disorders is no longer conjecture, because epidemiological studies show that environmental exposures to EDCs are associated with human diseases and disabilities. We conclude that when nonmonotonic dose-response curves occur, the effects of low doses cannot be predicted by the effects observed at high doses. Thus, fundamental changes in chemical testing and safety determination are needed to protect human health. (*Endocrine Reviews* 33: 378–455, 2012)

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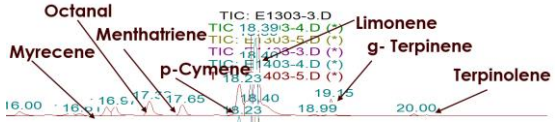
Abbreviations: A4, Androstenedione; AhR, aryl hydrocarbon receptor; BPA, bisphenol A; CDC, Centers for Disease Control and Prevention; DDE, dichlorodiphenyldichloroethylene; DDT, dichlorodiphenyltrichloroethane; DES, diethylstilbestrol; EDC, endocrine-disrupting chemical; EPA, Environmental Protection Agency; ER, estrogen receptor; FDA, Food and Drug Administration; GLP, good laboratory practices; LOAEL, lowest observed adverse effect level; mER, membrane-associated ER; NHANES, National Health and Nutrition Examination Survey; NIS, sodium/iodide symporter; NMDRC, nonmonotonic dose-response curve; NOEL, no observed effect level; NOAEL, no observed adverse effect level; NTP, National Toxicology Program; PIN, prostatic intraepithelial neoplasias; POP, persistent organic pollutants; ppb, parts per billion; SERM, selective ER modulator; TCDD, 2,3,7,8-tetrachlorodibenzo-*p*-dioxin; WoE, weight of evidence.

TABLE 4. Select examples of EDCs whose potential low-dose effects on animals remain to be studied

Chemical	Use	EDC action	Low-dose cutoff
Antiseptics and preservatives			
Butyl paraben	Preservative (cosmetics)	Estrogenic, antiandrogenic	2 mg/kg · d (EPA)
Propyl paraben	Antimicrobial preservative found in pharmaceuticals, foods, cosmetics, and shampoos	Estrogenic activity	LOAEL 10 mg/kg · d, NOEL 6.5 mg/kg · d (Europa)
Cosmetics and personal care products			
2,4-Dihydroxybenzophenone ⚠	UV absorber in polymers, sunscreen agent	Estrogenic activity	Not identified
3-Benzylidene camphor	UV blocker used in personal care products	Estrogenic activity	0.07 mg/kg · d (710)
4,4′-Dihydroxybenzophenone ⚠	UV light stabilizer used in plastics, cosmetics, adhesives, and optical fiber	Estrogenic activity	Not identified
Benzophenone-2 ⚠	Used in personal care products such as aftershave and fragrances	Estrogenic activity, changes in T_4, T_3, and TSH levels, alterations in cholesterol profile	NOEL 10–333 mg/kg · d (711)
Benzophenone-3 ⚠	UV filter	Estrogenic, PPARγ activator	200 mg/kg · d (Europa)
Multiple use (other)			
Melamine ⚠	Flame-retardant additive and rust remover; used to make laminate, textile, and paper resins; metabolite of cyromazine	Affects voltage-gated K^+ and Na^+ channels and Ca^{2+} concentrations in hippocampal neurons	63.0 mg/kg · d (FDA)
Resorcinol ⚠	Used in the manufacturing of cosmetics, dyes, flame retardants, hair dye formulations, pharmaceuticals, skin creams, and tires	Alters T_4 and TSH levels	80.00 mg/kg · d (Europa)
Pesticides			
Aldrin[a]	Insecticide	Estrogenic activity	0.025 mg/kg · d (Health Canada)
Alachlor	Herbicide	Decreases serum T_4, binds PR, weakly binds ER	1 mg/kg · d (EPA)
Amitrole	Herbicide	Decreases thyroid hormone	0.12 mg/kg · d (FAO)
Bitertanol	Fungicide	Alters aromatase	30 mg/kg · d (EPA)
Carbendazim	Fungicide	Affects FSH, LH, and testosterone levels; alters spermatogenesis and Sertoli cell morphology	8 mg/kg · d (712)
Diazinon	Insecticide	Alters glucocorticoids	0.065 mg/kg · d (CDC)
Endrin[a]	Insecticide	Stimulates glucocorticoid receptor	0.025 mg/kg · d (CDC)
Fenoxycarb	Insecticide	Alters acetylcholinesterase	260 mg/kg · d (CDC)
Mirex[a]	Insecticide	Decreases testosterone levels	0.075 mg/kg · d (CDC)
Zineb	Fungicide	Alters T_4 and dopamine levels	LOAEL 25 mg/kg · d (EPA)
Ziram	Fungicide	Alters norepinephrine levels	1.6 mg/kg · d (EPA)
Resins			
Bisphenol F ⚠	Used in polycarbonates	Alters T_4, T_3, and adiponectin levels, has estrogenic activity	LOAEL 20 mg/kg · d (713)
Styrene ⚠	Precursor to polystyrene	Alters dopamine	200 mg/kg · d (EPA)

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



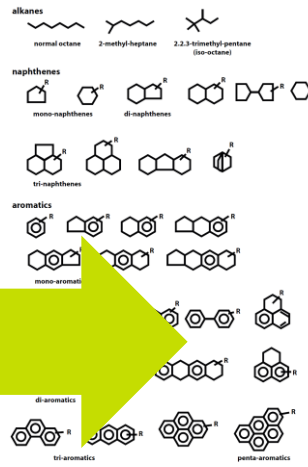
1. Filling and use of HDPE milk bottles
2. Recollection
3. Sorting

Foodgrade HDPE milk bottles

Suitable for Food Contact?

Recycling

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

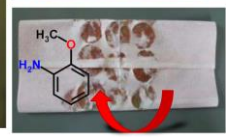


Paper and board contains large amount of residues from printing inks: aromatic (carcinogenic) and aliphatic **mineral oils** can be transferred without contact and lead to cross-contamination between materials

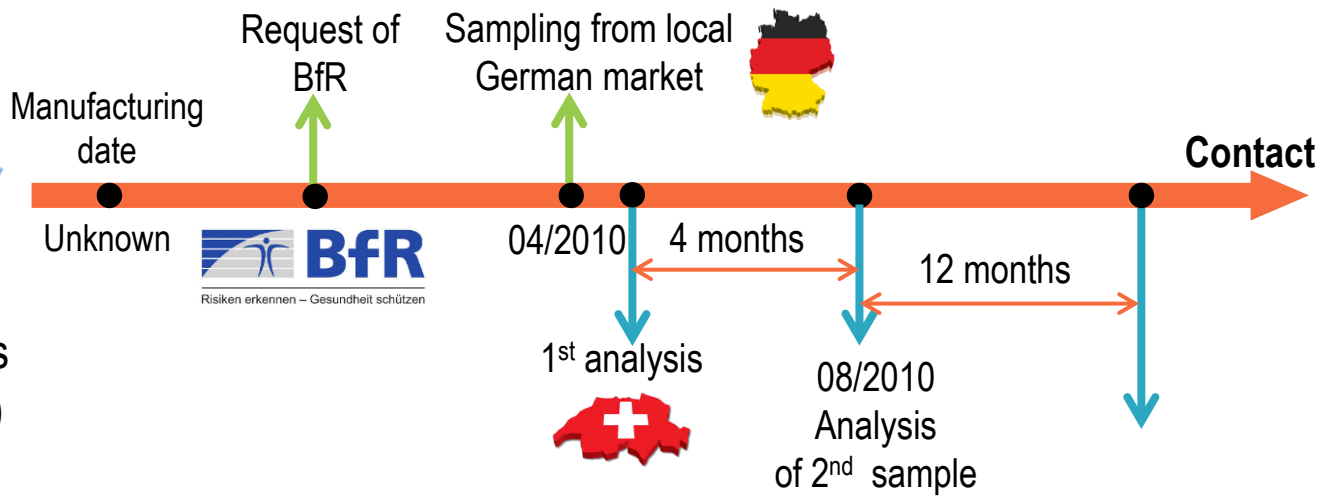
*J. of Chromatography A. 2013;**1293:107-19.***

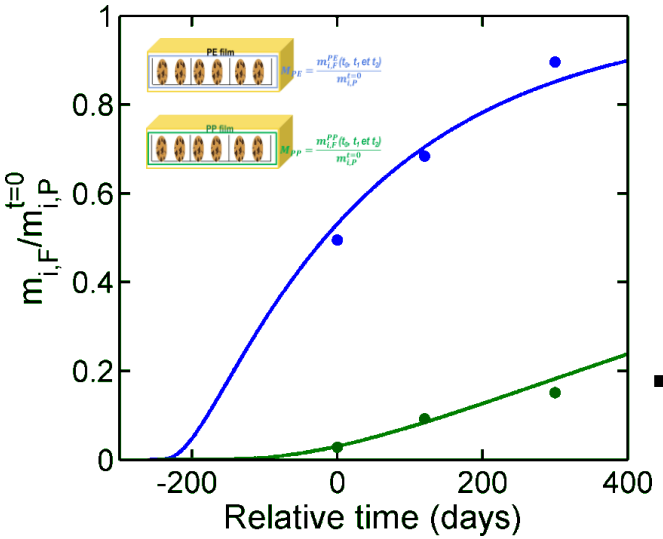
Recycling of PET vs other materials

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.



119 dry food products
(3 samples/category)
Biedermann et al. (2013)

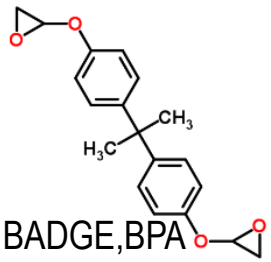


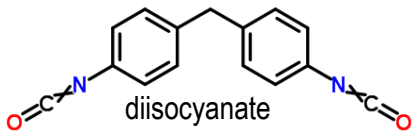


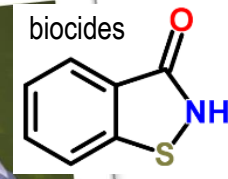
$$\rightarrow \frac{M_{PE}}{M_{PP}} \propto \frac{D_{i,PE}}{D_{i,PP}}$$

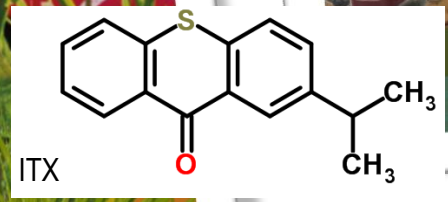
Paper and board = prevalent source of chemical contaminants in food

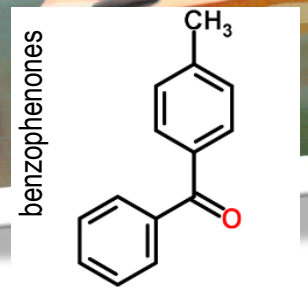
Mineral Oils, Printing inks, adhesives

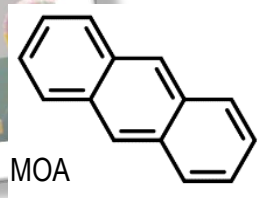

BADGE,BPA


diisocyanate


biocides


ITX


benzophenones


MOA

Food and Feed borne crises throughout the food chain

Nestlé
Good Food, Good Life

Bovine Spongiform Encephalopathy
B S E

Sudan red

Dioxins

Chloramphenicol
CAP

Mycotoxins

destroy consumer's confidence in food

But what about food packaging

Nestlé
Good Food, Good Life

Nonylphenol
NP

?

Semicarbazide/SEM

Organic solvents/
residues

Bisphenol A diglycidyl ether
(BADGE)

Italian police seize contaminated Nestle baby milk

22 Nov 2005 16:45:09 GMT
Source: Reuters

PREVIOUS | NEXT

Forest Ranger officials check a package of baby milk made by Swiss food group Nestle in a supermarket in Italy November 22, 2005. Italian police seized around 30 million litres of baby milk produced by Nestle on Tuesday after tests showed traces of ink, and the company said it was recalling the infant food in four European countries.
REUTERS/HO

(Adds Tetra Pak comment in paragraph 11)

By Massimiliano Di Giorgio and Isabel Strassheim

ROME/ZURICH, Nov 22 (Reuters) - Italian police seized around 30 million litres of baby milk produced by Swiss food giant Nestle <NESN.VX> on Tuesday after tests showed it was contaminated with traces of ink used in the packaging.

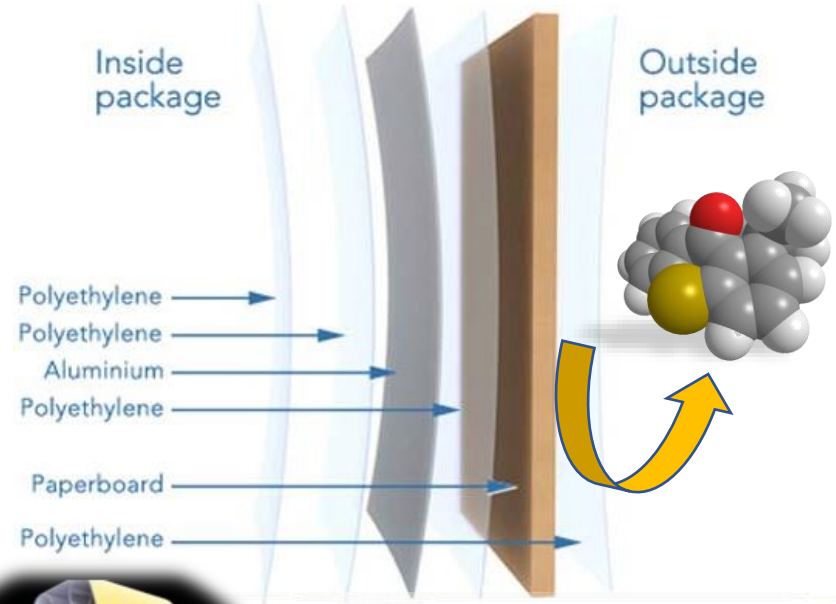
Nestle said the chemical substance was not harmful, but announced it was recalling the infant food in four European countries, including Italy, because of the problem, which related to Tetra Pak cartons.

Italian Agriculture Minister Gianni Alemanno demanded tests to see if babies given the contaminated milk over a prolonged period faced health risks.

"It is incredible that such defenceless beings as babies should face such serious risks in a product as widely used as milk," Alemanno said in a statement.

Italian officials said they had already seized about 2 million litres of Nestle baby milk earlier this month after finding traces of isopropylthioxanthone (ITX), an ink

"It is incredible that such defenseless beings as babies should face such serious risks in a product as widely used as milk"



REUTERS FOUNDATION AlertNet

INRAE

Regulations to orient policies

Transfer of responsibilities

"Markets are imperfect. So you do need regulation, knowing that the regulators are also human." – George Soros, USA

ROMA TREATY, 1957

PROHIBITION OF QUANTITATIVE RESTRICTIONS BETWEEN MEMBER STATES

Article 28

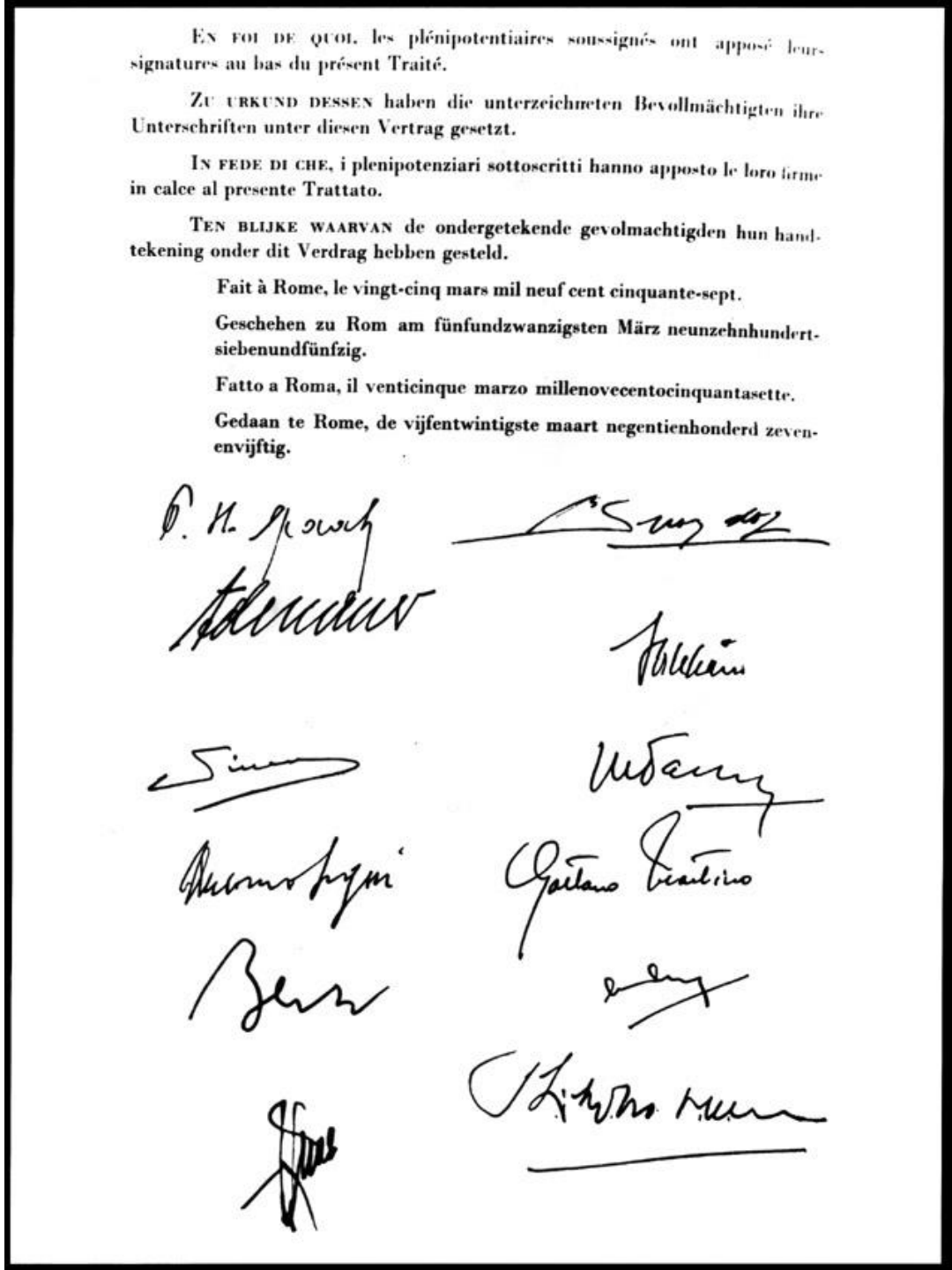
Quantitative restrictions on imports and all measures having equivalent effect shall be prohibited between Member States.

Article 29

Quantitative restrictions on exports, and all measures having equivalent effect, shall be prohibited between Member States.

Article 30

The provisions of Articles 28 and 29 shall not preclude prohibitions or restrictions on imports, exports or goods in transit justified on grounds of public morality, public policy or public security; the protection of health and life of humans, animals or plants; the protection of national treasures possessing artistic, historic or archaeological value; or the protection of industrial and commercial property. Such prohibitions or restrictions shall not, however, constitute a means of arbitrary discrimination or a disguised restriction on trade between Member States.



EN FOI DE QUOI, les plénipotentiaires soussignés ont apposé leurs signatures au bas du présent Traité.

ZU URKUND DESSEN haben die unterzeichneten Bevollmächtigten ihre Unterschriften unter diesen Vertrag gesetzt.

IN FEDE DI CHE, i plenipotenziari sottoscritti hanno apposto le loro firme in calce al presente Trattato.

TEN BLIJKE WAARVAN de ondergetekende gevolmachtigden hun handtekening onder dit Verdrag hebben gesteld.

Fait à Rome, le vingt-cinq mars mil neuf cent cinquante-sept.

Geschehen zu Rom am fünfundzwanzigsten März neunzehnhundertsiebenundfünfzig.

Fatto a Roma, il venticinque marzo millenovecentocinquantasette.

Gedaan te Rome, de vijfentwintigste maart negentienhonderd zevenenvijftig.

https://ec.europa.eu/food/safety/chemical_safety/food_contact_materials_en

FOOD

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European Commission

European Commission > Food Safety > Food > Chemical safety > Food Contact Materials

HEALTH | FOOD | ANIMALS | PLANTS | AMR

CHEMICAL SAFETY

- Contaminants
- Residues of Veterinary Medicines
- Hormones in Meat
- Pesticide Residues
- Food Contact Materials
  - Legislation
  - Authorisations
  - Non-harmonised
  - Consultation

ALL TOPICS

Food Contact Materials

Food comes into contact with many materials and articles during its production, processing, storage, preparation and serving, before its eventual consumption. Such materials and articles are called **Food Contact Materials (FCMs)**. Food contact materials are either intended to be brought into contact with food, are already in contact with food, or can reasonably be brought into contact with food or transfer their constituents to the food under normal or foreseeable use. **This includes direct or indirect contact.** Examples include:

- containers for transporting food
- machinery to process food
- packaging materials
- kitchenware and tableware

The term **does not cover fixed public or private water supply equipment**.

FCMs should be sufficiently inert so that their constituents neither adversely affect consumer health nor influence the quality of the food. To ensure the safety of FCMs, and to facilitate the free movement of goods, EU law provides for binding rules that business operators must comply with.

The EU Rules on food contact materials can be of general scope, i.e. apply to all FCMs or apply to specific materials only. EU law may be complemented with Member States national legislation if specific EU rules do not exist.

The safety of FCM is evaluated by the **European Food Safety Authority** (EFSA). At EFSA's website you can search for opinions on substances to be used in food contact materials.

The safety of Food Contact Materials is tested by the business operators placing them on the market, and by the competent authorities of the Member States during official controls. Scientific knowledge and technical competence on testing methods is being maintained by the **European Reference Laboratory for Food Contact Materials (EURL-FCM).** Its website provides guidelines and other resources concerning the testing of food contact materials.

Principles for EU legislation

Union legislation on food contact materials at EU level aims to:

- Protect consumers' health
- Ensure the effective functioning of the internal market

Contacts

- SANTE-fcm@ec.europa.eu
- National authorities
- European professional organisations
- European Reference Laboratory on Food Contact Materials (EURL-FCM)
- European Food Safety Authority

Training

For government officials engaged in food and feed safety inspection of selected countries training on food contact materials is provided free of charge under BTSF. Also refer to the European Training Platform for Safer Food.

Share

RELATED LINKS

- Food Contact Materials Database
- Multi-language versions of brochures and guidance

RELATED DOCUMENTS

- EU guidelines on conditions and procedures for the import of polyamide and melamine kitchenware originating in or consigned from China and Hong Kong
- EU Guidance to the Commission Regulation (EC) No 450/2009 on active and intelligent materials and articles intended to come into contact with food

QUICK LINKS

- Rapid Alert for Food and Feed (RASFF)
- Health and food audits and analysis
- European Food Safety Authority (EFSA)
- Better Training for Safer Food (BTSF)
- E-News
- Events
- Videos

Legislation

I. General legislation

The framework Regulation

Regulation (EC) No 1935/2004 provides a harmonised legal EU framework. It sets out the general principles of safety and inertness for all Food Contact Materials (FCMs).

The principles set out in Regulation (EC) No 1935/2004 require that materials do not:

- Release their constituents into food at levels harmful to human health
- Change food composition, taste and odour in an unacceptable way

Moreover, the framework pr

- for special rules on inert)
- powers to enact addi
- the procedure to per FCMs involving the E
- rules on labelling inc bottle, or a soup sp information, please r contact materials.
- for compliance docun

Regulation on Good Manu

Regulation (EC) No 2023/2 so that the specifications fo

- premises fit for purpo
- documented quality premises, and
- selection of suitable s the safety and inertn

Good manufacturing rules a materials, although the proc

II. EU legislation

In addition to the general cellulose film, plastics (in materials — are covered by starting substances used to

- Plastic Materials
- Active and Intelligent M
- Recycled Plastic Materi
- Ceramics
- Regenerated Cellulose Film

III. Other Legislation

Legislation on Specific Substances

- Regulation 1895/2005/EC - restricting use of certain epoxy derivatives in materials and articles intended to come into contact with food
- Directive 93/11/EEC - release of N-nitrosamines and N-nitrosatable substances from rubber teats and soothers

EU LEGISLATION ON FCM

Framework Regulation (EC) 1935/2004
General requirement to all FCM
Specific measures to some FCM & Substances

Regulation (EC) 2023/2006
Good Manufacturing Practices (GMP)
Applicable to all FCM

Specific measures on Materials
17 Materials identified in Annex I

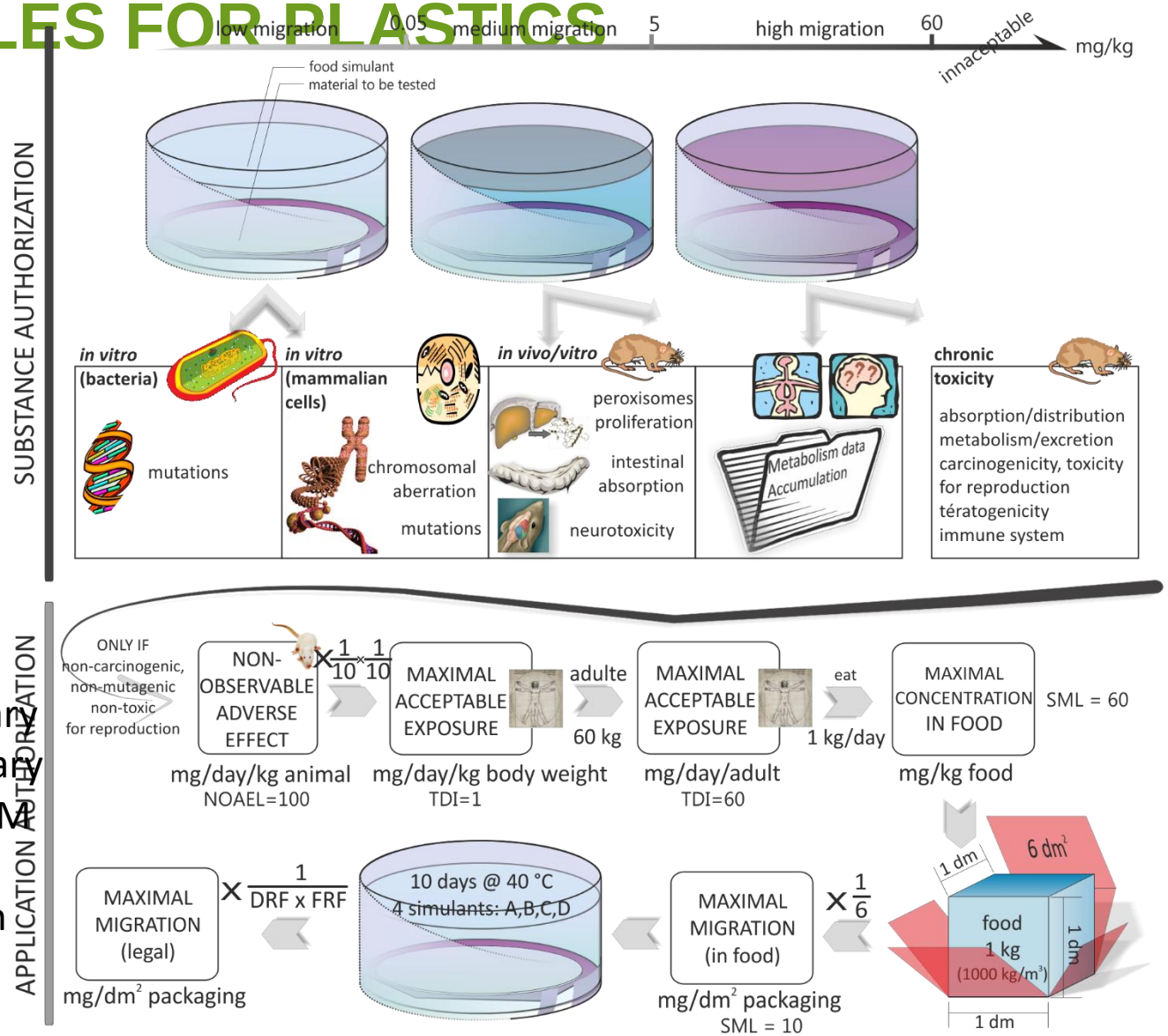
Specific Measures on substances

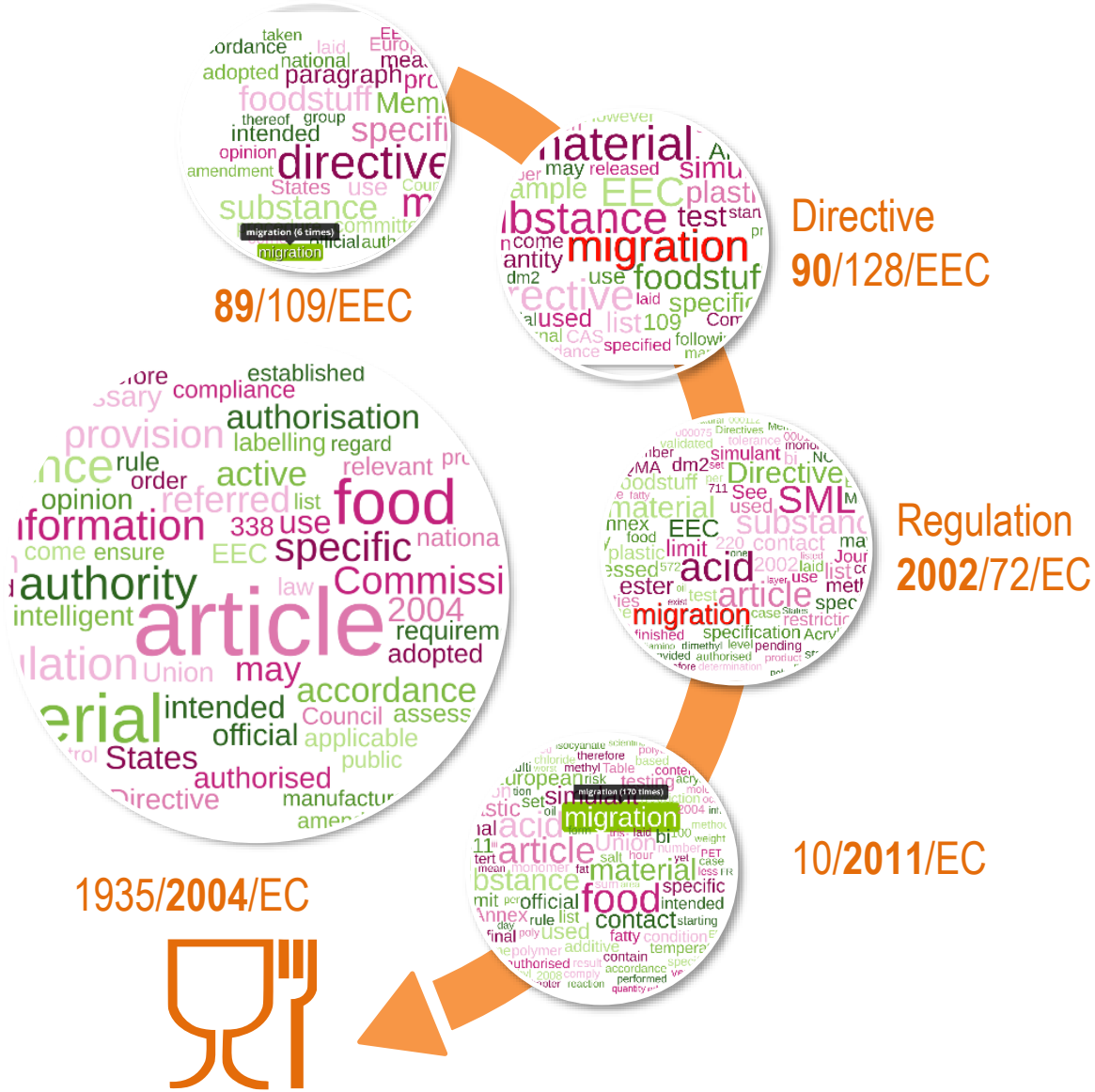
In place for 4/17 materials	Not in place for 13/17 materials	Vinyl chloride monomer
Ceramics	Inks, Coatings	BADGE, BFDGE, NOGE
Regenerated cellulose	Paper & board	Nitrosamines & N-nitrosables
Plastics	Rubber, Adhesives	
Plastics recycled	Etc.	
Active and Inteligent Meterials		

SPECIFIC RULES FOR PLASTICS

COMPLIANCE ISSUES

Ex-Post Impact Assessment Unit of the European Parliamentary Research Service (EPRS) between December 2015 and February 2016. It seeks to assess the implementation of existing EU FCM rules, and, in particular, framework Regulation (EC) No 1935/2004, which is the focus of a dedicated Implementation Report being prepared by the EP Committee on Envi





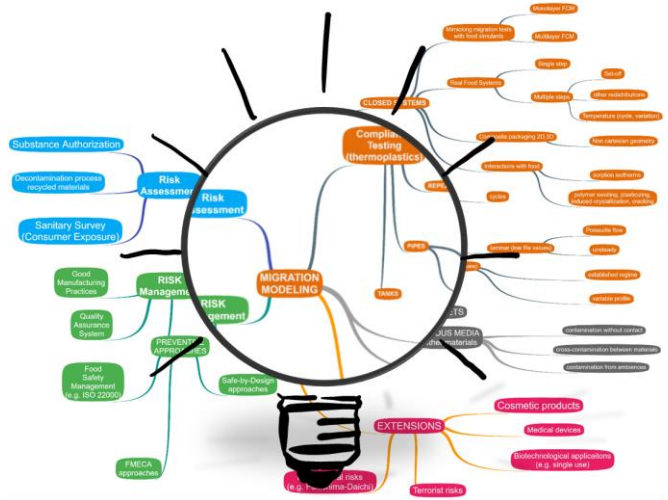
Food Additives and Contaminants, January 2005; 22(1): 73–90

Taylor & Francis
Taylor & Francis Group

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

T. BEGLEY[1], L. CASTLE[2], A. FEIGENBAUM[3], R. FRANZ[4], K. HINRICHS[5], T. LICKLY[6], P. MERCEA[7], M. MILANA[8], A. O'BRIEN[9], S. REBRE[10], R. RIJK[11], & O. PIRINGER[7]

[1]*Food & Drug Administration, 5100 Paint Branch Parkway, College Park, MD 20740, USA,* [2]*Central Science Laboratory, Sand Hutton, York Y041 1LZ, UK,* [3]*INRA — CPCB, Moulin de la Housse, F-51697 Reims Cedex 2, France,* [4]*Fraunhofer-Institut IVV, Giggenhauser Straße 35, D-85354 Freising, Germany,* [5]*Cognis GmbH, Henkelstraße 67, D-40551 Dusseldorf, Germany,* [6]*DOW, 1803 Building, Midland, MI 48674, USA,* [7]*Fabes GmbH, Schragenhofstraße 35, D-80992 Munich, Germany,* [8]*Istituto Superiore de Sanita, Viale Regina Elena, 299, I-0161 Rome, Italy,* [9]*PIRA International, Leatherhead KT22 7RU, UK,* [10]*Atofina, Rue Danton 95, F-92300 Levallois-Perret, France, and* [11]*TNO, Utrechtseweg 48, NL-3700 AJ Zeist, the Netherlands*



FDA
CSL
INRA SCIENCE & IMPACT
Fraunhofer IVV
BASF We create chemistry
DOW
FABES
ISTITUTO SUPERIORE DI SANITÀ
SMITHERS PIRA
ARKEMA
TNO

INRA SCIENCE & IMPACT

Contribution of INRA

https://www.plasticseurope.org/application/files/2615/2933/0926/The_Role_of_Food_Packaging_2018.pdf

Inside Food Contact Materials

PlasticsEurope
FCA Food Contact Additives

WHAT YOU NEED TO KNOW

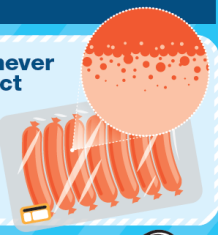
Plastic Food Contact Materials play a crucial role in preserving food from contaminants and **preventing food waste.** Yet, some worry about the chemicals that are required in the production of these important materials.

What are Food Contact Materials?

"Food Contact Materials", or FCMs for short, refers to all *materials* that come into contact with food.

Natural migration occurs whenever two materials come into contact with each other

Migration is a natural and unavoidable phenomenon that occurs **in all materials.** Whenever two materials come into contact with each other, substances can migrate from one material into another. This also happens with food packaging and food.



Risk assessments make sure that Food Contact Materials are safe

A risk assessment is based on different elements to assess potential health risks associated with exposure to substance migration into the food.

HAZARD IDENTIFICATION:
Identifies potential health effects in humans and/or environment, caused by chemicals.

EXPOSURE ASSESSMENT:
Evaluates the potential chemical exposures to humans and the environment from the production, distribution, use, disposal and recycle of a chemical substance.

RISK CHARACTERIZATION:
Integrates those identification and assessment results to determine the probability of occurrence of health and/or environmental effects in a given population.

THE RESULT ENSURES SAFE USE OF PRODUCTS

EFSA The European Food Safety Authority performs a risk assessment of the substance to ensure a high level of human health protection. The safety limit is based on the toxicological profile of each substance.

Quantity is key

Even natural substances can interact with the body but would only cause adverse effects from a certain dose. It is the **quantity** which **sets the risk.**

Water:

Water is vital for leading a healthy lifestyle. We need water to remain hydrated and energised.

Adequate Daily Intake: around 2.5 litres[1]

Water intoxication can occur when a person drinks so much that the water dilutes the concentration of sodium in the blood, creating an electrolyte imbalance. Water intoxication, known as hyponatremia, is mostly a risk for endurance athletes.

Coffee:

Coffee has antioxidants and nutrients that contribute to good health. Coffee increases your focus and can improve energy levels.

ADI: 400 milligrams[2]

Too much caffeine can cause insomnia, restlessness, nausea, irregular heartbeat, muscle tremors, anxiety and headaches.

Soy sauce:

Soy sauce has some great health benefits: it is low in calories and very high in natural antioxidants.

ADI: 2 tablespoons (32 grams)[3]

If consumed in too large a portion, it increases blood sodium levels, potentially leading to neurological problems.

Why is packaging so important?

Food waste is a huge problem, in Europe and beyond...

16%[4] — the amount of food that the average EU consumer wastes

According to the WHO, in the less developed world up to **50%** of all food is wasted between harvest and home[4].

... and food poisoning is a massive problem as well...

351.000[5] people have globally **died** per year as a result of food poisoning.

In the UK, more than **1 million people** per year have been poisoned by deteriorated food, leading to **500 deaths**[6].

... But adequate food packaging could change this!
Packaging plays an important role in ensuring the freshness of food, extends its shelf life and helps to improve the quality of products for consumers.

In a **sustainable society**, using modern packaging and storage systems, wastage is reduced dramatically to around **3%**[4]

[1] EFSA (2009), "Dietary reference values for water": https://www.efsa.europa.eu/en/efsajournal/pub/1459
[2] EFSA, "Caffeine": http://www.efsa.europa.eu/sites/default/files/corporate_publications/files/efsaexplainscaffeine150527.pdf
[3] Calculated based on EFSA (2005), "EFSA provides advice on adverse effects of sodium": https://www.efsa.europa.eu/en/press/news/050622. 1 tbsp. (16g) of soy sauce contains 0.9g of sodium.
[4] European Commission (2015), 'Average EU consumer wastes 16% of food; most of which could be avoided': https://ec.europa.eu/jrc/en/news/average-eu-consumer-wastes-16-food-most-which-could-be-avoided?rs=dnl
[5] Time (2015), "351,000 People Die of Food Poisoning Globally Every Year": http://time.com/3786003/351000-people-die-of-food-poisoning-globally-every-year/
[6] UK government (2011), FOODBORNE DISEASE STRATEGY: https://www.food.gov.uk/sites/default/files/multimedia/pdfs/fds2015.pdf

Inside Food Contact Materials

PlasticsEurope
FCA Food Contact Additives

HOW CAN WE BE SURE THAT THEY ARE SAFE?

A SCIENCE-BASED ANALYSIS IS PERFORMED TO ENSURE THE SAFE USE OF AN ADDED SUBSTANCE

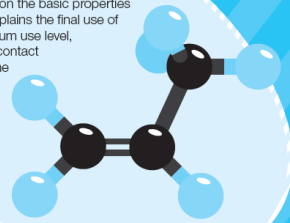
EFSA

Technical dossier

The technical dossier is part of a scientific and regulatory process which determines the safe use of an added substance

1 Identity and physico-chemical properties of the substances

The goal is to understand the substance and how it migrates. The applicant provides information on the basic properties (e.g. solubility and stability) and explains the final use of the substance, including: maximum use level, function, in which plastic(s), in contact with which foods, what are the contact conditions (time, temperature…), etc.



2 Data on the residual content of the substance in the Food Contact Material

The objective is to understand how much of the substance is present and what type of specific migration can be expected.

Residual content is the actual content in the final material placed on the market.

3 Migration data of the substance

The purpose is to comprehend how much of a substance is migrating into food. This is done by testing different types of food and real storage conditions (time/temperature).

4 Toxicological data and microbiological properties of the substance

The applicant needs to demonstrate that, in case of microbiological properties of a substance, these have no effect on the food. To demonstrate that levels of migration into food are safe for human consumption, the applicant provides the adequate toxicological reports.

5 Evaluation of existing assessments

The applicant provides information on whether a substance is already approved in a consumer application elsewhere.

Conclusions

EFSA reports its conclusions to the European Commission. If approved, the substance can be used in FCMs. The substance is safe and suitable to be used in food contact according to the descriptions included in the technical dossier.

INSIDE FOOD CONTACT MATERIALS

PlasticsEurope
Association of Plastics Manufacturers
FCA Food Contact Additives
A sector group of Cefic
EUPC

HOW CAN WE MAKE SURE THAT MIGRATION IS SAFE?

MIGRATION OF SUBSTANCES INTO FOOD OCCURS WITH ALL PACKAGING

Migration is a physical process and happens whenever packaging — of any type — comes into contact with food. It is natural. The key point is ensuring the level of migration remains safe.

PLASTICS ARE RIGOROUSLY TESTED TO MAKE SURE THAT MIGRATION - IF ANY - IS SAFE

Testing conditions are specified legally, and need to be used by all actors performing tests in the value chain (from raw materials to packaging producers and to food packers). The test are done at several stages in the value chain to ensure that the plastic sample is suitable in its end-use.

Variables can include:

- Temperature
- Time
- Contact surface
- Food type

Take a sample of the plastic

Test in contact with a food simulant

Food simulants - as prescribed by law, (e.g. olive oil) - mimic the properties of different food types under typical / worst case conditions.

Monitor migration under standardised conditions

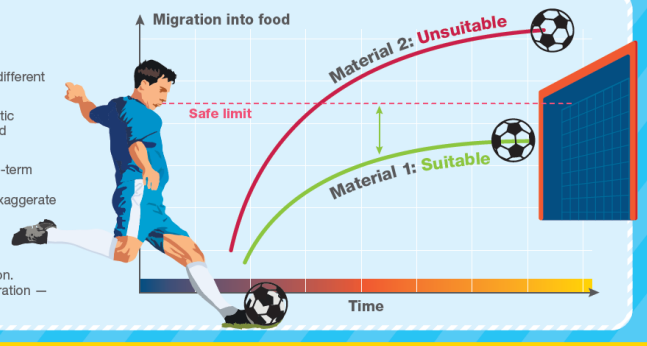
Analyse the results to verify that safety limits are met

WHAT DO THE TESTS SHOW?

The tests show how migration occurs in different food types under various conditions.

The tests enable us to determine if a plastic packaging can be used for given food and conditions of use.

For example, it may be beneficial for long-term storage, unless they are suitable for high temperature. The tests are designed to exaggerate the real use scenario and therefore to make sure there is a safety margin, e.g. by assuming that all the food is in contact with the packaging, and by exaggerating levels of consumption. These testing conditions ensure that migration — if any — is far below the safety level.



WITH ALL THESE DATA, WE CAN ENSURE THE SAFE USE OF THE PACKAGING

INSIDE FOOD CONTACT MATERIALS

PlasticsEurope
Association of Plastics Manufacturers
FCA Food Contact Additives
A sector group of Cefic
EUPC

HOW CAN WE MAKE SURE THAT MIGRATION IS SAFE?

At all stages of the value chain, materials are produced in a controlled, safe and consistent way.

NINE GOLDEN RULES OF ENSURING SAFETY THROUGHOUT THE SUPPLY CHAIN:

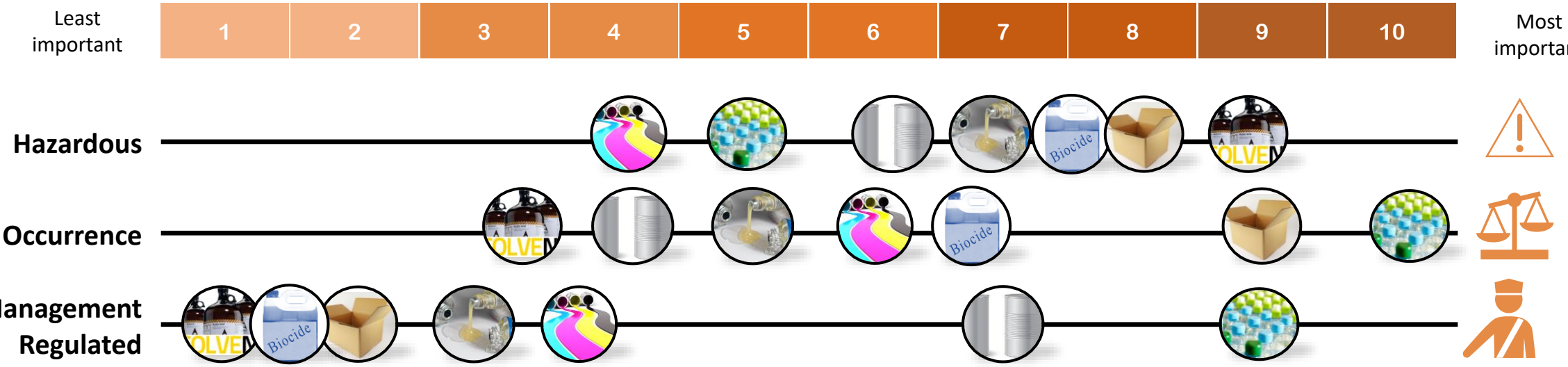
- Assign management responsibilities for ensuring product safety, and train all operational personnel.
- Implement quality assurance systems and policies to ensure compliance with applicable regulations.
- Have procedures in place at production level to prevent contamination.
- Adhere to a stringent hygiene policy.
- Document all relevant information (e.g. product formulation, operating procedures), ensure correct labelling, and implement traceability procedures.
- Conduct internal risk assessment of the quality controls and specifications in order to ensure ongoing effective implementation.
- Have a system for complaint handling, product recall and incident management in place.
- Regularly carry out internal and supplier audits.
- Ensure that procedural changes are managed and implemented properly.

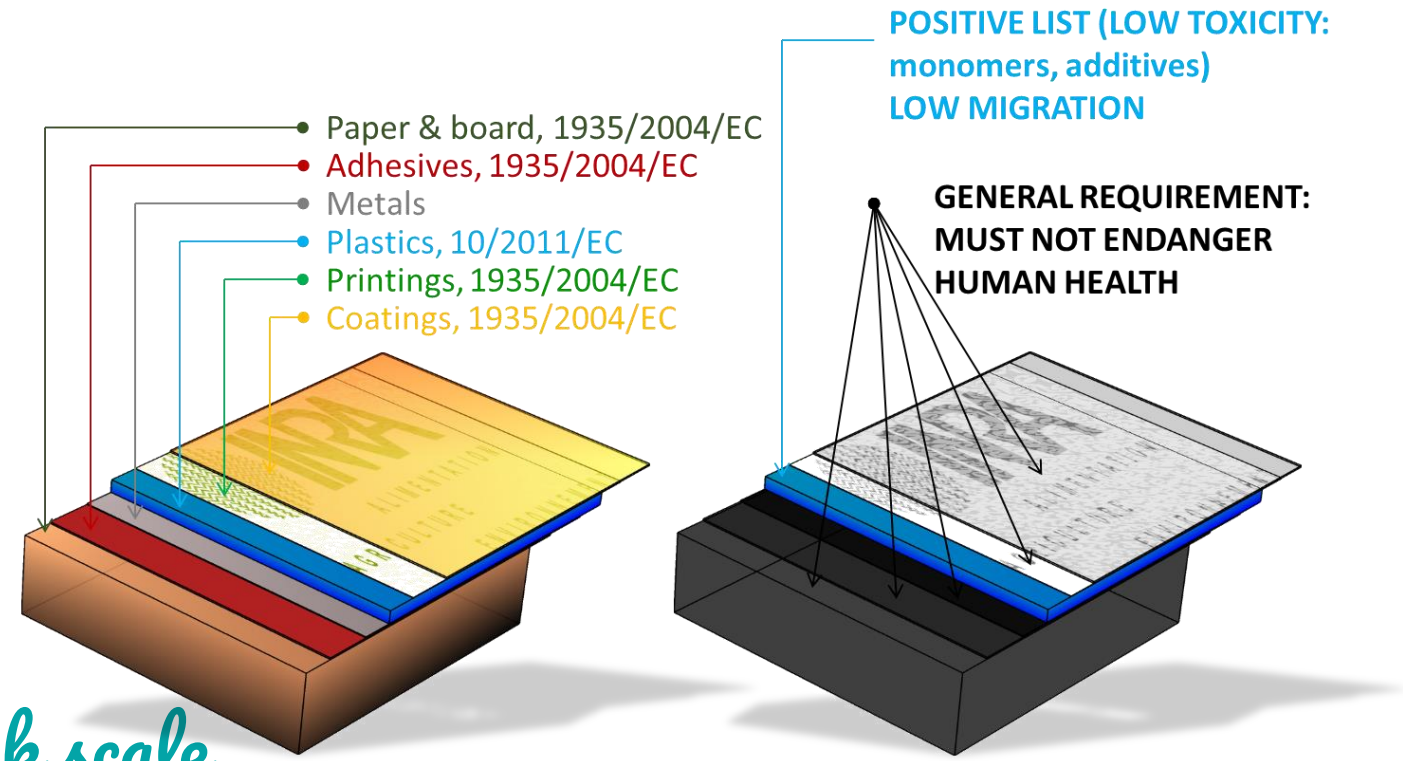
WHO ENSURES THE SAFETY OF FOOD CONTACT MATERIALS?

All of the different parties involved are required to issue a declaration of compliance that states product safety.

PROCESS FOLLOWS EFSA'S RISK ASSESSMENT PRINCIPLES

ALL THIS ENSURES SAFE FOOD CONTACT MATERIALS

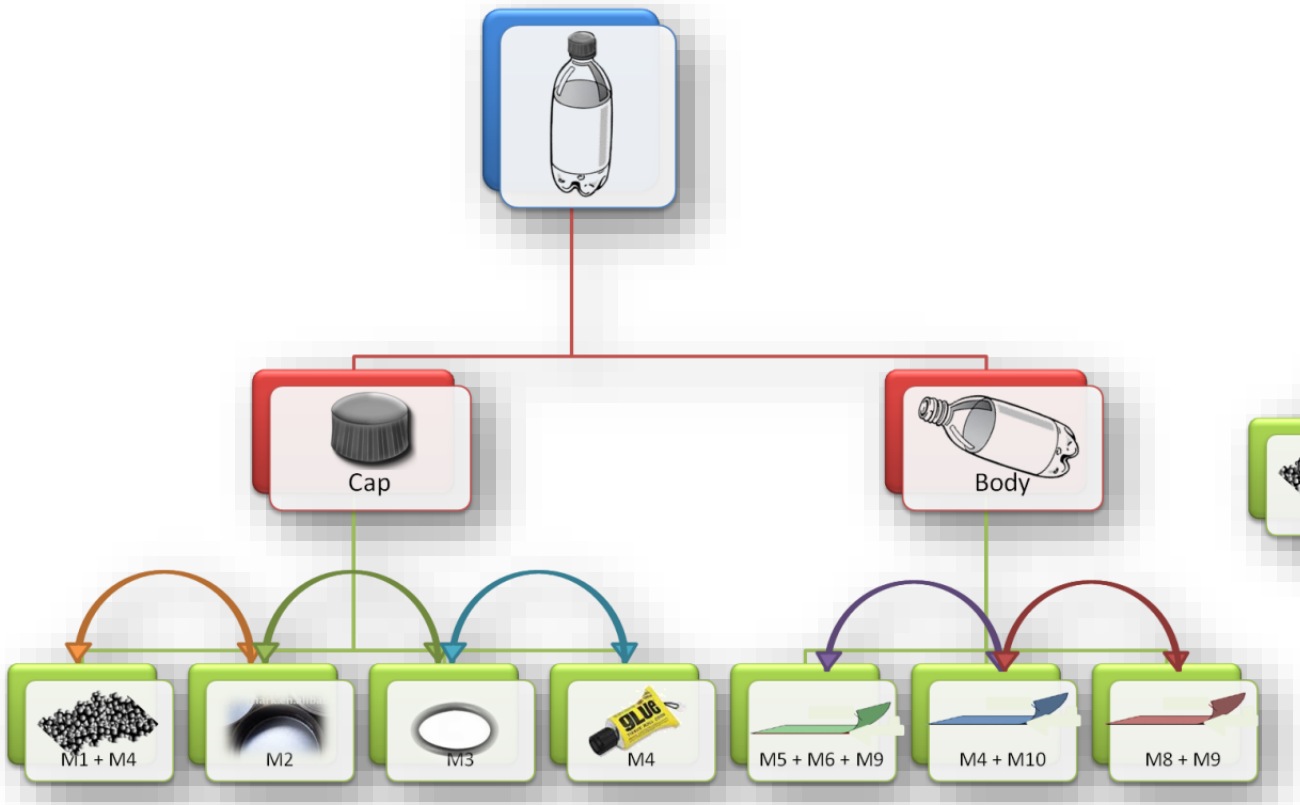


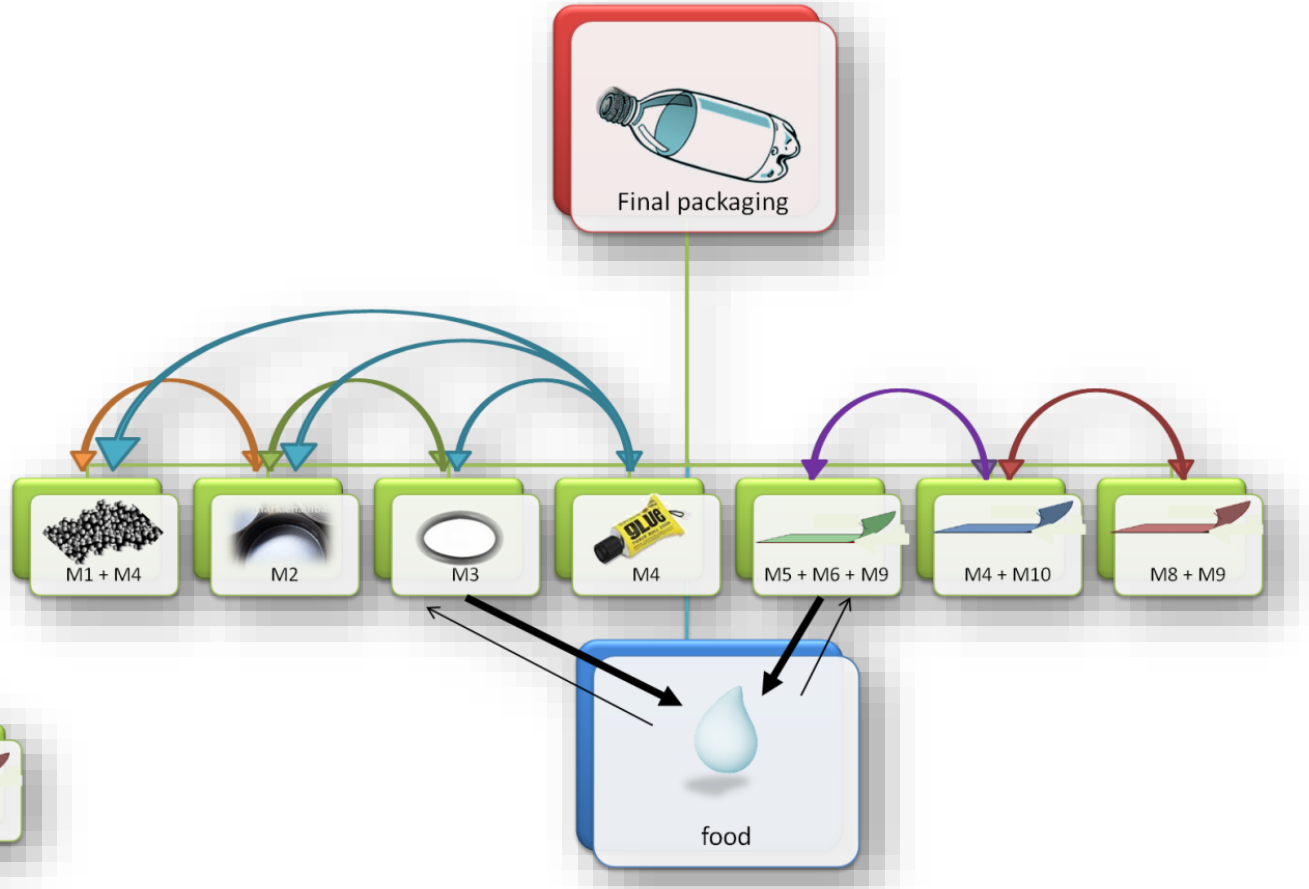


Contradictions and risk scale

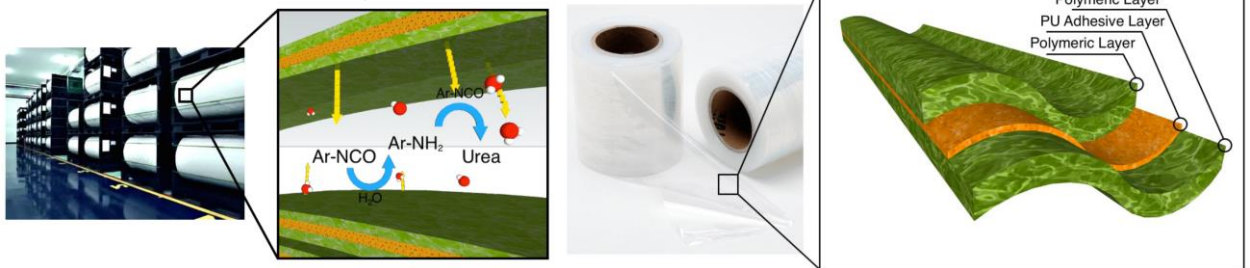
Risk management requires the full cooperation of the supply chain

How to establish the responsibility of stakeholders?

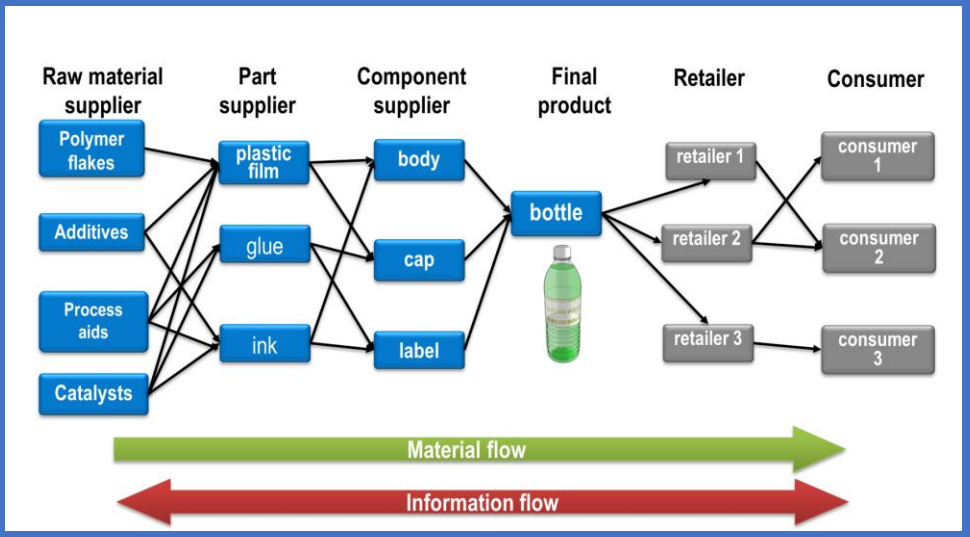


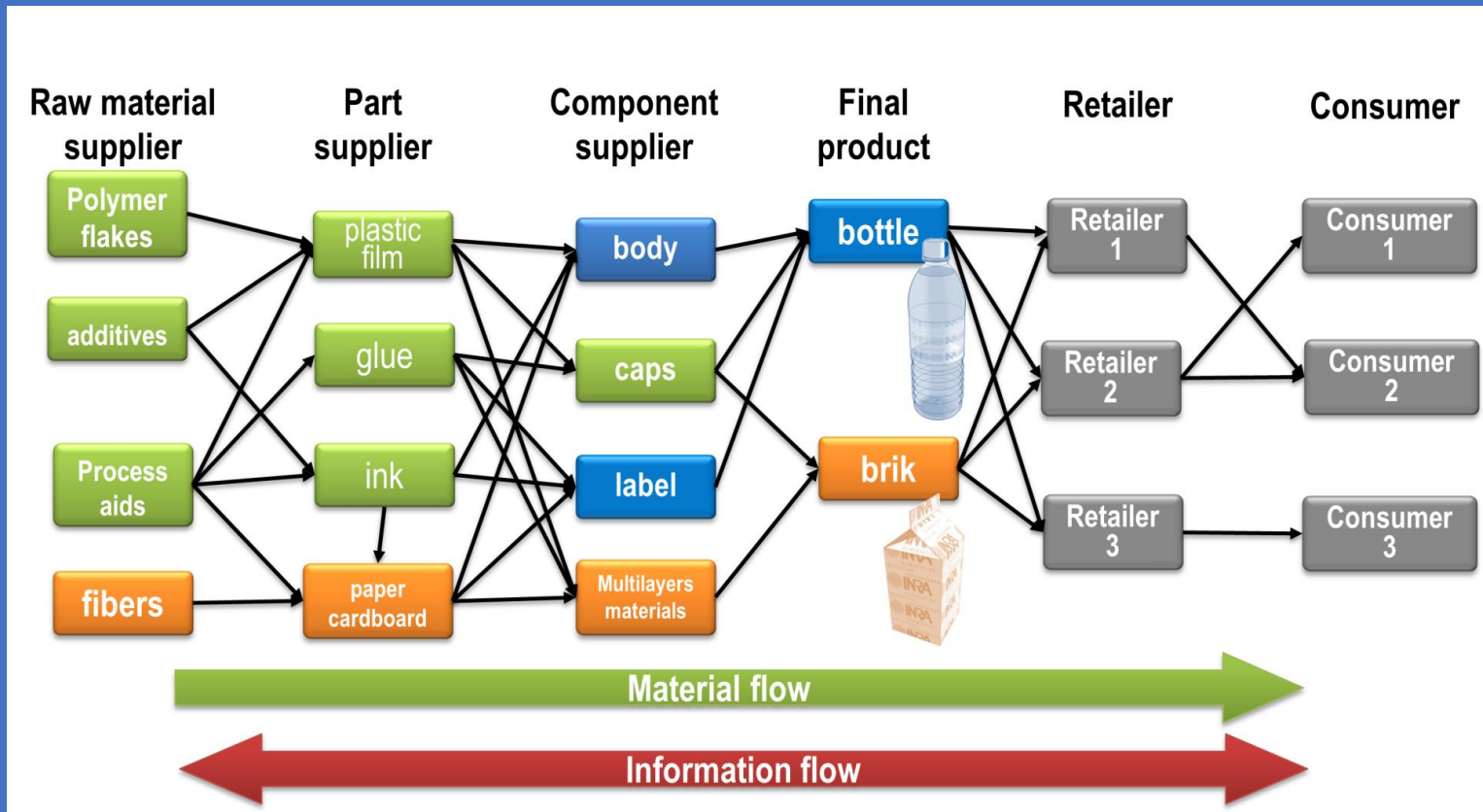


Most of the packaging systems are composite



Developing the cooperation along the supply chain



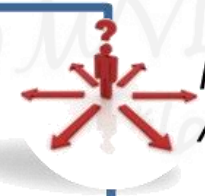


Preventive approaches

From preventive approaching to integrated engineering

Safety concepts

Current Approaches



Future Approaches

Low Migration

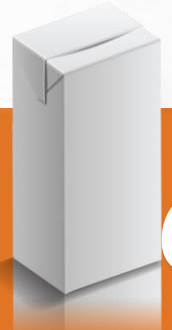
Low Toxicity

Low Consumer Exposure

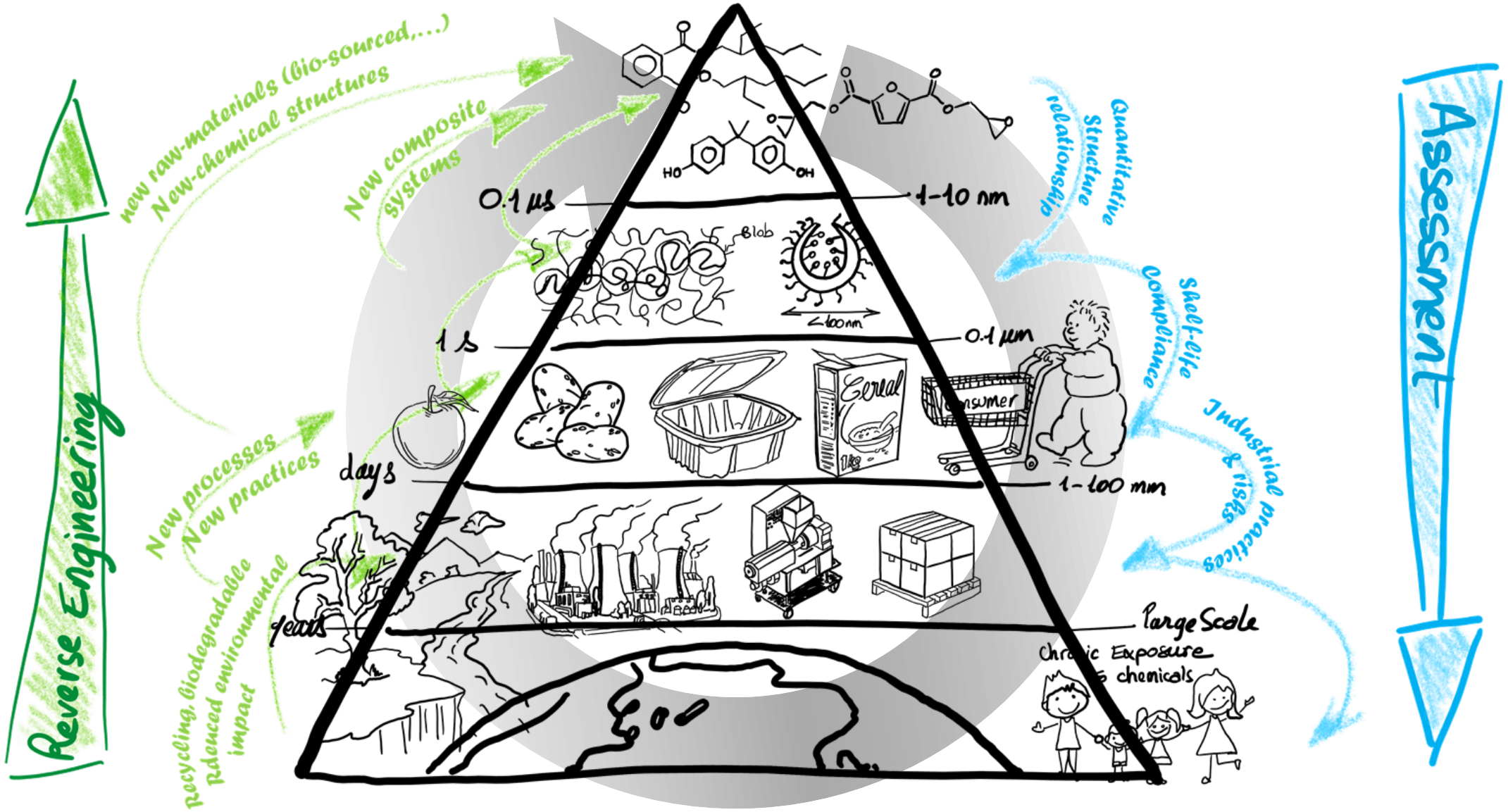
Safe-by-Design

+VOLUNTARY APPROACHES & LOCAL ORDINANCES

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

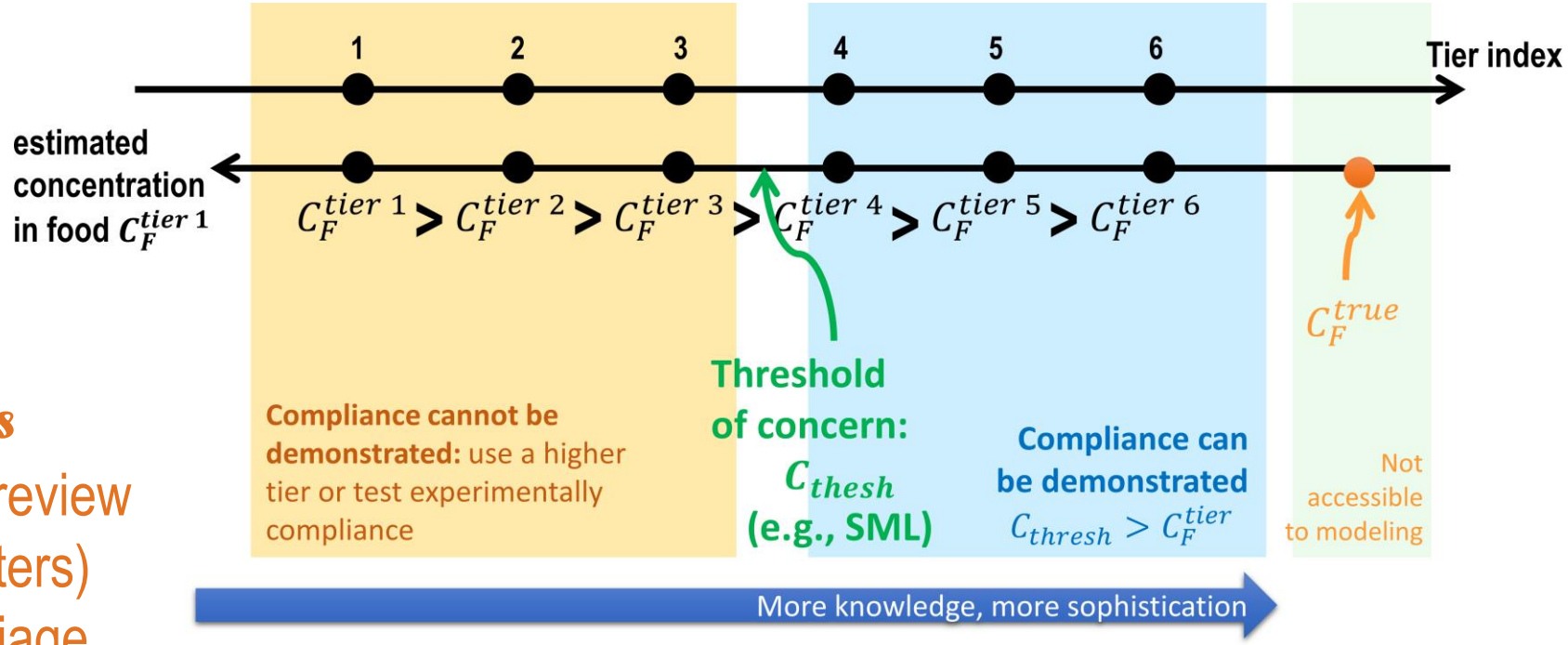


Our recommendations



Linked decisions with complex ramifications at various scales

Modeling across the scales the next frontier for supporting public and industrial decisions



Tier modeling

- ***"Mandatory" in public models*** with legal and safety issues for review (help to identify influent parameters)
- Can be used for prioritization, triage and future refinements
- ***Good practices*** exist in EU and US for risk assessment
- ***Approved for compliance testing*** in EU, US and China

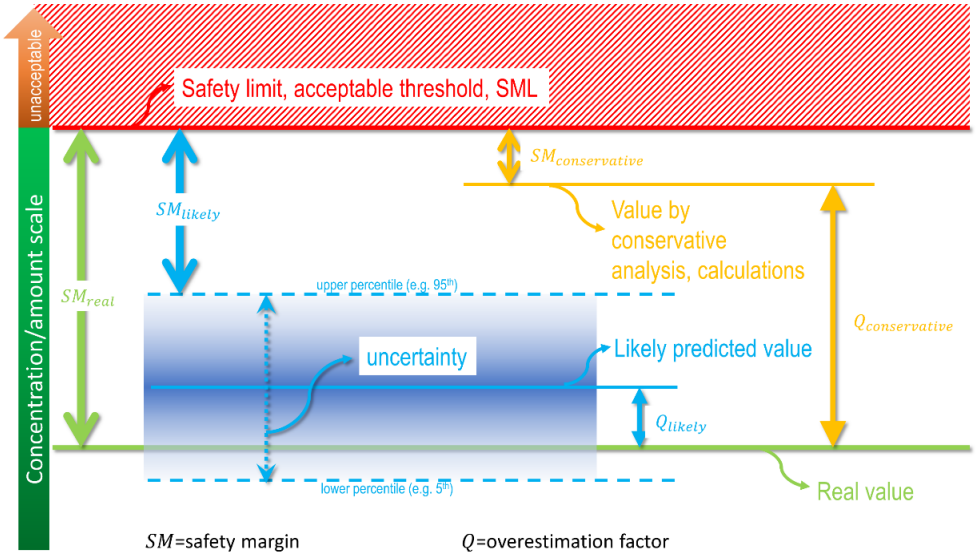
E. J. Hoekstra, R. Brandsch, C. Dequatre, P. Mercea, M.-R. Milana, A. Störmer, X. Trier, O. Vitrac, A. Schäfer and C. Simoneau, in: E. Hoekstra (Ed.): JRC Scientific and technical Reports EUR 27529 EN, European Commission, Ispra (Italy), **2015**.

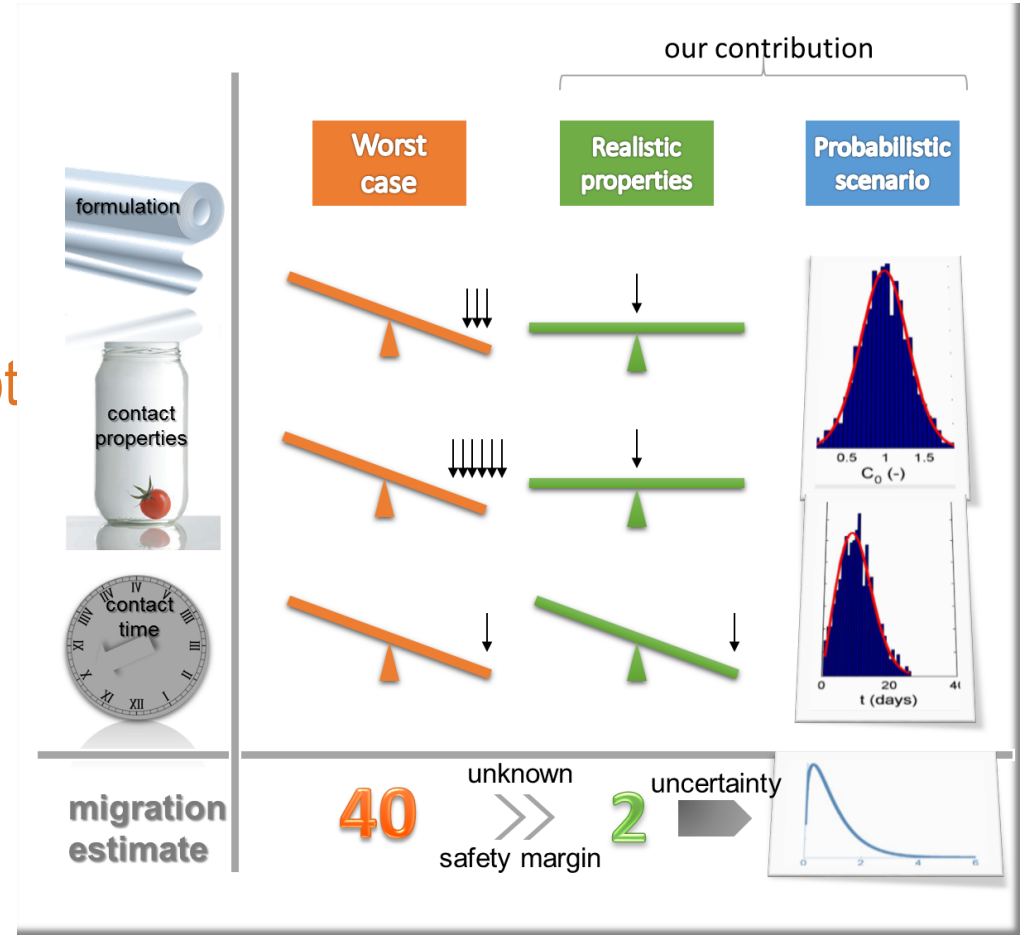
INRA SCIENCE & IMPACT

Progressive enrichment instead of brute force

Uncertainty vs ignorance

- "*scientia*" (science) vs "*opinio*" (belief)
- Conventional modeling assumes complete knowledge and epistemologic transformation of information into knowledge.
- How to code "vagueness", "skeptism", "error", "doubt





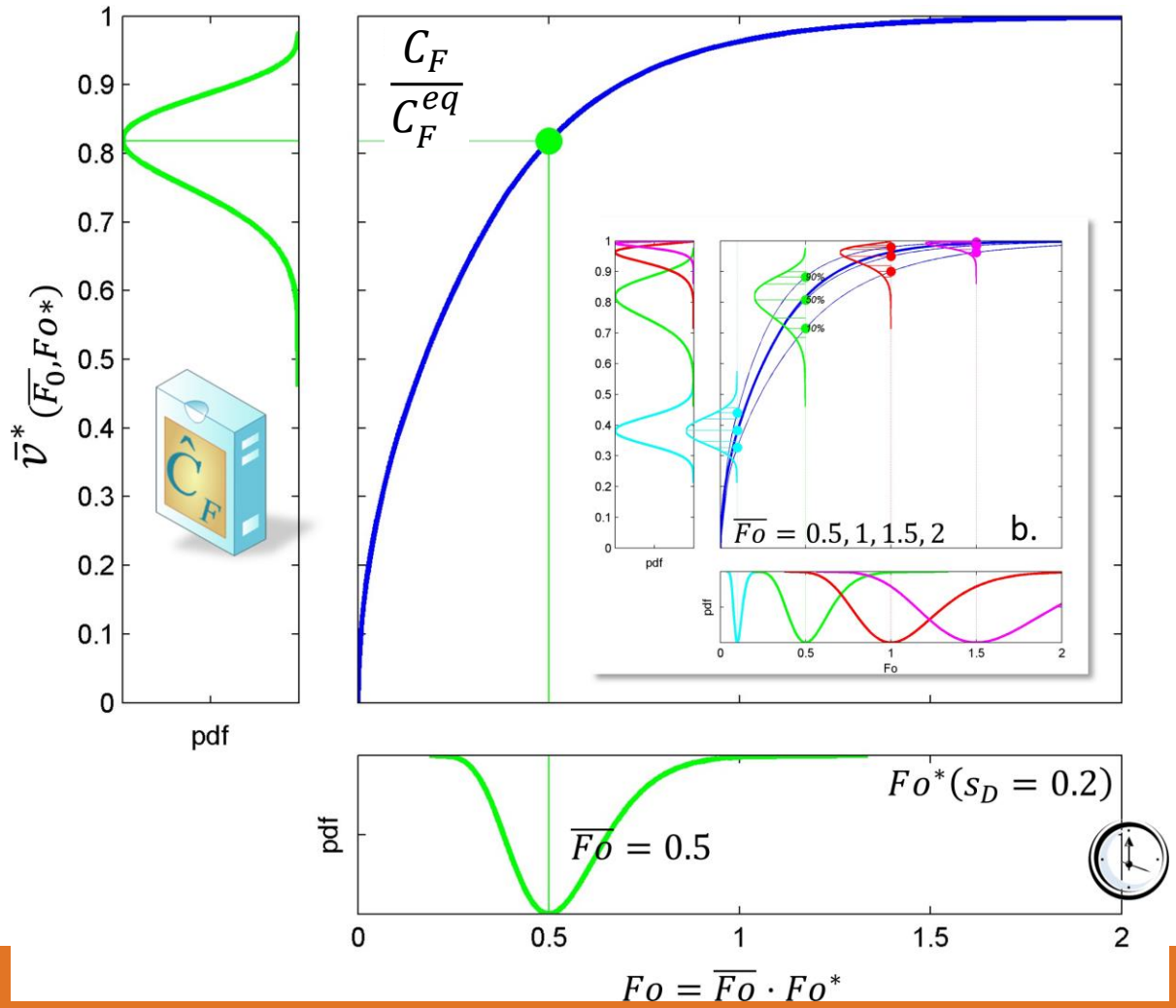
Y. Zhu, P.-M. Nguyen and O. Vitrac in: G. Robertson (Ed.); Elsevier Food Science Reference Module, Elsevier, Amsterdam, NL, 2019, pp. 64

Probabilistic modeling

- Part of best practices
- "Mandatory" for risk assessment
- Uncertainty ≠ variability, it can be reduced by additional knowledge or model details.
- Monte-Carlo sampling can be avoided in several situations to reach almost real time simulation.

$$f_{\bar{v}^*}(v) = \sum_{k=1}^{p} f_{Fo}\left(\bar{v}^{*-1}\big|_{Fo\in Y_k}(v)\right)\left|\frac{d}{dv}\bar{v}^{*-1}\big|_{Fo\in Y_k}(v)\right|^{-1}$$

E.g., monotonic model



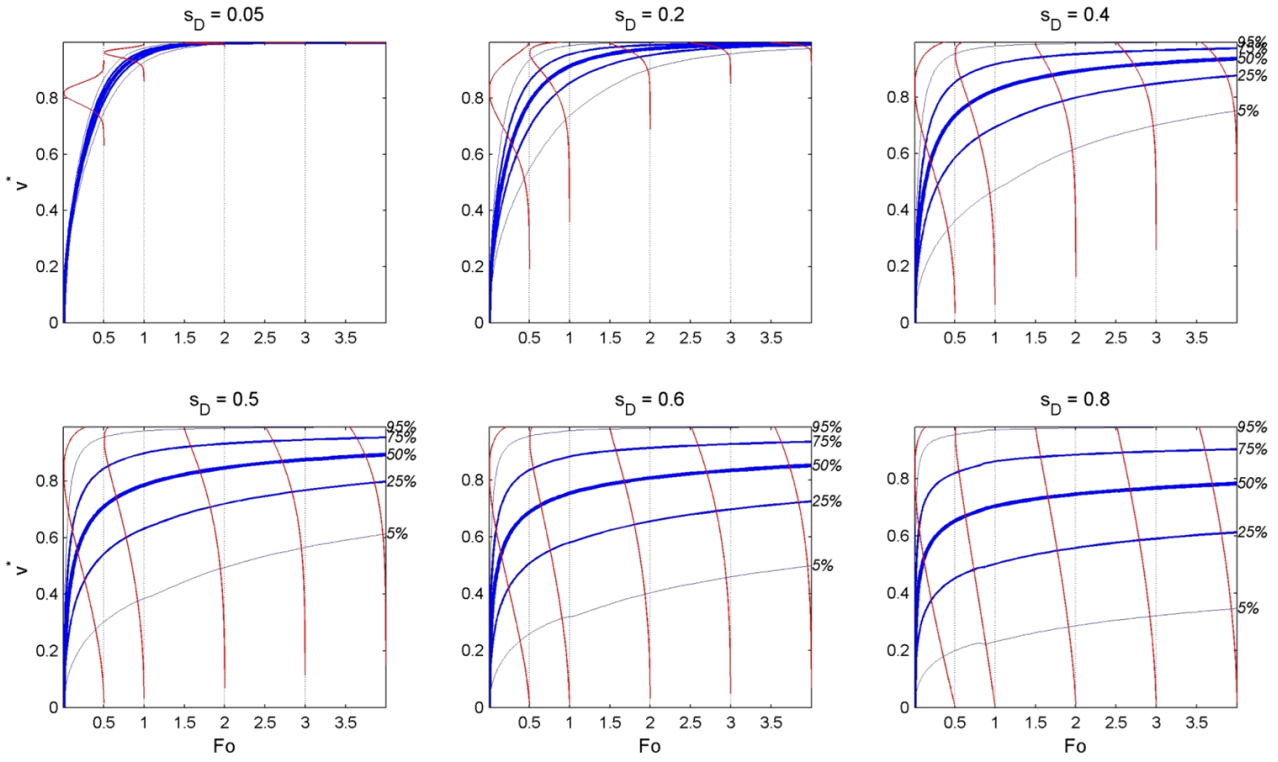
O. Vitrac and M. Hayert, *Aiche Journal* **2005, 51, 1080-1095.**
O. Vitrac, B. Challe, J.-C. Leblanc and A. Feigenbaum, *Food Additives and Contaminants t* **2007, 24, 75-94.**

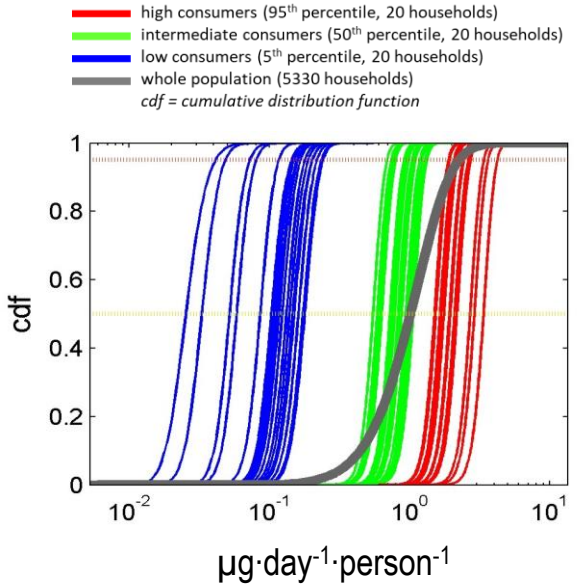
$$p_{\underset{product\ scale}{r}}\ C \le x\ = f\begin{pmatrix}\text{food, packaging, migrants}\\ \text{storage cond., uncertainty}\end{pmatrix}$$

$$p_{\underset{household\ scale}{r}}\ E \le y\ = g\begin{pmatrix}\text{food products, packaging materials, migrants}\\ \text{storage conds., uncertainty}\\ \text{consumption scenarios}\end{pmatrix}$$

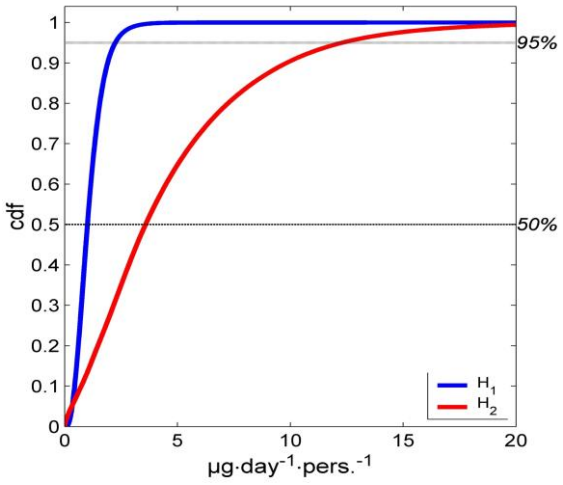
$$E_k = \frac{c_0 \cdot \overline{v}^*_\infty}{365 \cdot P_k} \cdot \sum_{i=1}^{N_k} \overline{v}^*_i \quad Fo_i, Bi, K, L$$

6122 Households
221,190 Purchases
1,930,257 Purchased units





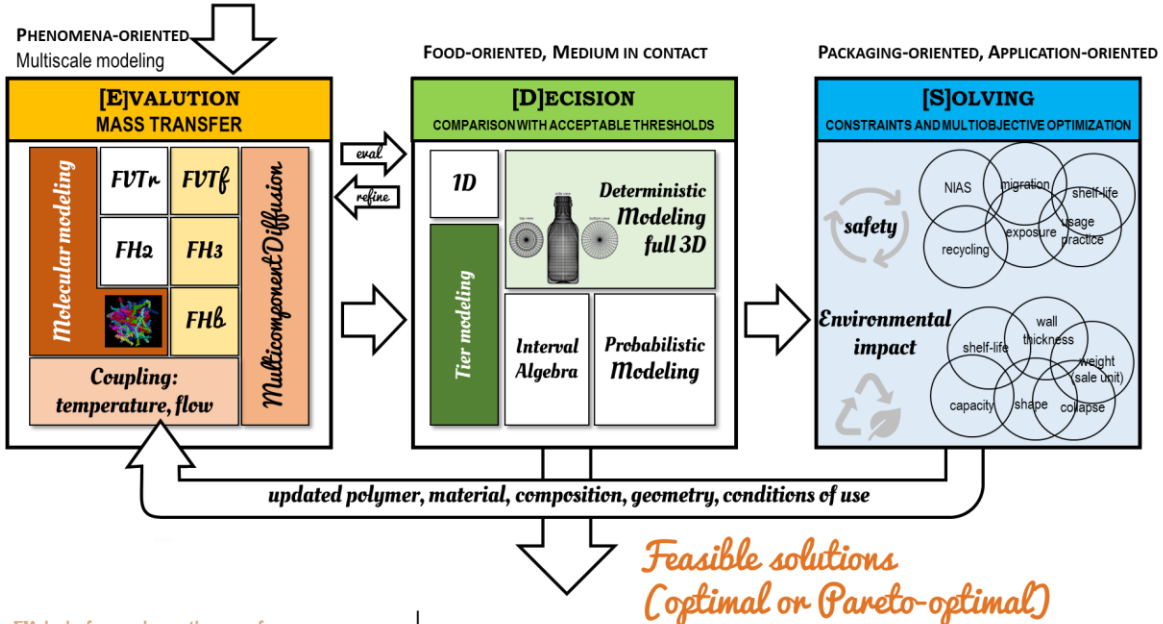
2 physico-chemical scenarios



O. Vitrac and J.-C. Leblanc, *Food Additives and Contaminants Part a-Chemistry Analysis Control Exposure & Risk Assessment* ***2007, 24, 194-215.***

premises
Market demand, new food products
New regulations (*e.g.*, ban of materials or substances)
Life cycle analysis considerations
First solution from known problem-solving tools (TRIZ, Six Sigma approach, etc.)
Diagnostic from root cause analysis, seek of preventive actions

Our research **Computer-aided drafting**



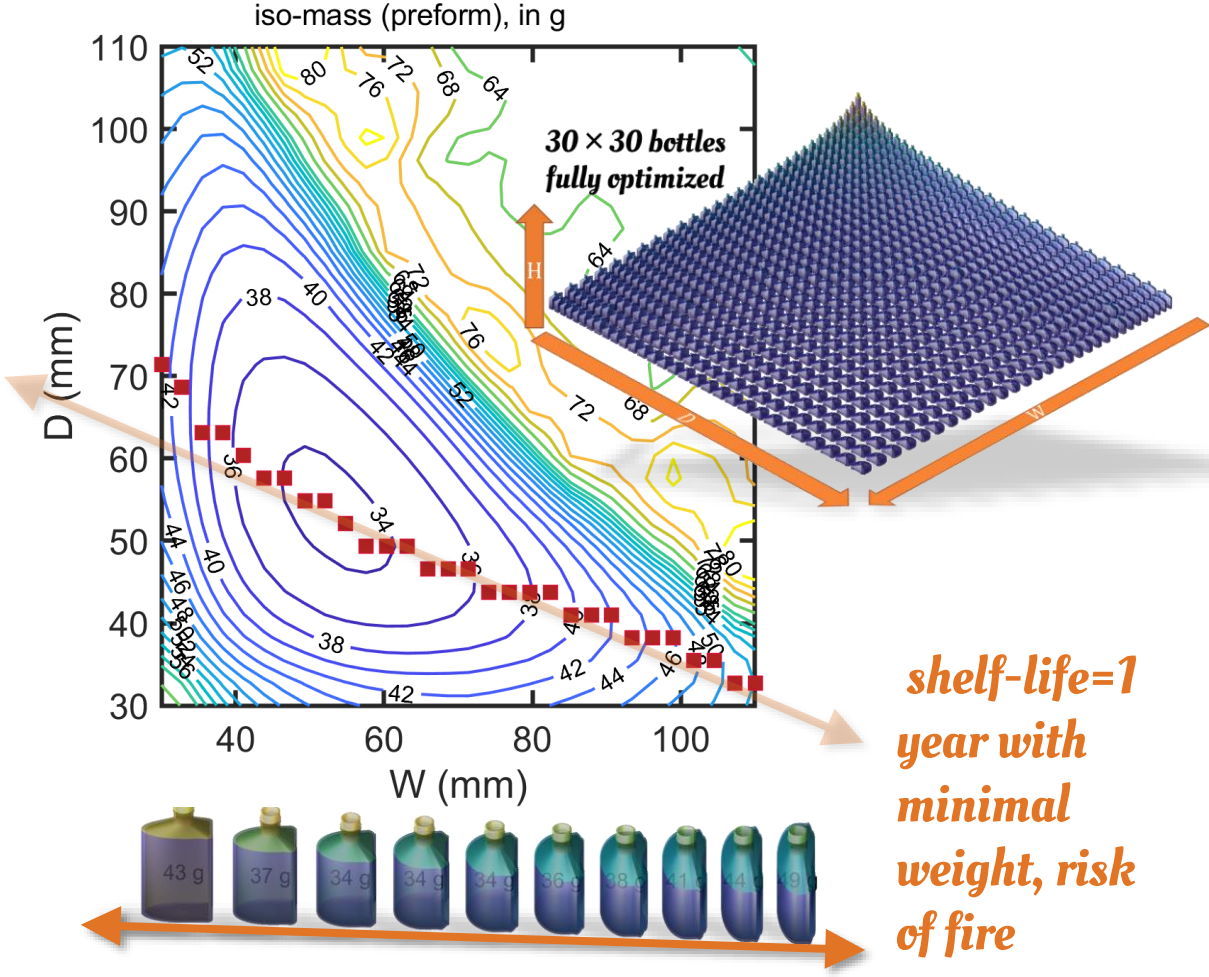
Feasible solutions
(optimal or Pareto-optimal)

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

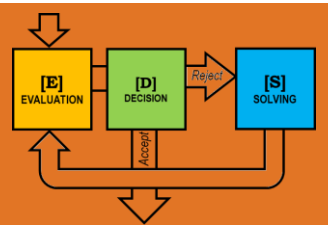
FH: Flory Huggins approximation of chemical affinities and temperature effects
(*2*=binary and *3*=ternary mixturres, *b*= formulation for block polymers)

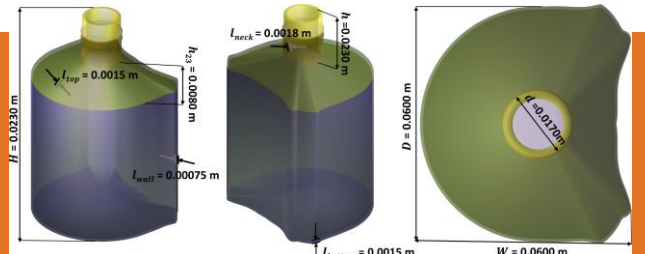
Our research **Rapid prototyping**

applications
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



shelf-life=1 year with minimal weight, risk of fire

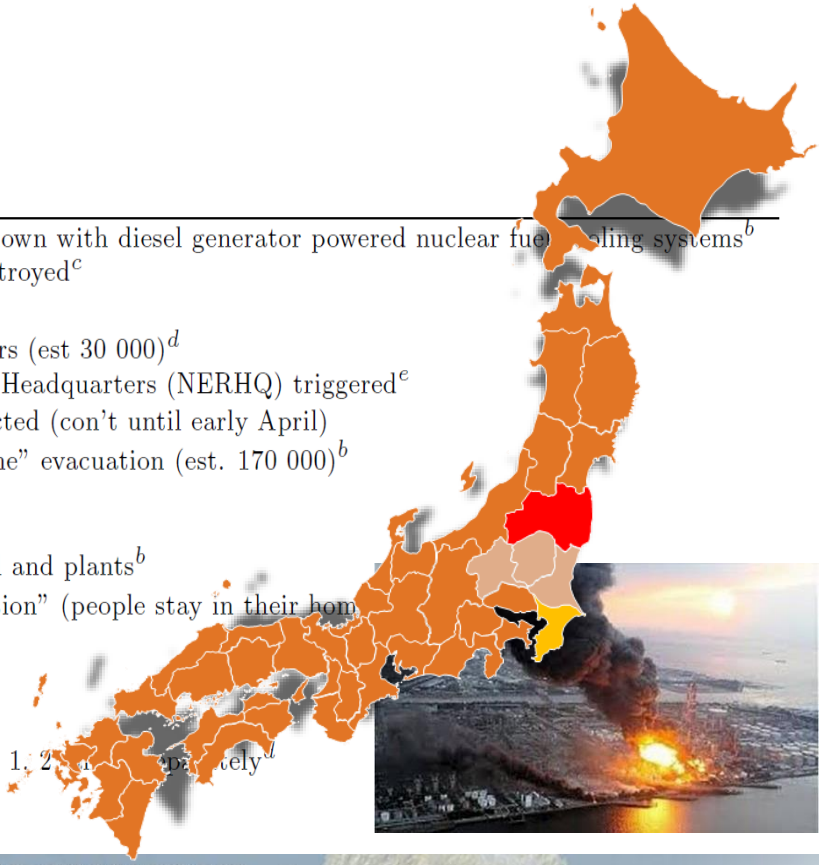




Packaging design

Minatures PET bottles for alcoholic beverages served in planes

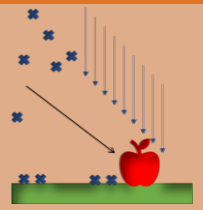
Day (2011)	Event	INES[a]	Results
March 11	Earthquake		All operating reactors at FNPP begin emergency shutdown with diesel generator powered nuclear fue ling systems[b]
	Tsunami		Four of the six reactors damaged, diesel generators destroyed[c]
			Evacuation of 3 km radius surrounding FNPP[d]
	d+1: Airborne contamination		Unevacuated residents within 10 km told to stay indoors (est 30 000)[d]
			Emergency declared and Nuclear Emergency Response Headquarters (NERHQ) triggered[e]
March 12	Airborne sampling begins		Significant radionuclide release of ^{137}Cs and ^{131}I detected (con't until early April)
			20 km radius around PP "stay-away" or "restricted zone" evacuation (est. 170 000)[b]
		4	"Accident with Local Consequences" applied to Unit 1
March 15	Contamination NW of FNPP	4	significant deposition due to precipitation[g]
	Environmental sampling begins	4	^{137}Cs and ^{131}I detected in significant quantities in soil and plants[b]
	d+4: evacuation ≤ 20 km	4	Arc from 20 to 30 km away designated "indoor evacuation" (people stay in their hom
		4	Evacuation of 20 km zone completed (185 000)[d]
March 16	Monitoring of food begins[b]	4	
March 17	Provisional regulation values (PRV)[h] set	4	
March 18		5	"Accident with Wider Consequences" applied for Units 1, 2 ately[d]
	d+10: contamination 200 km S	3	"Serious Incident" applied for Unit 4[d]
March 21	Contamination 200 km south of FNPP[g]	5,3	
	First restrictions on food items[b]	5,3	11 days after initial accident
April 12		7	"Major Accident" for Units 1, 2, and 3 c
June 16	Evacuation updated	7	Spots of "evacuation recommended" base
July 17	"Stable cooling" of reactors established[b]	7	
Dec 16	"Cold shutdown" of all reactors[b]	7	

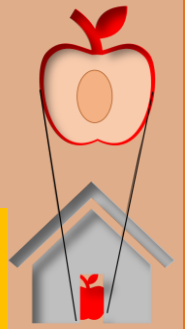


Nov 2017: end of export restrictions to EU

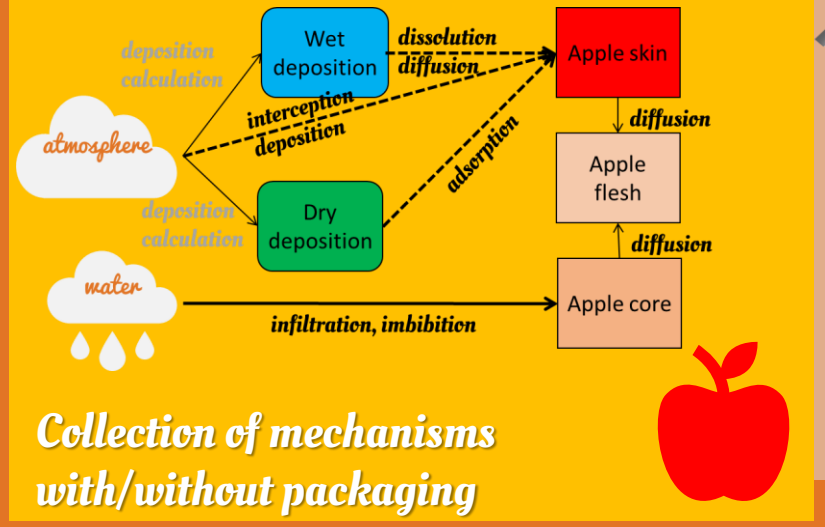
INRA SCIENCE & IMPACT

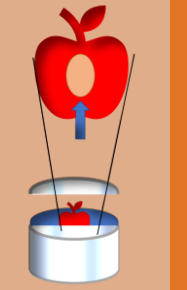
Scenarios of food exposure accounting for storage and packaging conditions





Apple plugin

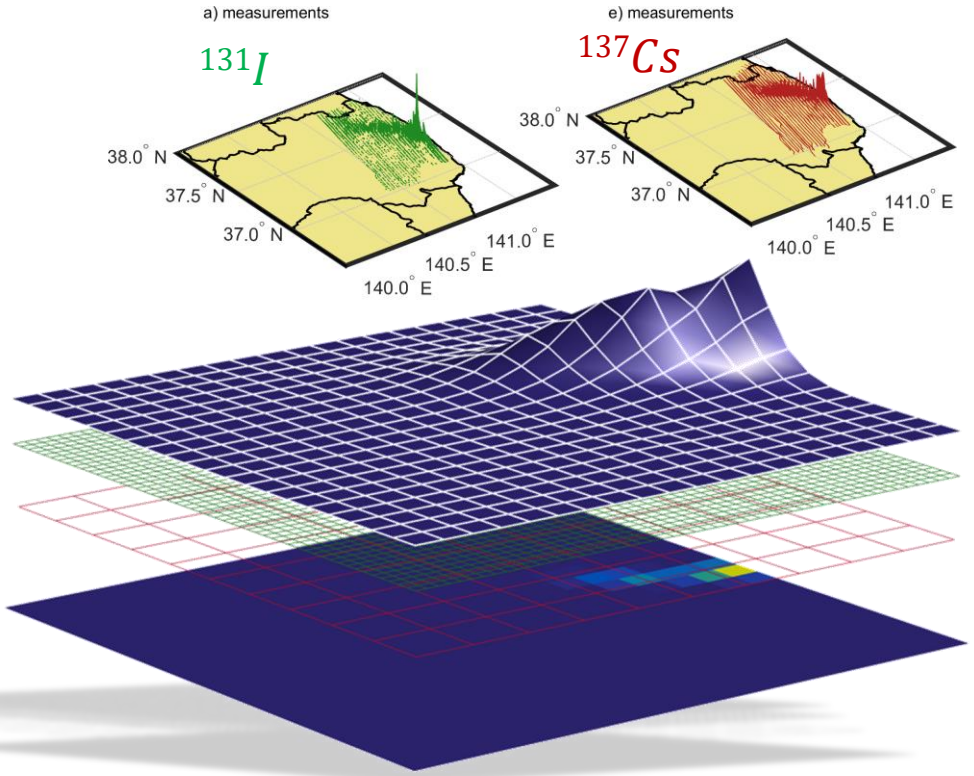




^{131}I
^{90}Sr
^{137}Cs

Collection of mechanisms with/without packaging

Relatively volatile radionuclide can contaminate large areas

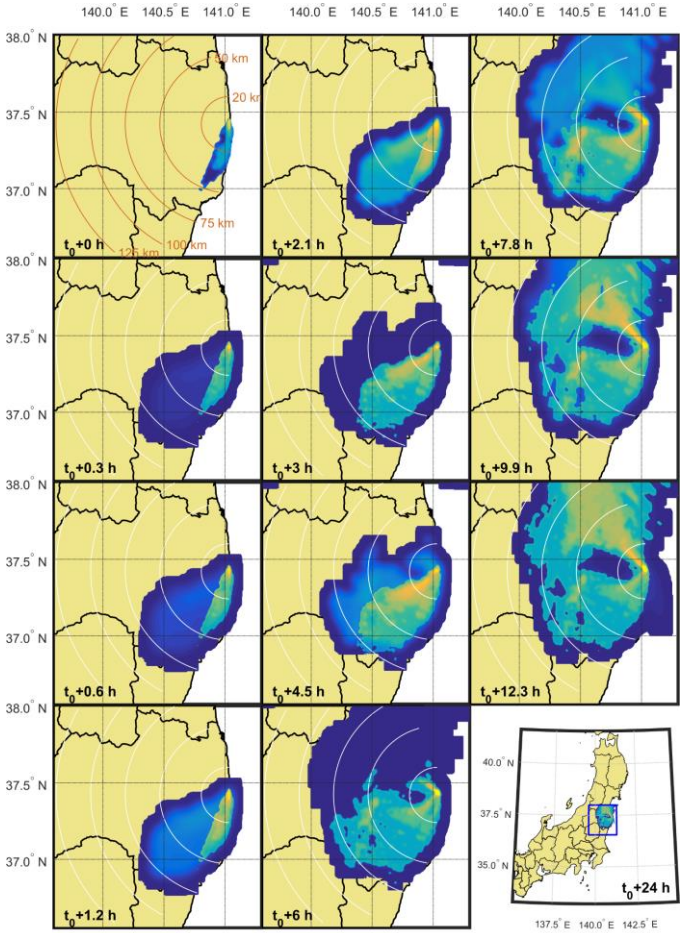


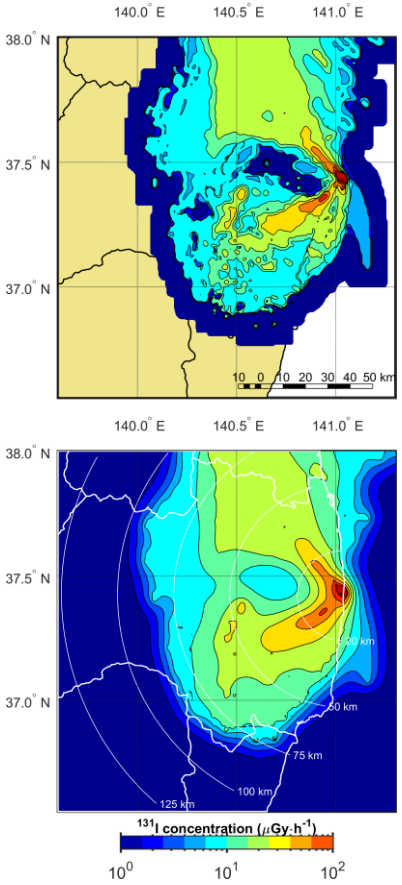
Combining multiple information with different resolutions and obtained on different periods

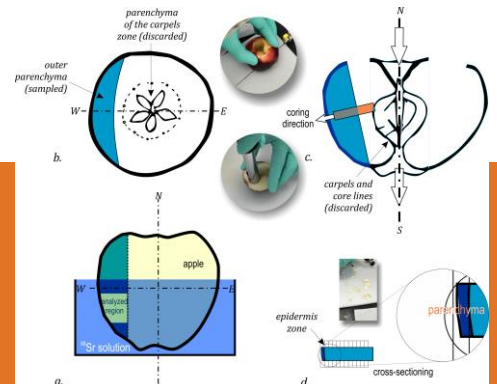
- Meteorological data
- Dispersion data (measured, simulated)

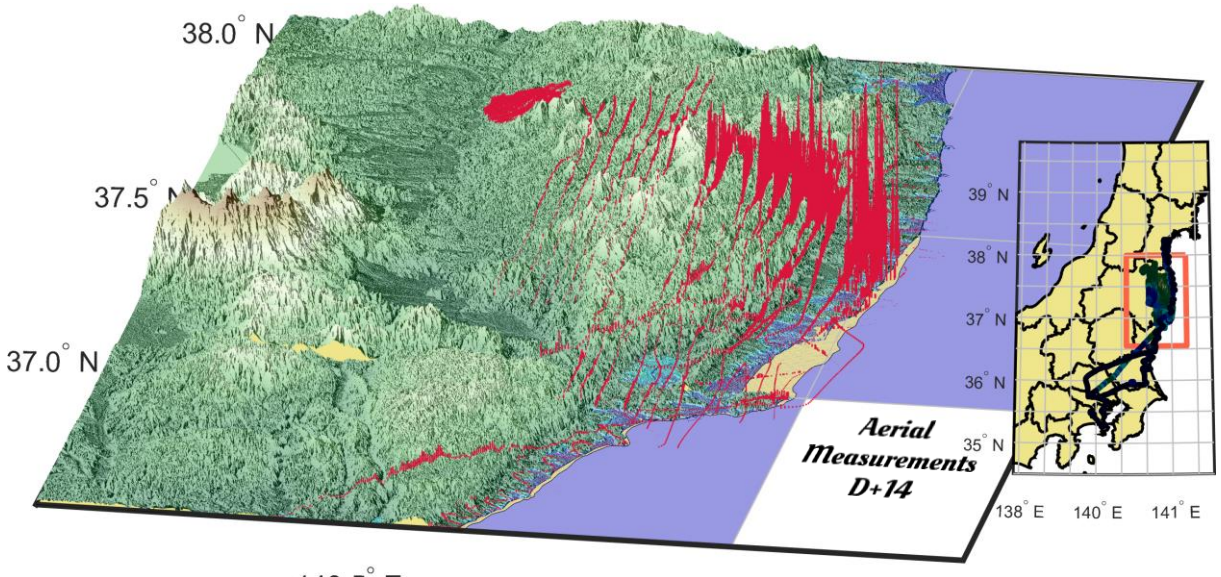
Collaborations
FDA (WEAC, Boston, MA,USA)
IRSN (Fontenay-les-Roses, France)

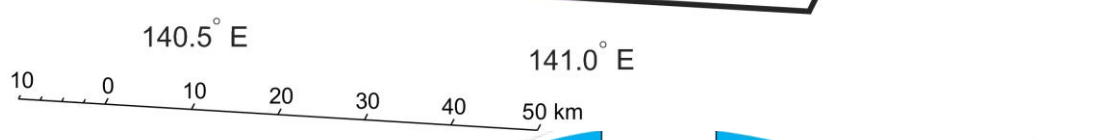
Contamination of food products after a nuclear disaster

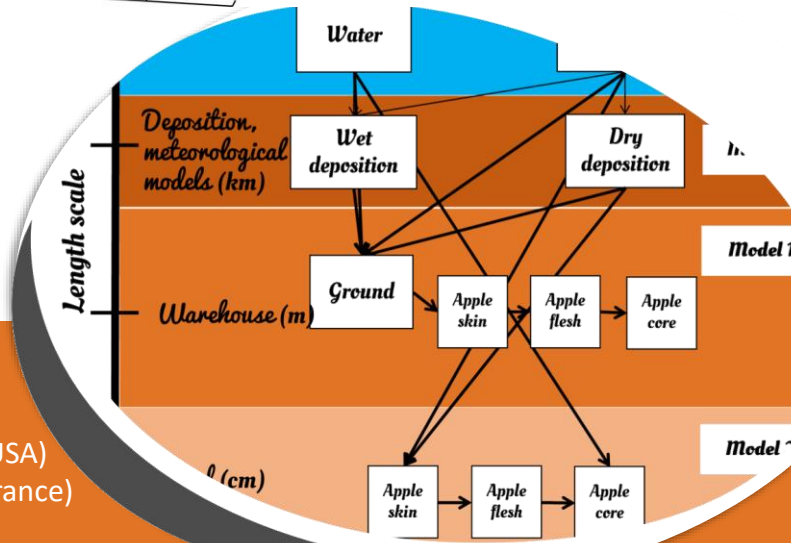






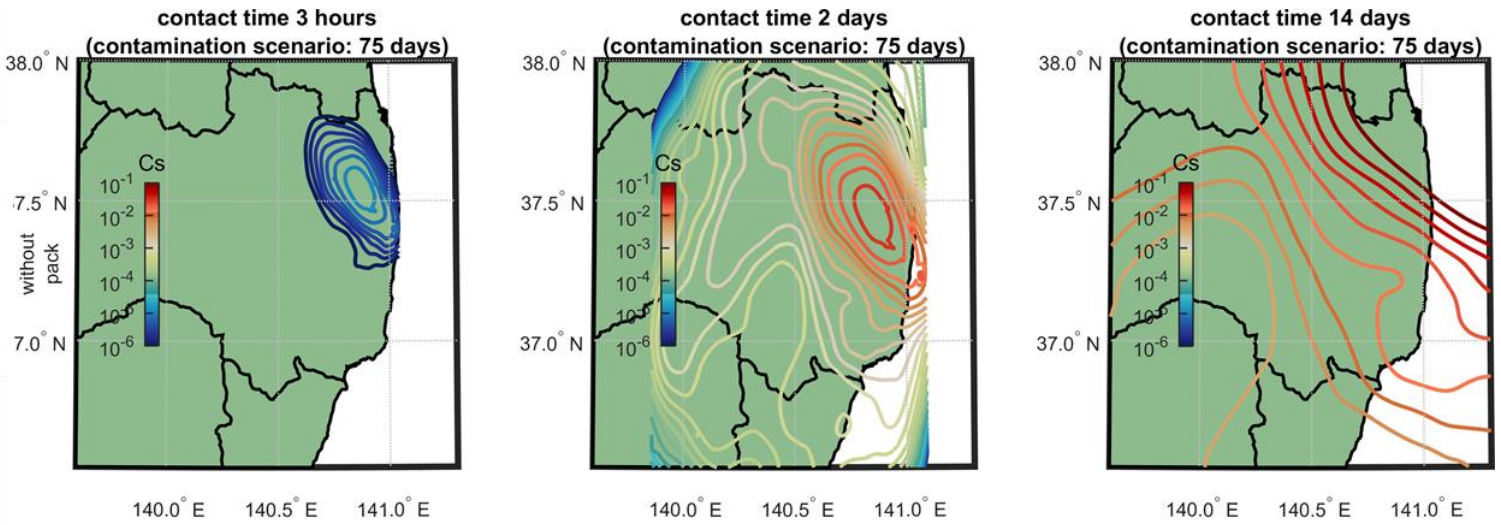


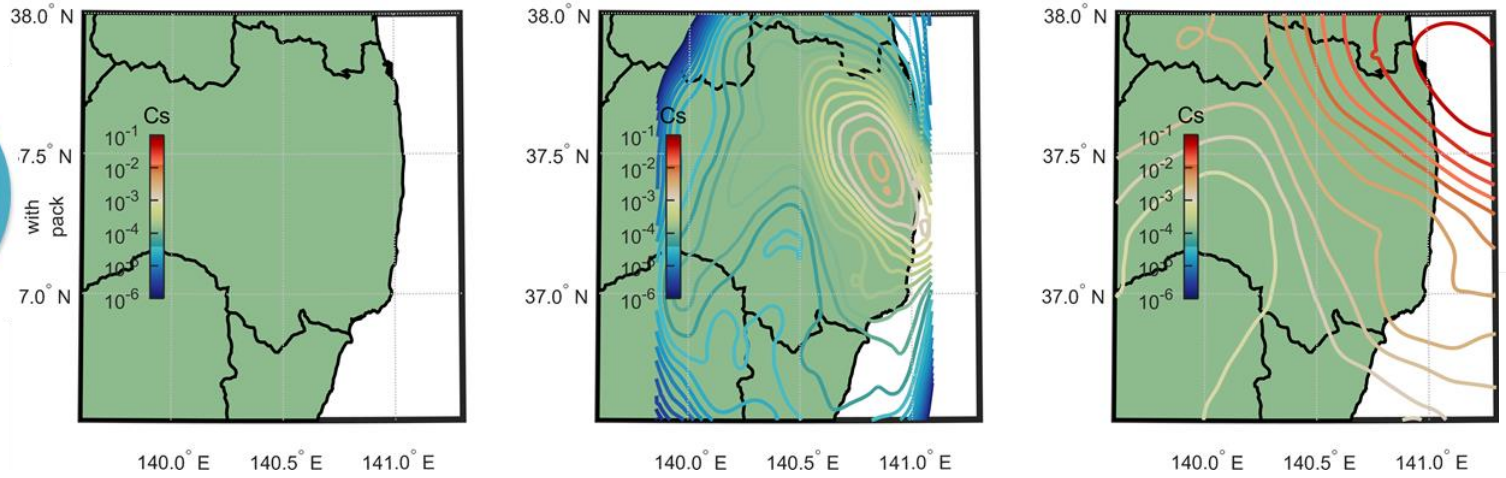




Collaborations

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

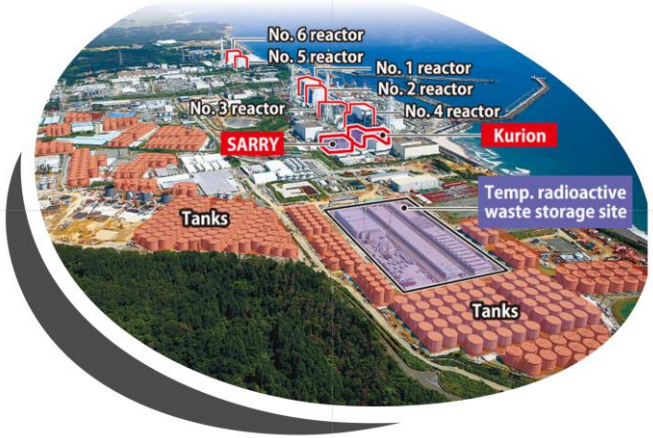




A tool for first responders

- *triage*
- *orienting future tests*

The Fukushima plant today



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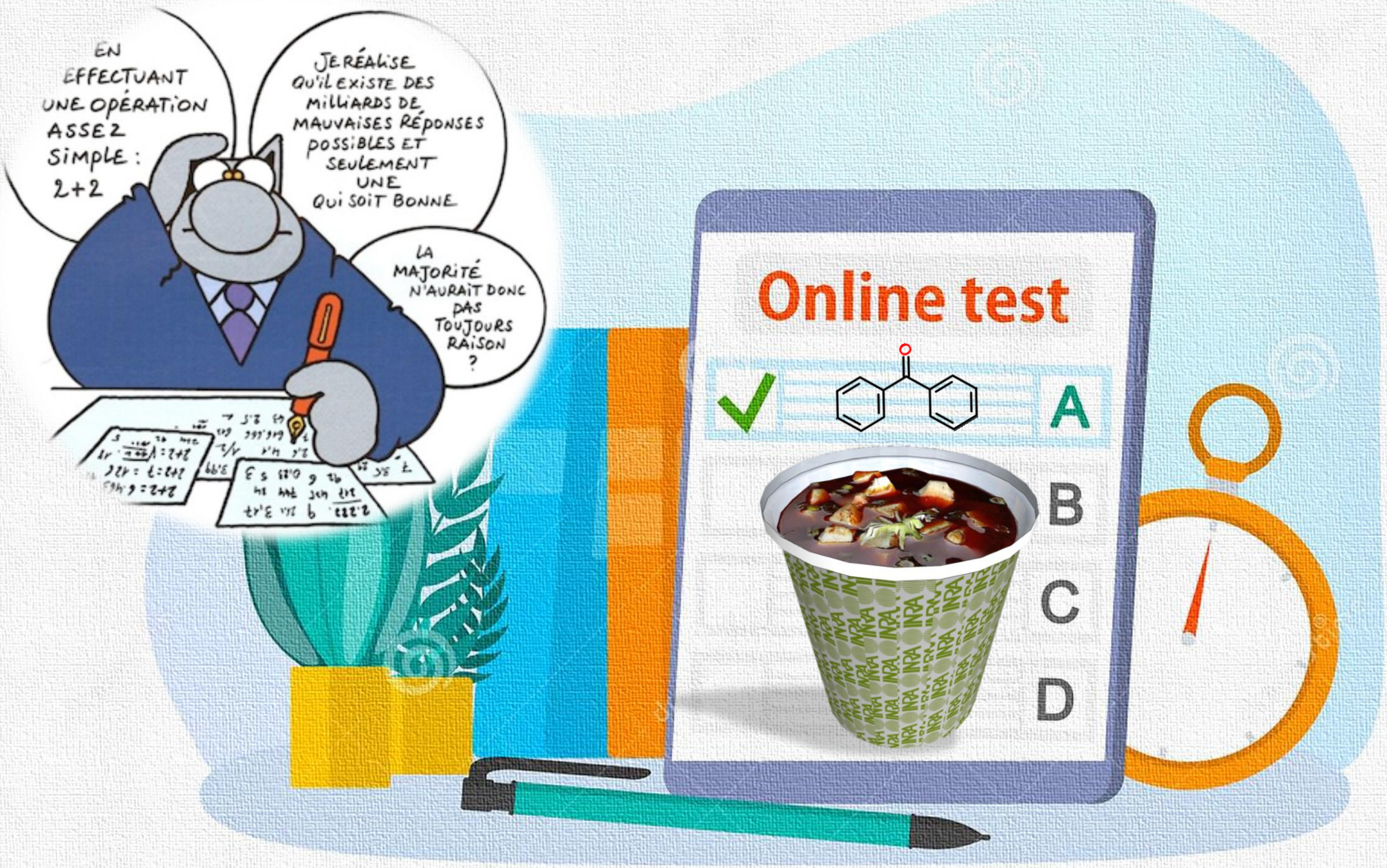
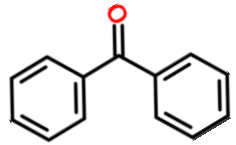
Work in progress wit IRSN

"real-time" dispersion model (1.1 km, 1 hour)

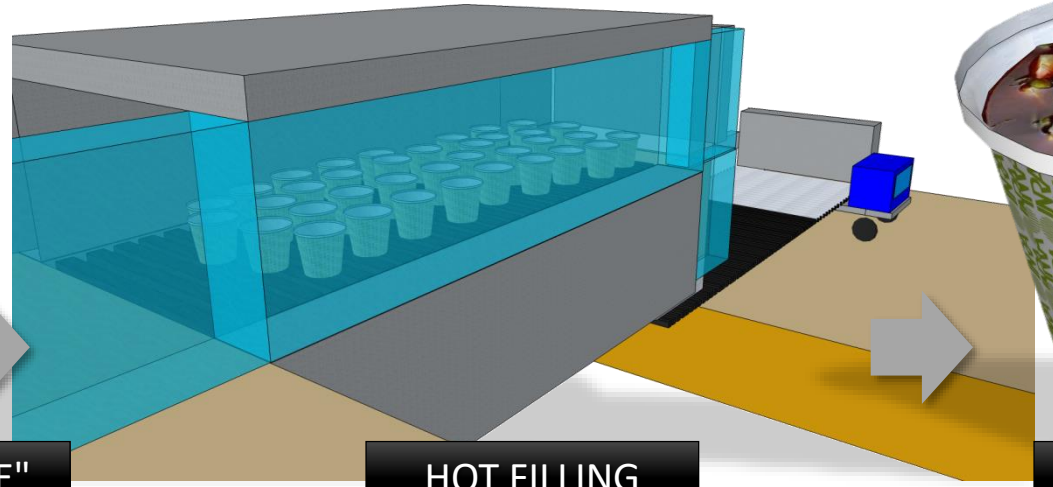

EN EFFECTUANT UNE OPÉRATION ASSEZ SIMPLE : 2+2
JE RÉALISE QU'IL EXISTE DES MILLIARDS DE MAUVAISES RÉPONSES POSSIBLES ET SEULEMENT UNE QUI SOIT BONNE
LA MAJORITÉ N'AURAIT DONC PAS TOUJOURS RAISON ?
Online test
A
B
C
D
INRA

CHAINED STEPS: where is the critical step?

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

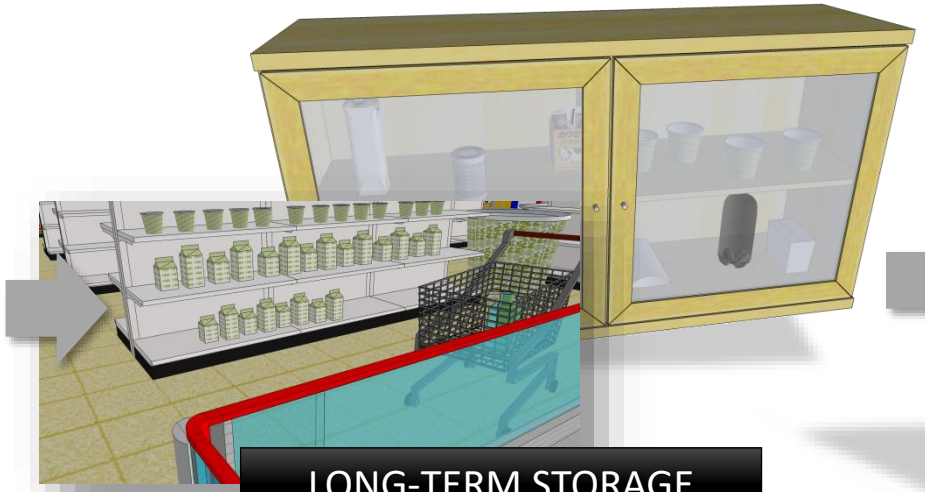


STORAGE "BEFORE USE"



HOT FILLING

FATTY CONTACT

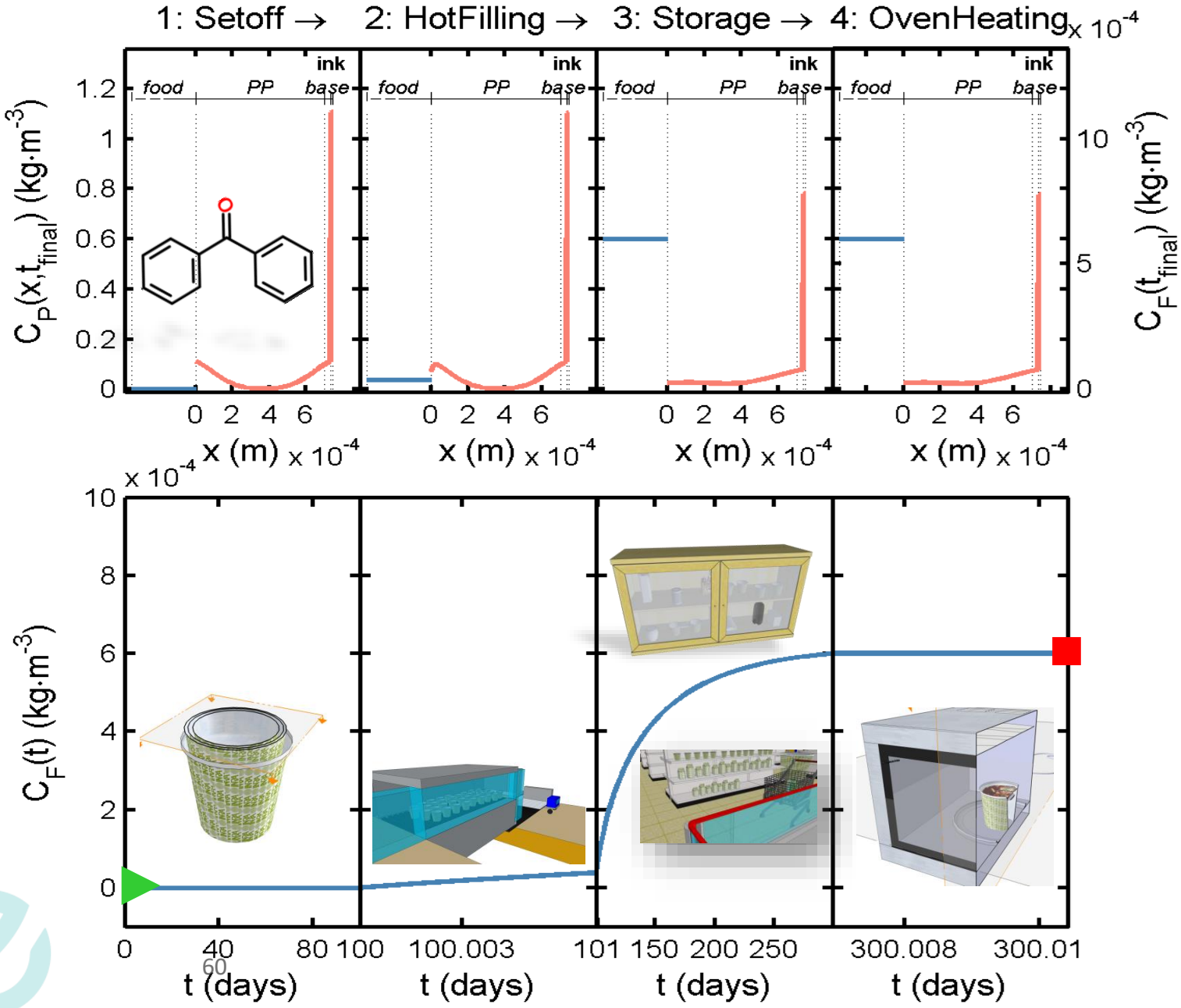


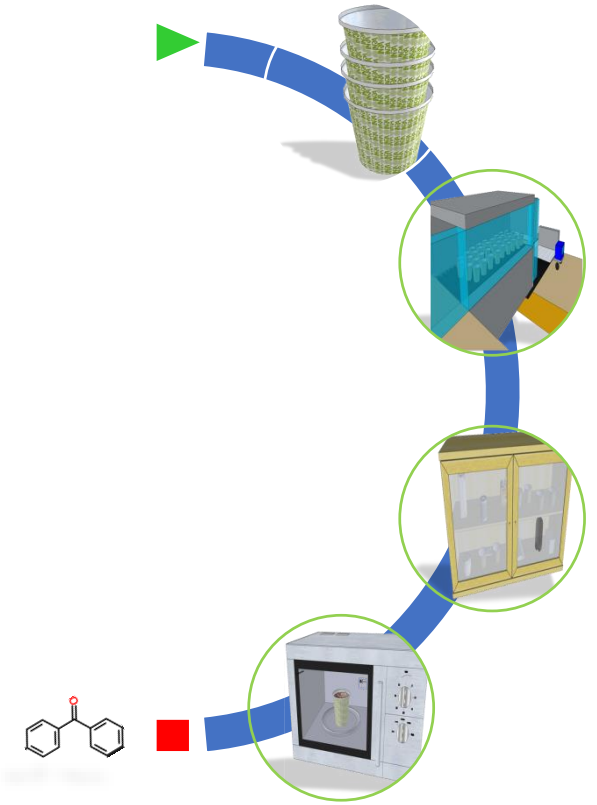
LONG-TERM STORAGE

MICROWAVE OVEN HEATING

CHAINED STEPS

UV-curing printing ink

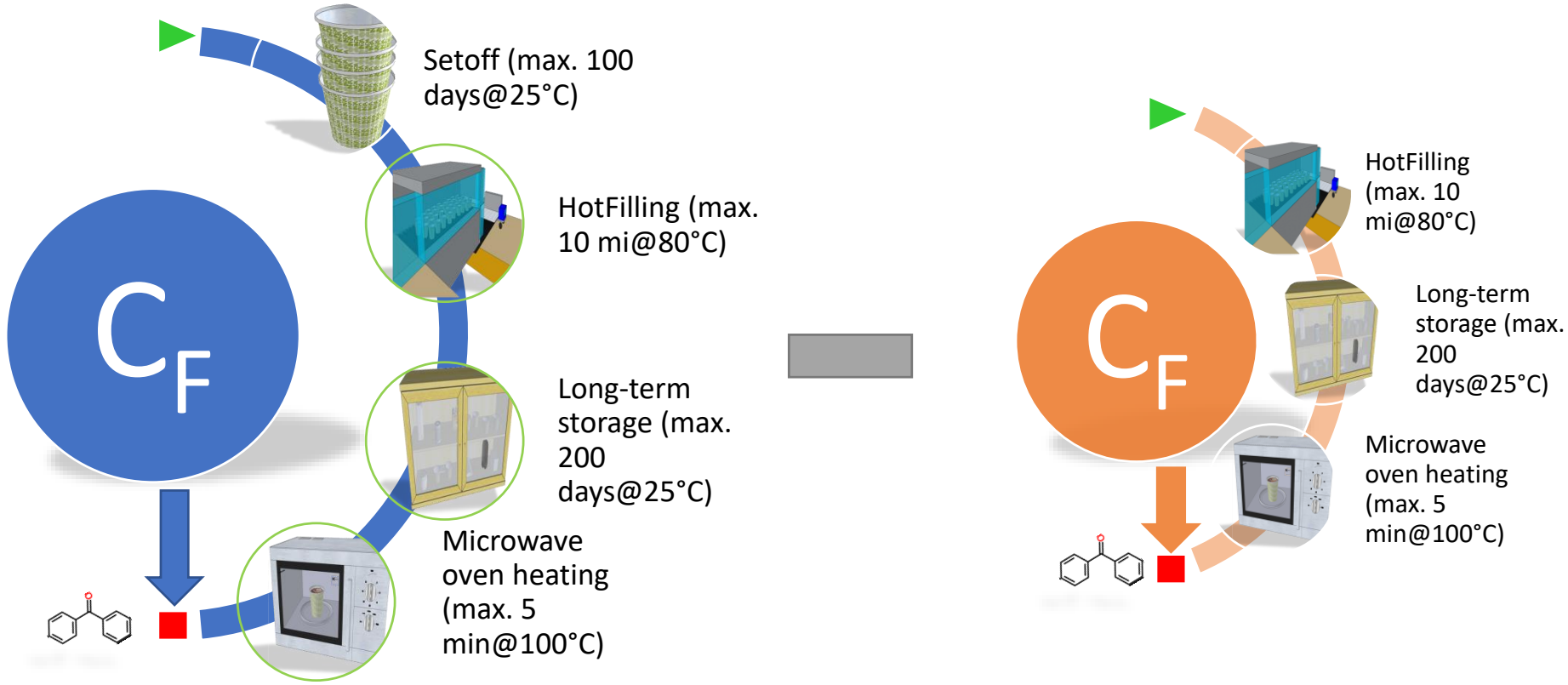




ASSESSING THE SEVERITY OF A SINGLE STEP

CASE OF "SETOFF" STEP

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



comparison with step i alone

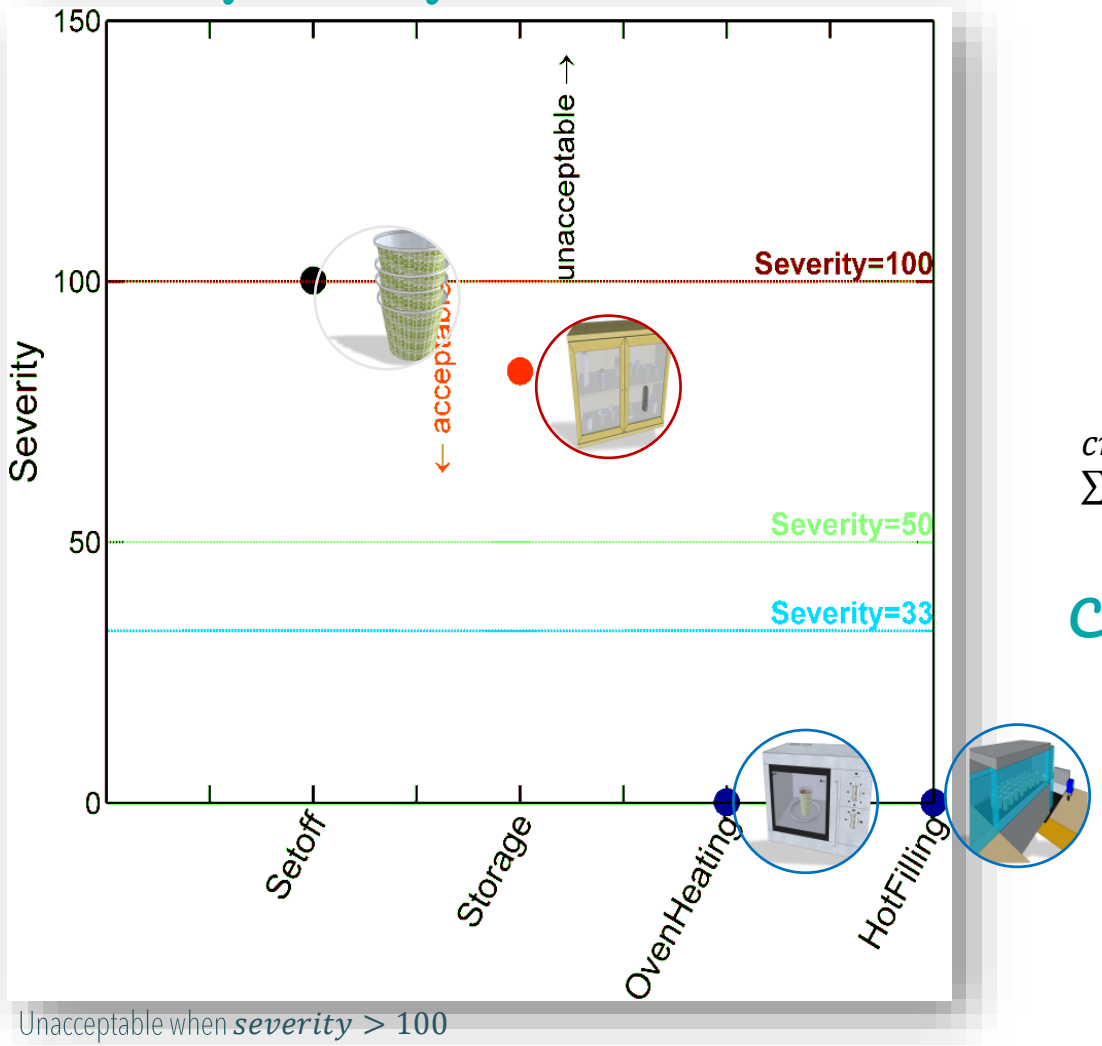
$$\text{Severity}\left(\hat{C}_F(step\,i)\right) = f\left(\max\left(C_{F_M}|_{1\to2\to\cdots\to M} - C_{F_M}|_{1\to2\to\cdots\to M/i}, C_{F_i}|_i\right)\right)$$

comparison with step i removed

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

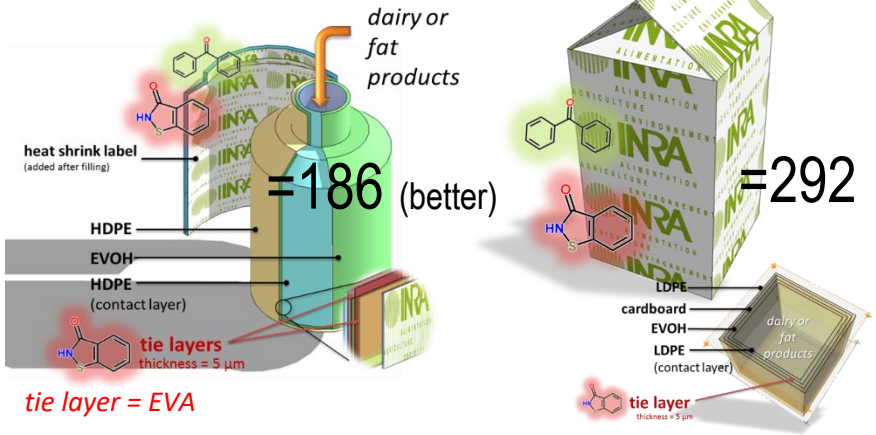
$$severity = 100 \times \frac{C_F}{SML}$$

Critical step (severity scale)



Unacceptable when $severity > 100$

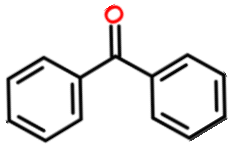
Concurrent design (criticality scale)



tie layer = EVA

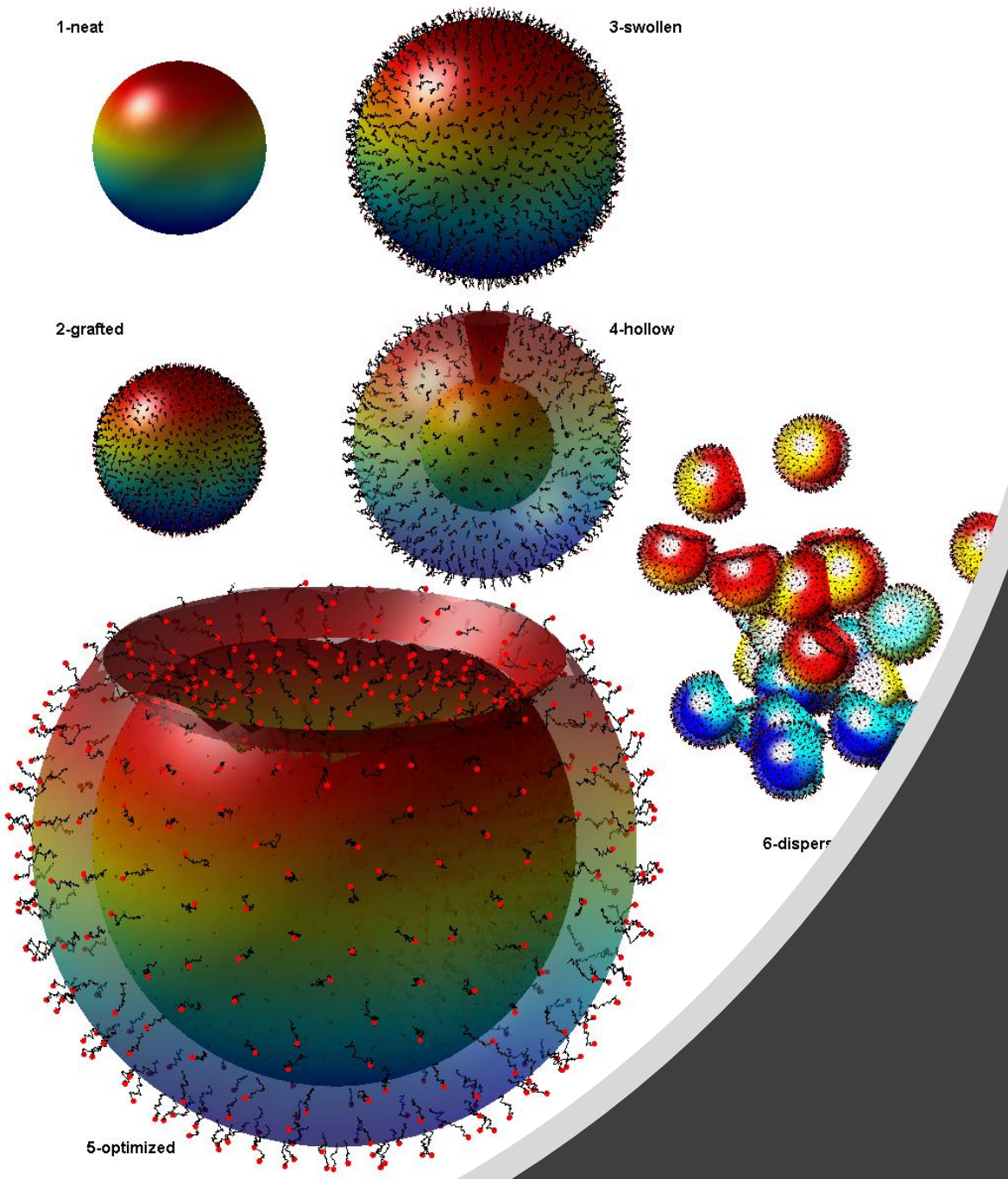
$$criticality = \sum_{all\ components} \sum_{all\ substances} \sum_{all\ modalities} pr(modality) \times severity$$

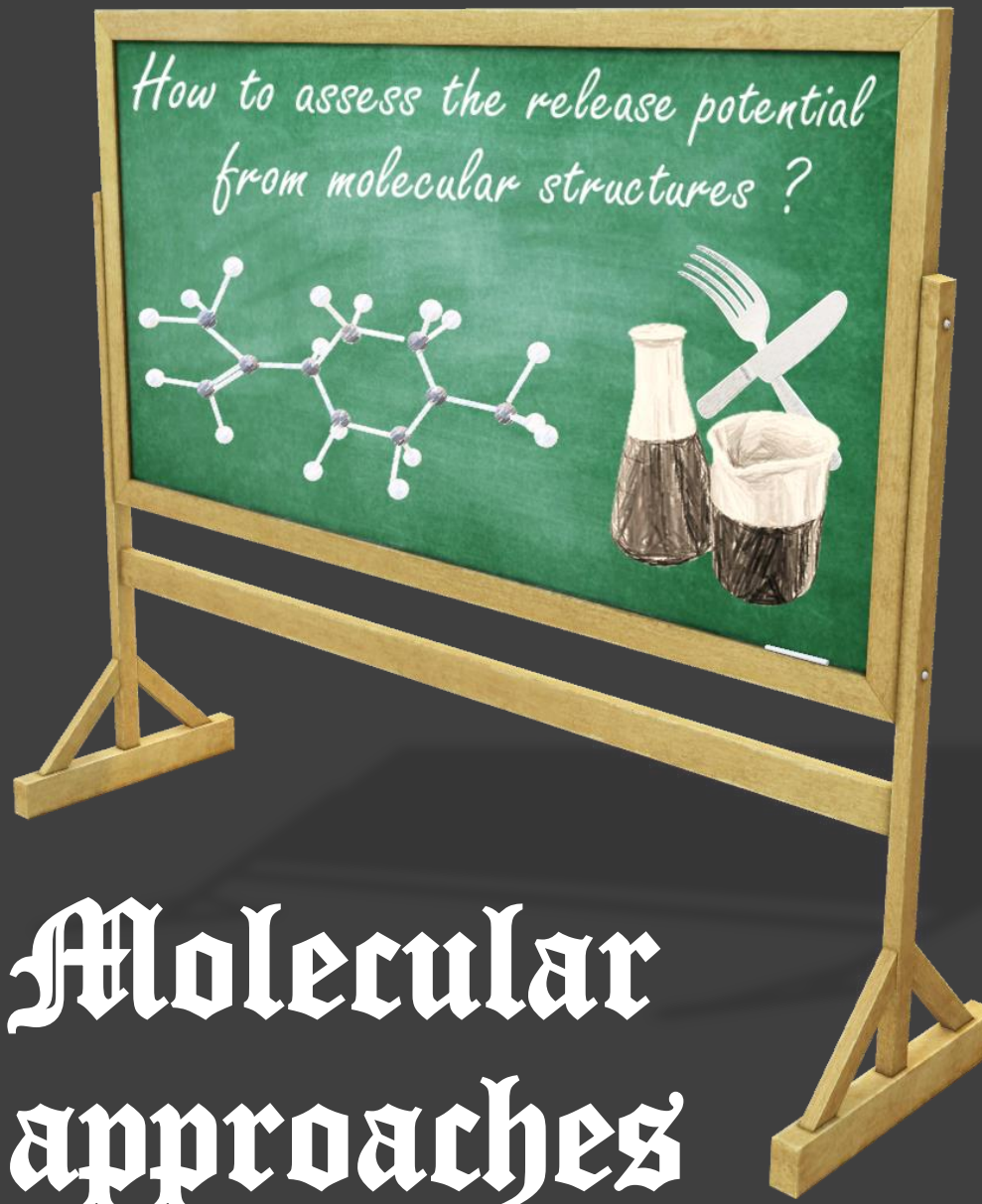
Critical substance



=115
(almost acceptable)

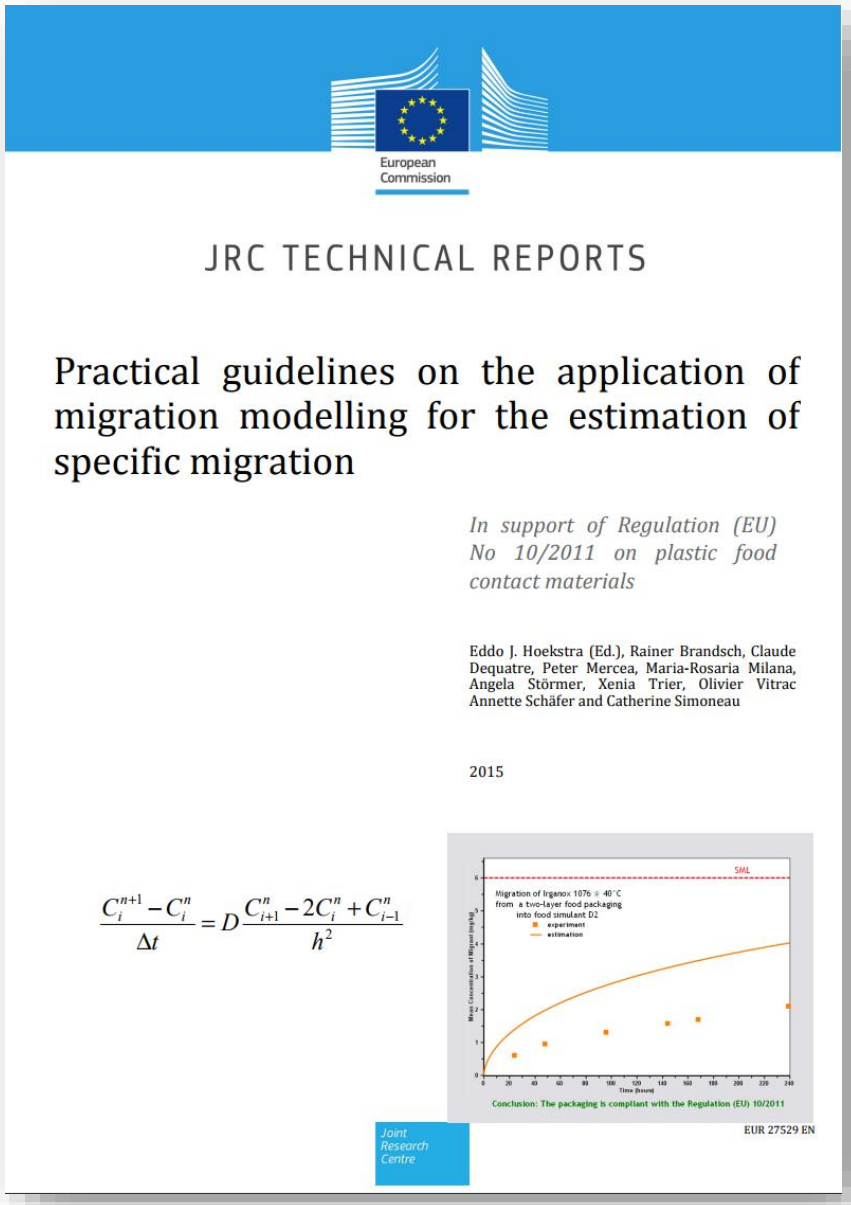
=124



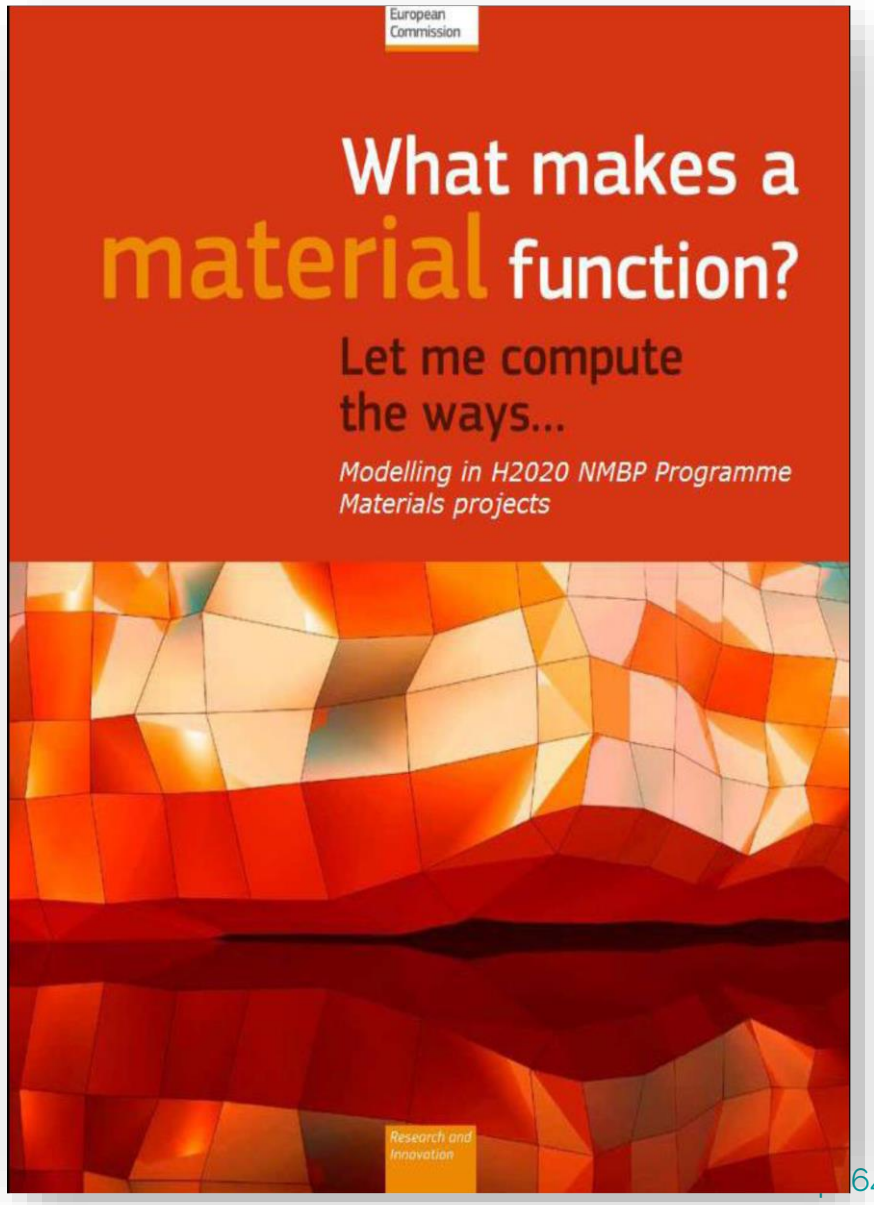


Molecular approaches

Towards a common approach for risk and design

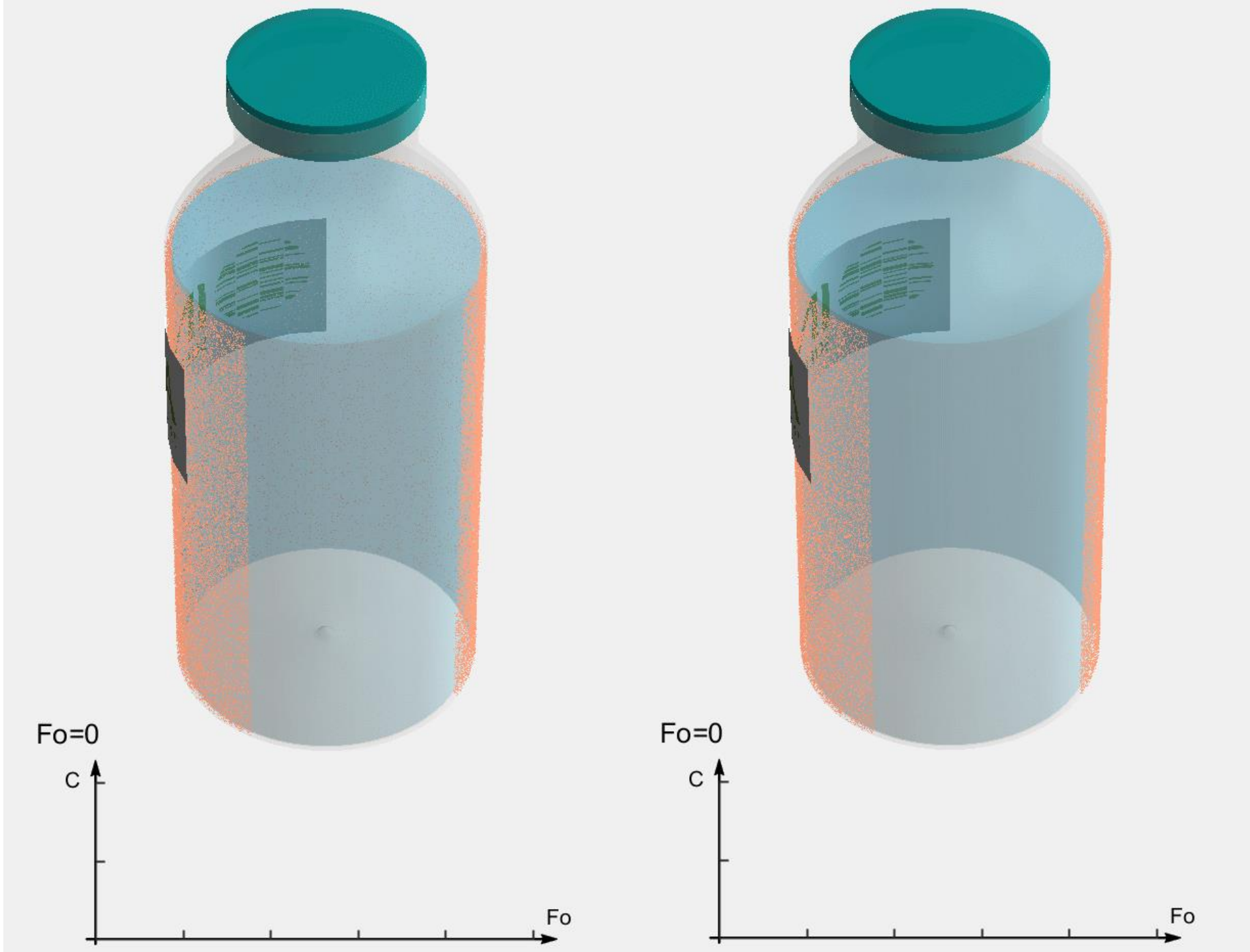


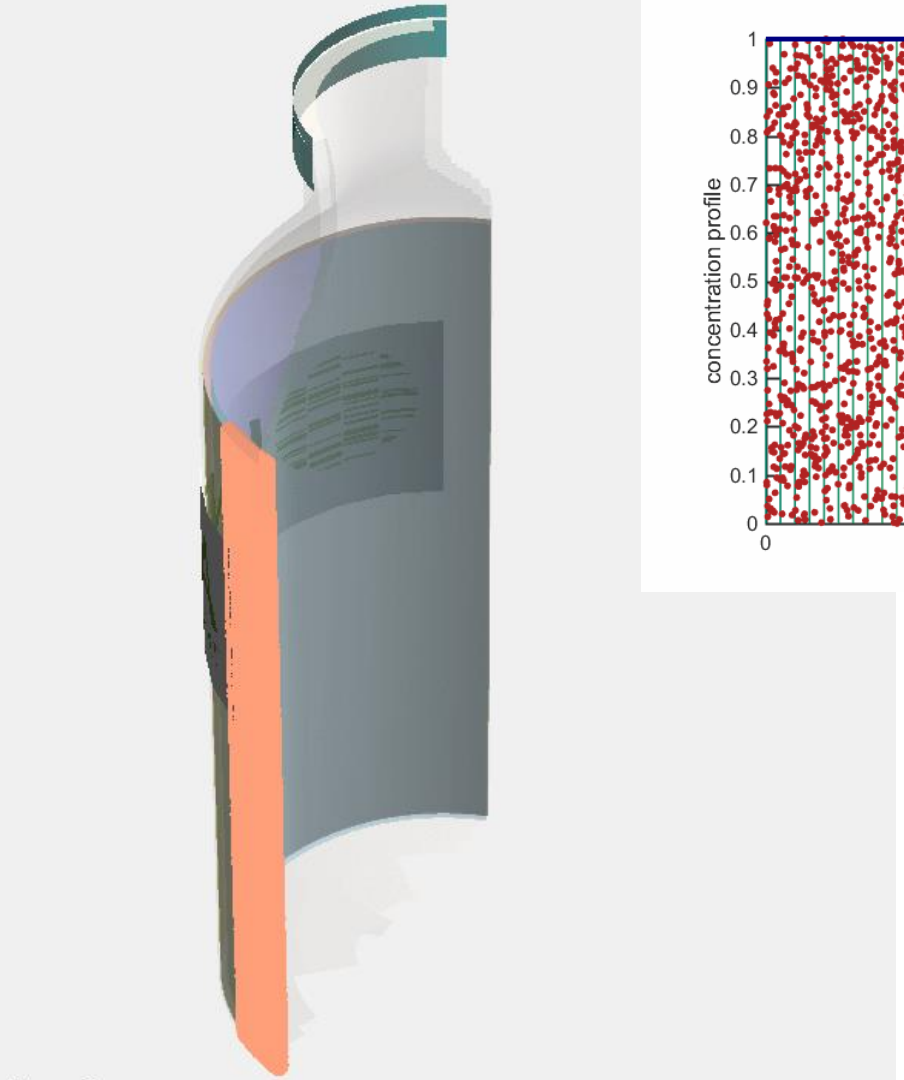
http://publications.jrc.ec.europa.eu/repository/handle/JRC98028

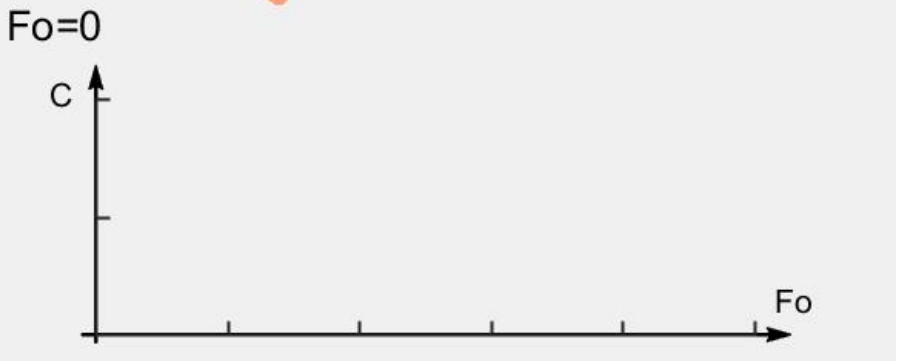


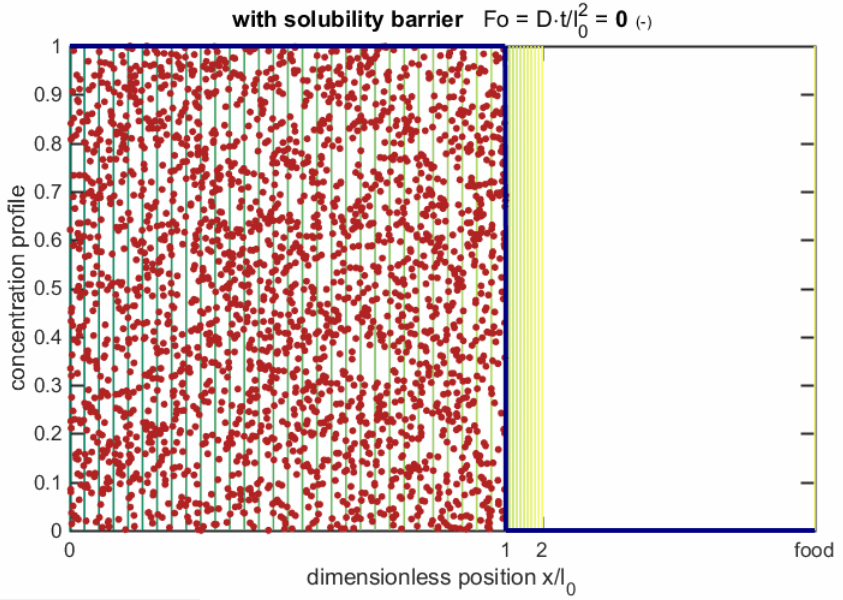
https://publications.europa.eu/en/publication-detail/-/publication/e0845ae1-1b60-11e7-aeb3-01aa75ed71a1

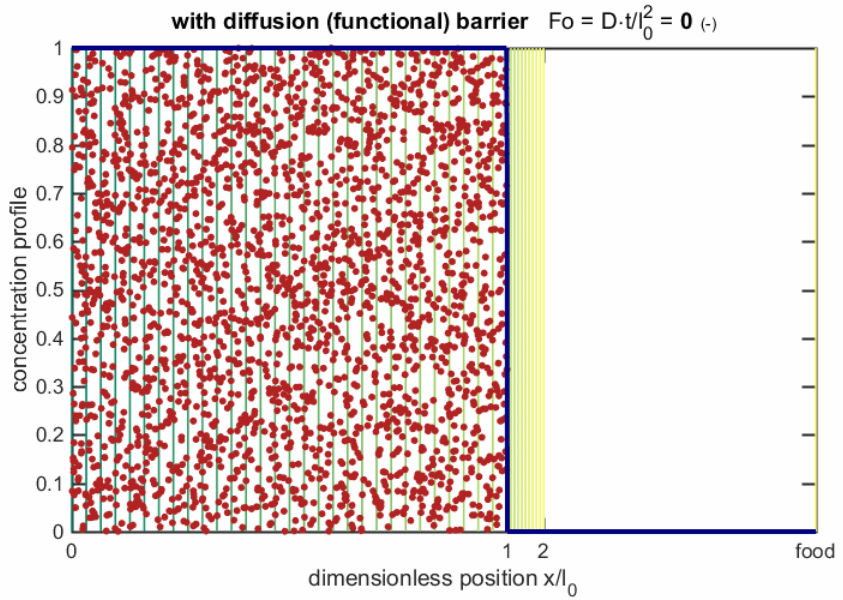
The problem at stake

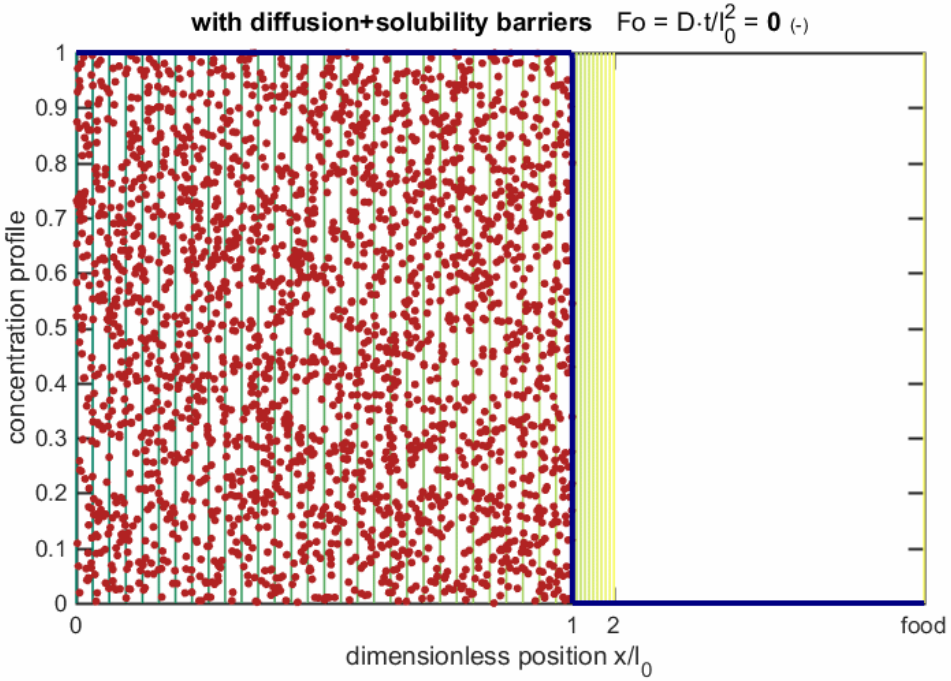


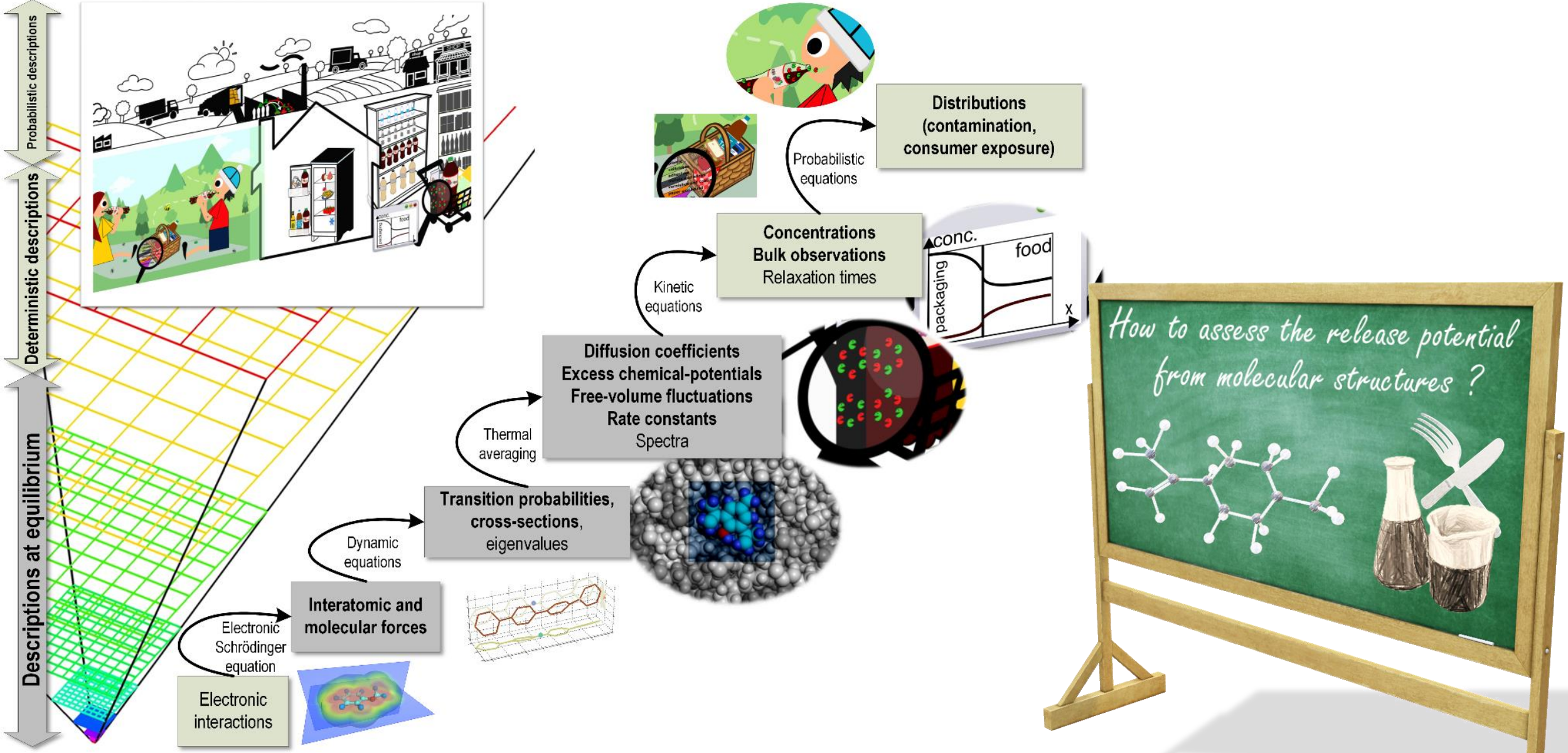



Fo=0
c
Fo


with solubility barrier Fo = D·t/l0² = 0 (-)
concentration profile
dimensionless position x/l0
food

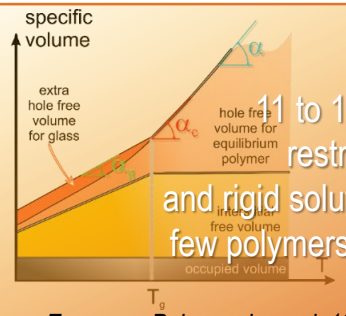
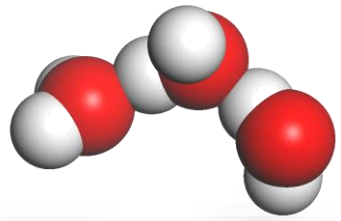
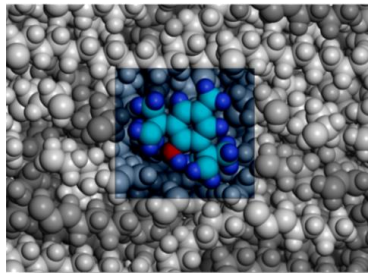

with diffusion (functional) barrier Fo = D·t/l0² = 0 (-)
concentration profile
dimensionless position x/l0
food

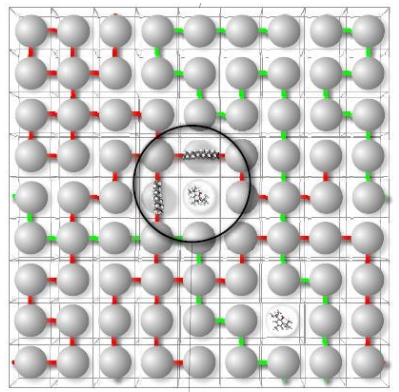

with diffusion+solubility barriers Fo = D·t/l0² = 0 (-)
concentration profile
dimensionless position x/l0
food

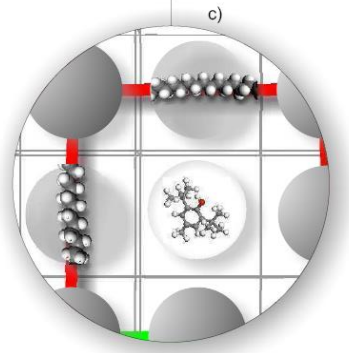

Probabilistic descriptions
Deterministic descriptions
Descriptions at equilibrium
Distributions (contamination, consumer exposure)
Probabilistic equations
Concentrations
Bulk observations
Relaxation times
Kinetic equations
conc.
food
packaging
x
Diffusion coefficients
Excess chemical-potentials
Free-volume fluctuations
Rate constants
Spectra
Thermal averaging
Transition probabilities, cross-sections, eigenvalues
Dynamic equations
Interatomic and molecular forces
Electronic Schrödinger equation
Electronic interactions
How to assess the release potential from molecular structures ?

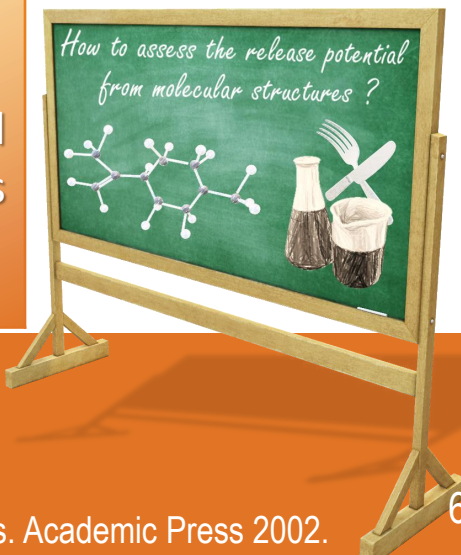
coarse

detailed

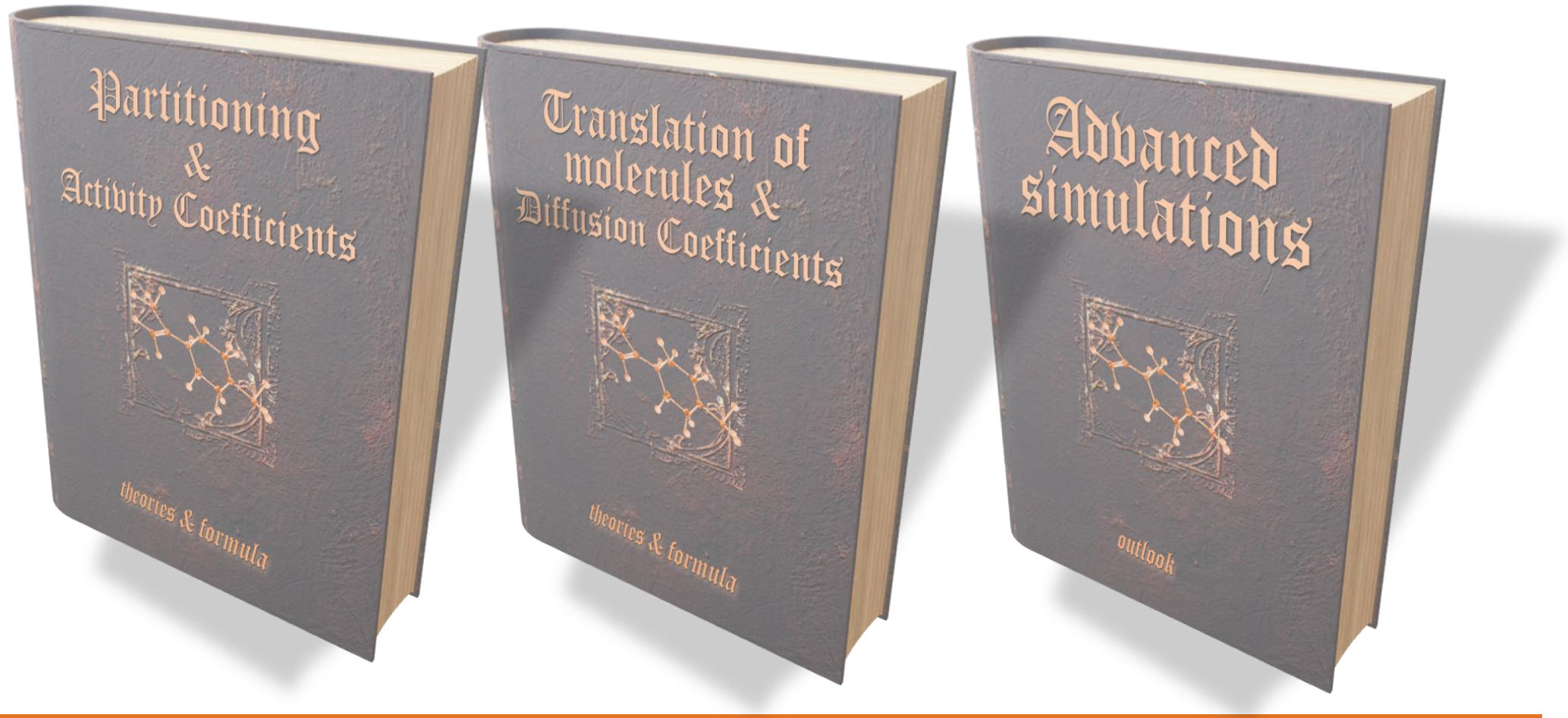
	TRANSPORT diffusion coefficients D and their activation E_a	THERMODYNAMICS chemical affinity (Flory-type isotherms)
Worst-case approaches (arbitrary)	For compliance testing (Piringer's equation) *Food Additives and Contaminants. 2005;**22:73-90.***	$K_{F/P} = 1 \; or \; 10^{-3}$ JRC Scientific and Technical Reports EUR 27529 EN. Ispra (Italy): European Commission; 2015.
Group contribution methods (fitting)	Decision tree *Journal of Applied Polymer Science. 2006;**101:2167-86.***	UNIQUAC, UNIFAC, Flory—Huggins Prausnitz, Lichtenthaler & de Azevedo. Molecular Thermodynamics of Fluid-Phase Equilibria: Pearson Education; 1998.
Theory from first principles (statistical physics)	Free-volume theory (Vrentas-Duda)  11 to 13 parameters restricted to small and rigid solutes (solvents) few polymers documented *European Polymer Journal. 1998;**34:797-803.***	Self-association theory  Kontogeorgis & Folas. Thermodynamic Models for Industrial Applications: From Classical and Advanced Mixing Rules to Association Theories: Wiley; 2009.
Full atomistic simulation or coarse-grained (no assumptions)	for $D \geq 10^{-14} \; m^2 \cdot s^{-1}$  *Journal of Chemical Physics. 2010;**132:194902.***	 Tailored calculations *Industrial & Engineering Chemistry Research. 2010;**49:7263-80.***







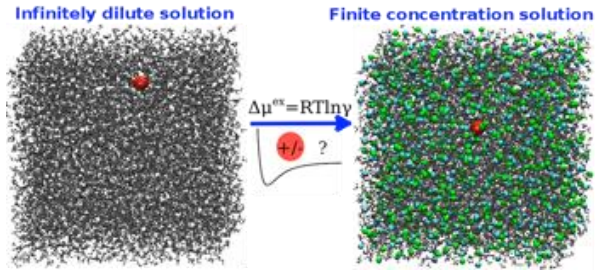
State of the art



ONLINE COURSES & WORKSHOPS (O. Vitrac, visiting scientist at Michigan State University in 2015 – East Lansing, MI, USA)

- 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
- https://mediaspace.msu.edu/media/Dr.+Olivier+Vitrac+presentsA+Diffusion+coefficients+of+organic+solutes+in+polymersA/1_zz20dgt9
- https://mediaspace.msu.edu/media/WorkshopA+Prediction+of+the+migrationA+beyond+conventional+estimates%2A/1_won1m7aw


assess the release potential
structures ?
Food Research International. 2017;88, Part A:91-104.
Industrial & Engineering Chemistry Research. 2017;56:774–87
J. Polymer Science Part B: Polymer Physics. 2014;52:1252-8.
International Journal of Chemical Reactor Engineering. 2010;8.
Industrial & Engineering Chemistry Research. 2010;49:7263-80.
Industrial & Engineering Chemistry Research. 2009;48:5285-301.
Partitioning
&
Activity Coefficients
theories & formula
>> FMECAKairP limonene
3 assessions found for 'limonene'
extraction of ChemSpiderID=20939 ('limonene')
completed in 3.17 s
ans =
4.5034e-05



$K_{i,F/P}$ = 50 × more chemical affinity for P | 50 × more chemical affinity for F

1/50 | 50

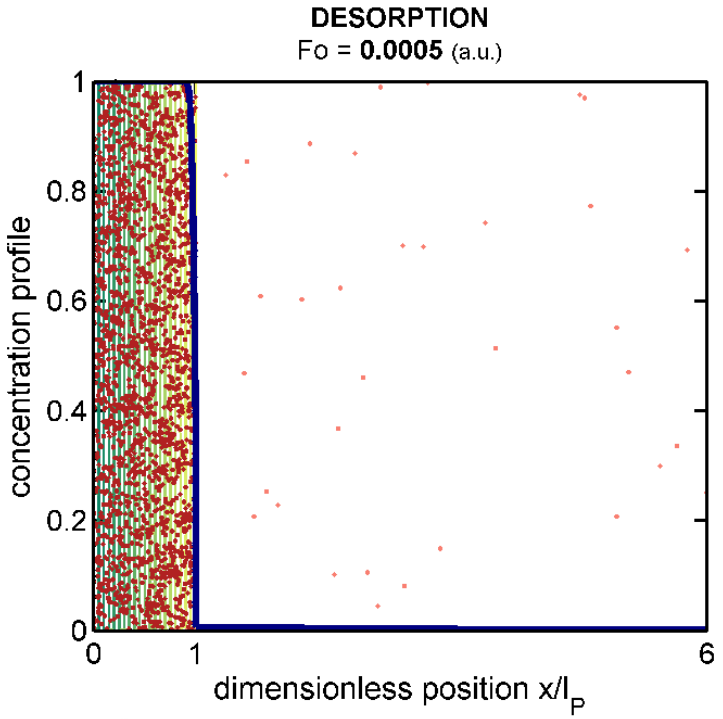
- **Free energy perturbation**

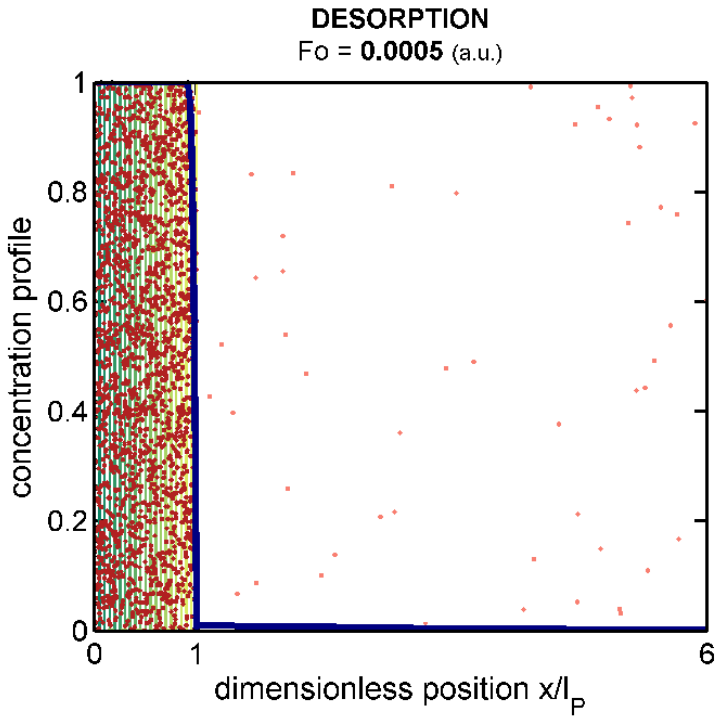
$$\exp\left(-\frac{F_1 - F_0}{k_B T}\right) = \left\langle \exp\left(-\frac{U_1 - U_0}{k_B T}\right)\right\rangle_0$$

- **based on Jarsynski's equality** (1997)

$$\exp\left(-\frac{F_1 - F_0}{k_B T}\right) = \left\langle \exp\left(-\frac{W_{\text{fast}}}{k_B T}\right)\right\rangle_0$$

- **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





$\langle\ \rangle_0$ =ensemble average for a given state 0

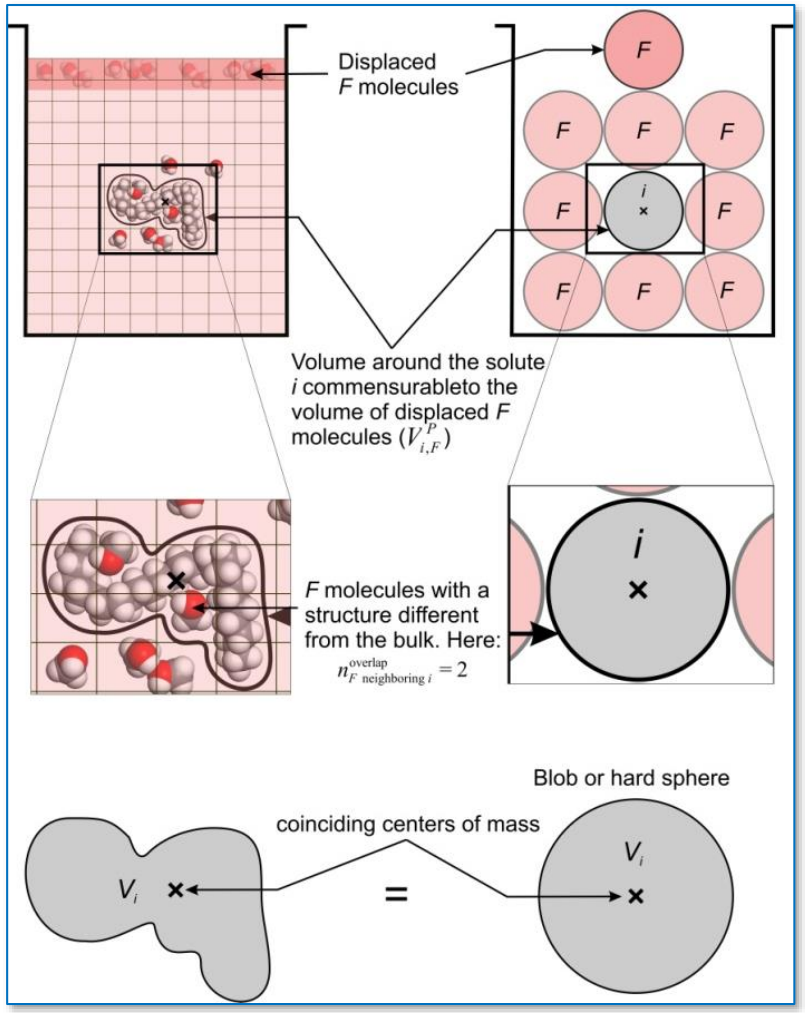
(averaging over 0 may be required)

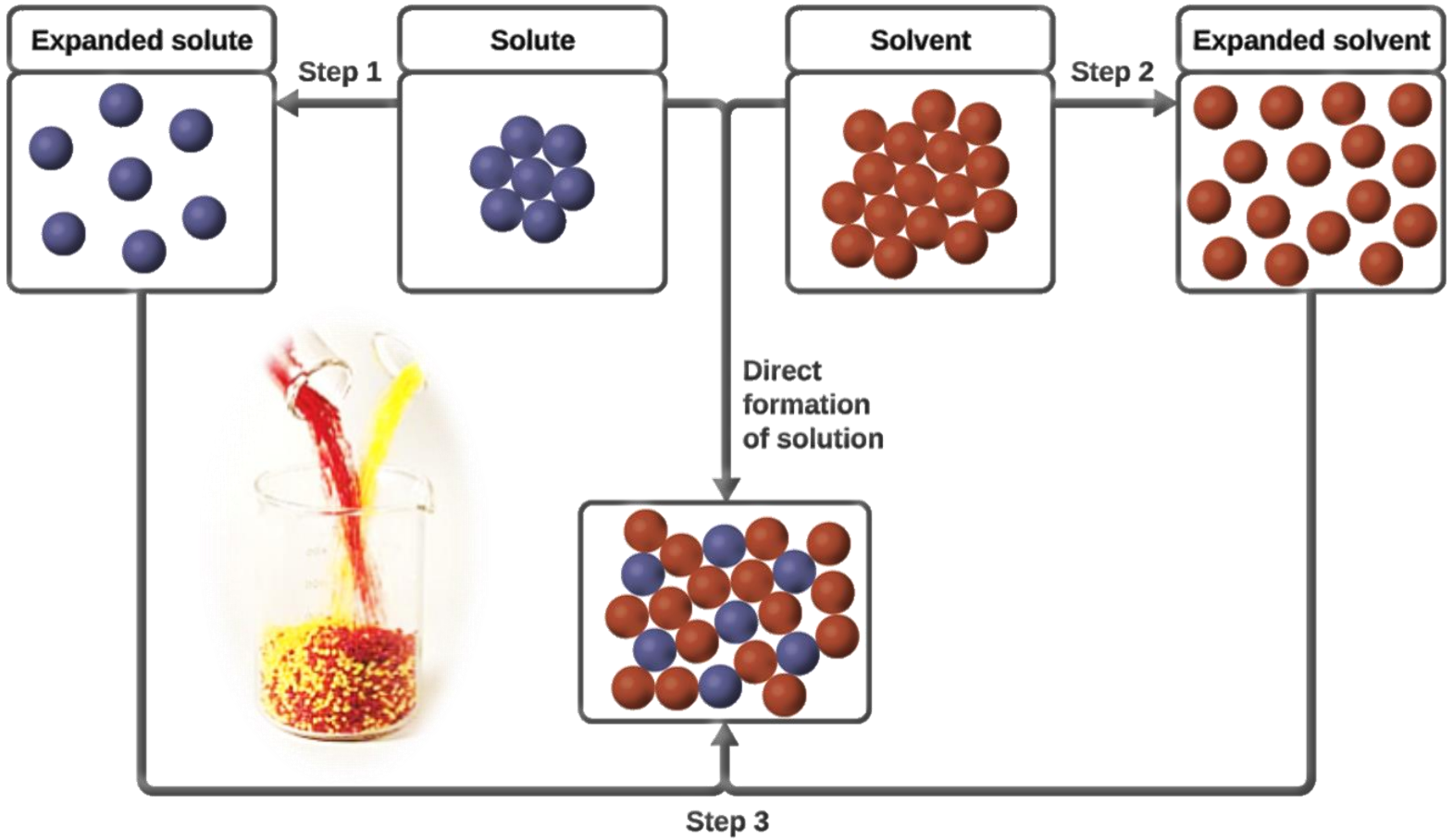
$$K_{i,F/P} = \frac{C_{i,F}^{eq}}{C_{i,P}^{eq}} = \frac{1}{1 - crystallinity} \frac{\gamma_{i,P_{amorphous}}^{v}}{\gamma_{i,F}^{v}}$$

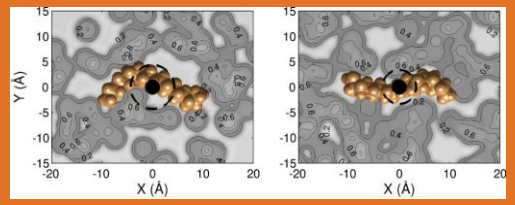
P = POLYMER
F = FLUID, FOOD

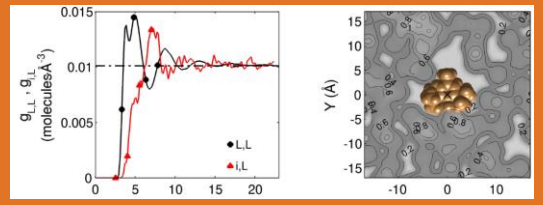
BEYOND COMPRESSIBLE REPRESENTATION

EFFECT OF LOCAL COMPOSITION





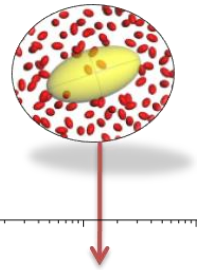


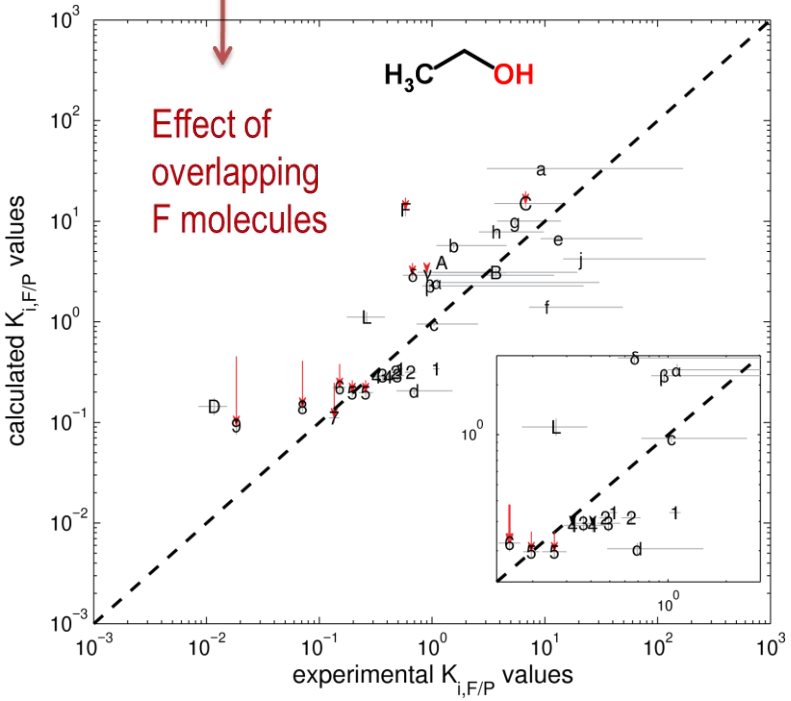


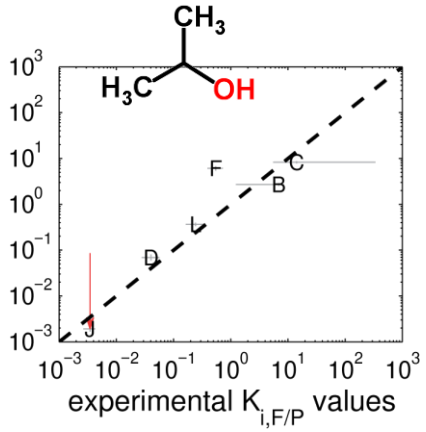
EXAMPLE OF PREDICTIONS FOR POLYETHYLENE

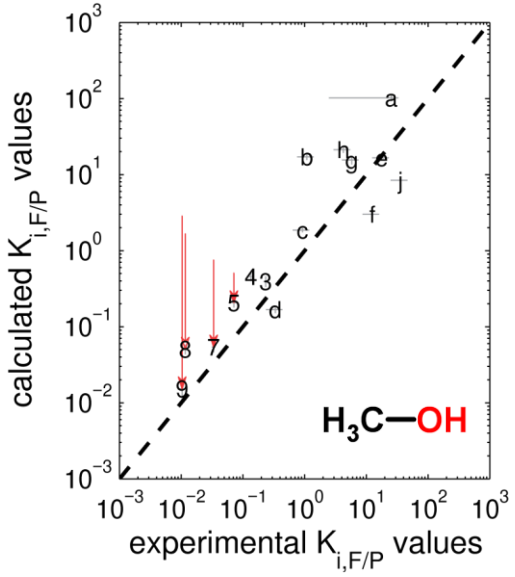
PROPANOL, ETHANOL, METHANOL, WATER

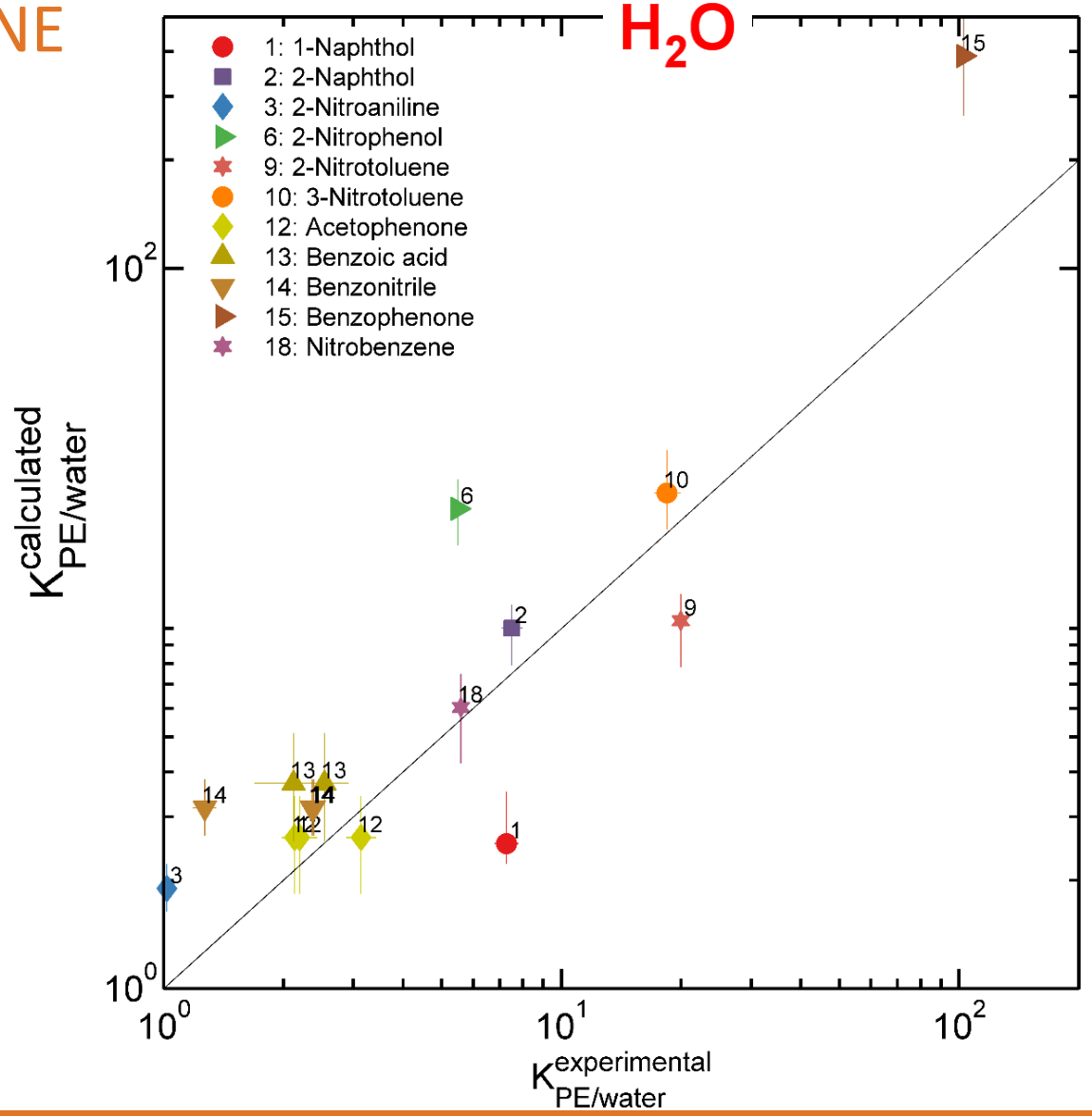
↗ *polarity*







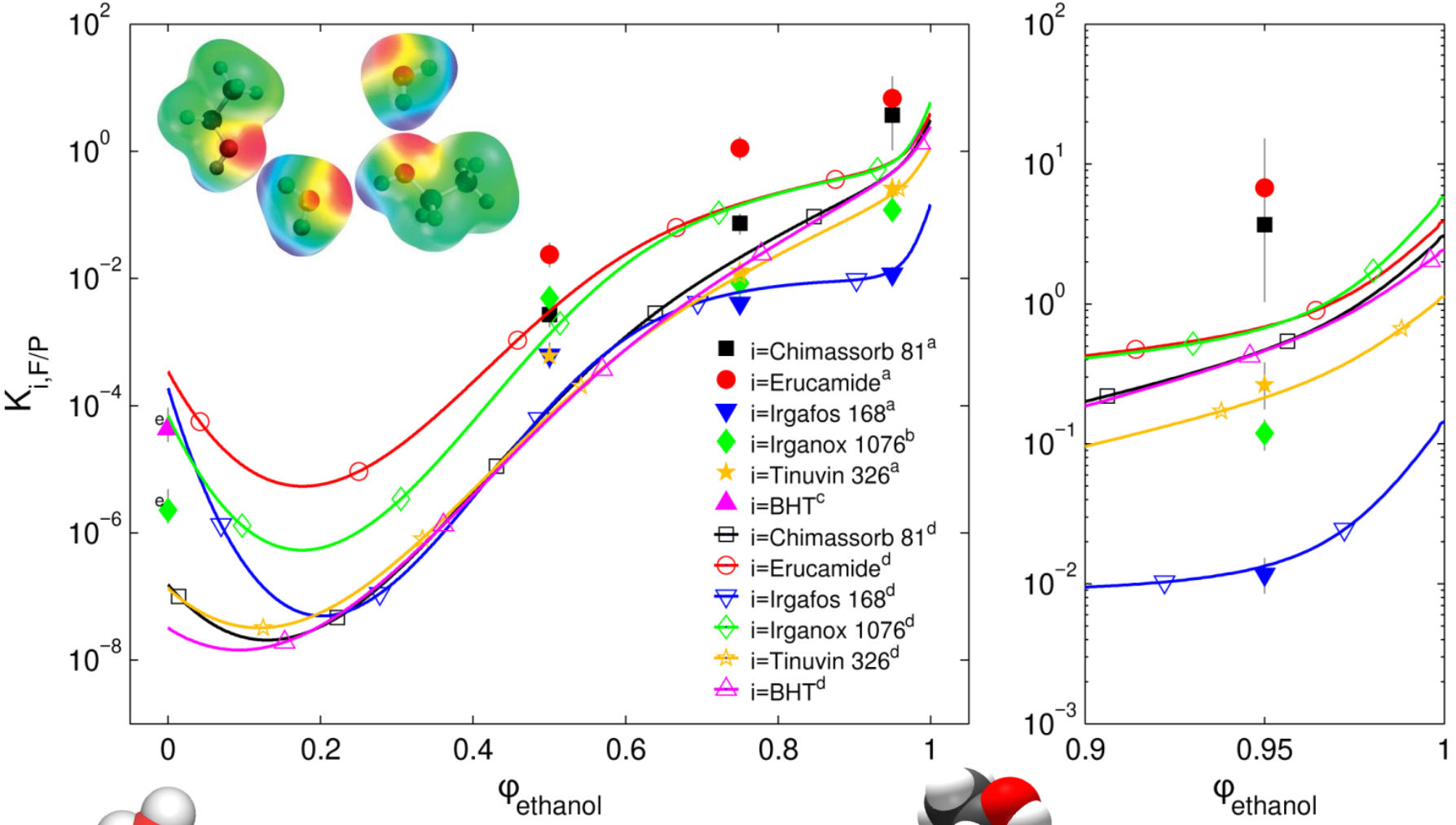


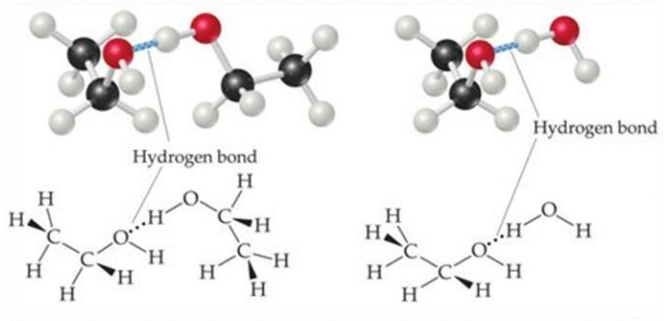


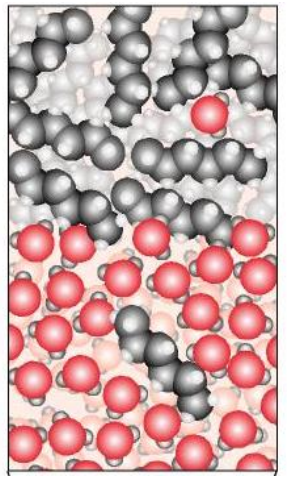
*International Journal of Chemical Reactor Engineering. 2010;**8.***
*Industrial & Engineering Chemistry Research. 2010;**49:7263-80.***
*Industrial & Engineering Chemistry Research. 2009;**48:5285-301.***

EXAMPLE OF PREDICTIONS FOR POLYETHYLENE

WATER-ETHANOL MIXTURES

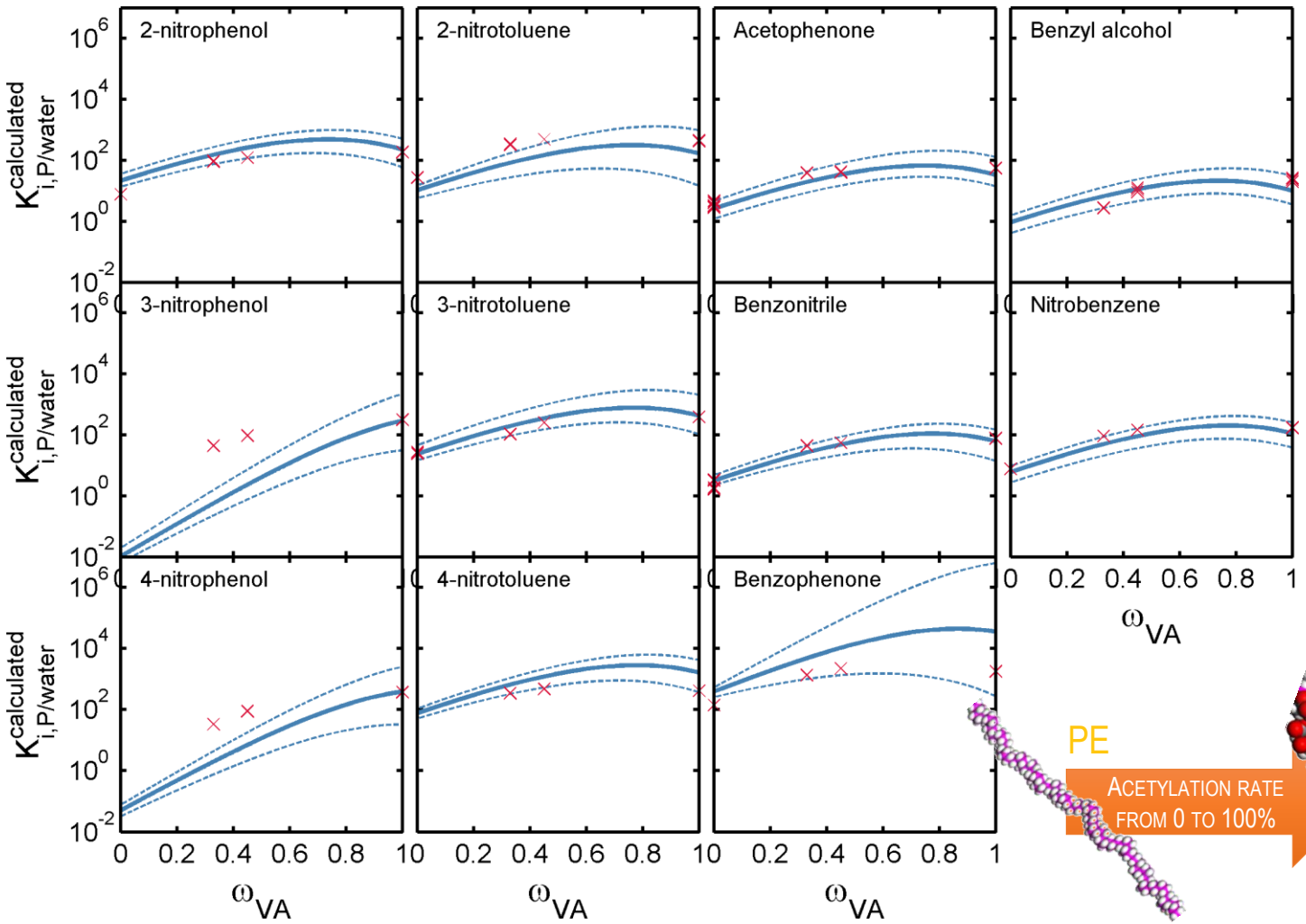




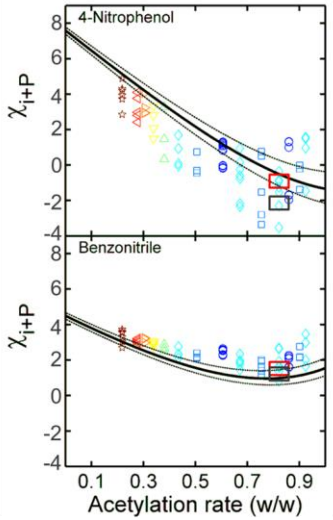


EXTENSIONS TO COPOLYMERS

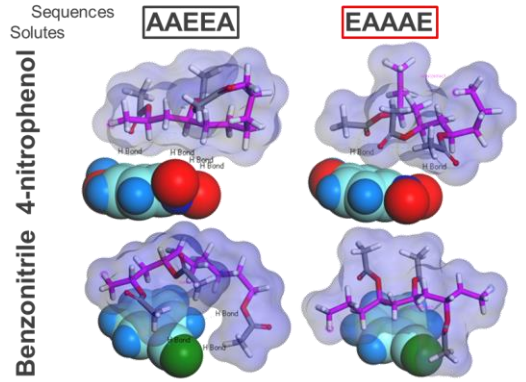
EFFECT OF ACETYLATION RATE



Effect of acetylation rate on χ



Configurations of minimal energies : n = 5
(acetylation rate w/w = 0.82)

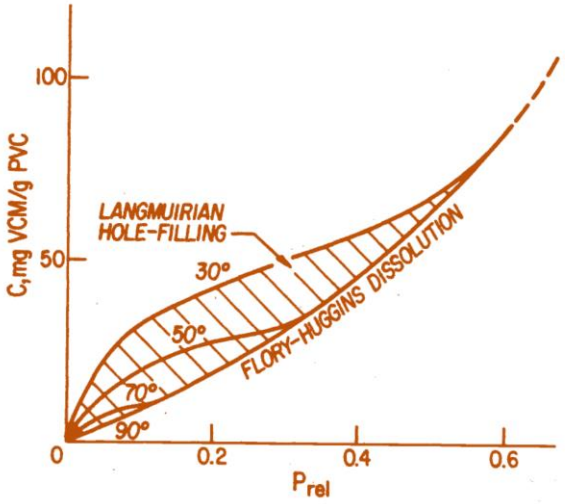


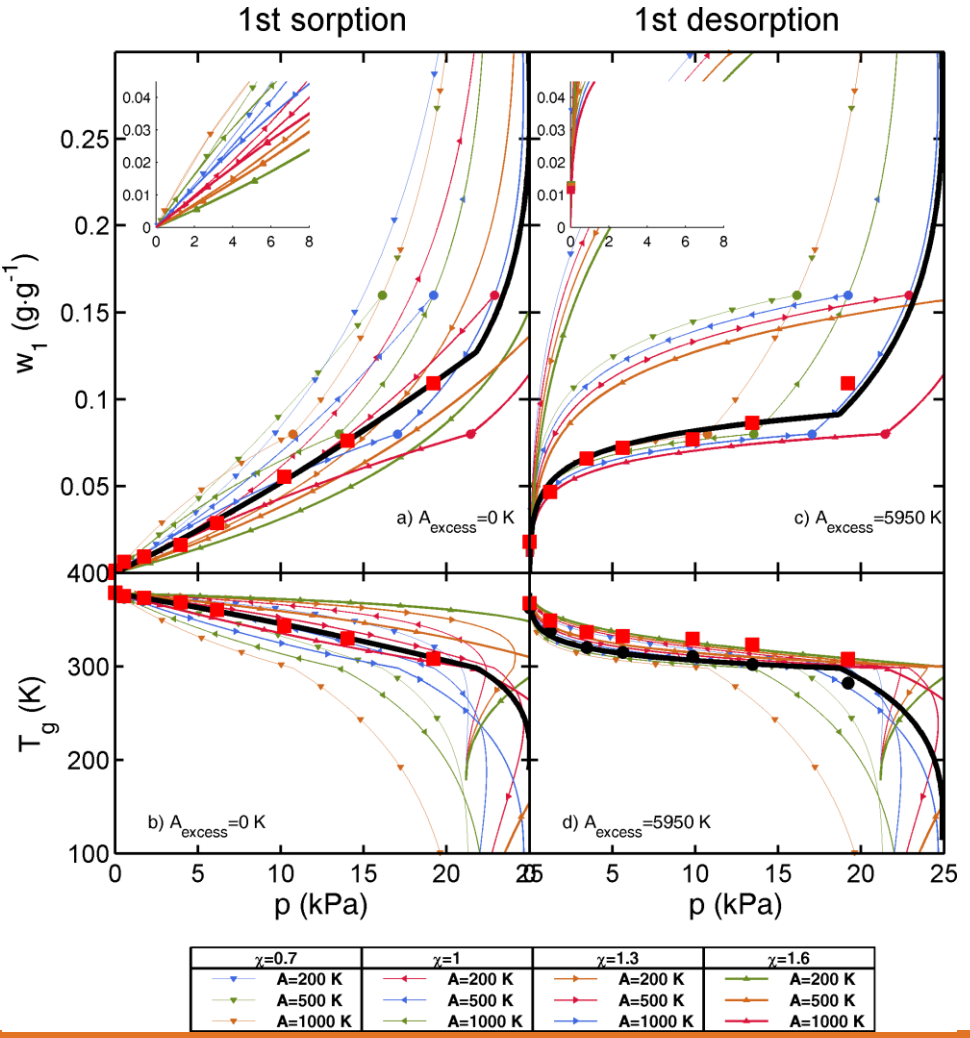
Microscopic calculations

mean field approximation

PLASTICIZATION AND HISTORY EFFECTS ON SORPTION/DESORPTION

DEVIATION TO IDEALITIES: SORPTION OF N-HEXANE IN PS AT 298 K





$$p = p_s \cdot \emptyset_1 \cdot \exp\left[(1-\emptyset_1) + \chi \cdot (1-\emptyset_1)^2\right] \cdot \exp(F)$$

where

$$F = \frac{\mathrm{MW}_1 \cdot w_2^2 \cdot (c_p - c_{pg}) \cdot A}{R \cdot T} \cdot \left(\frac{T}{T_{gm}} - 1\right)$$

For $T < T_{gm}$

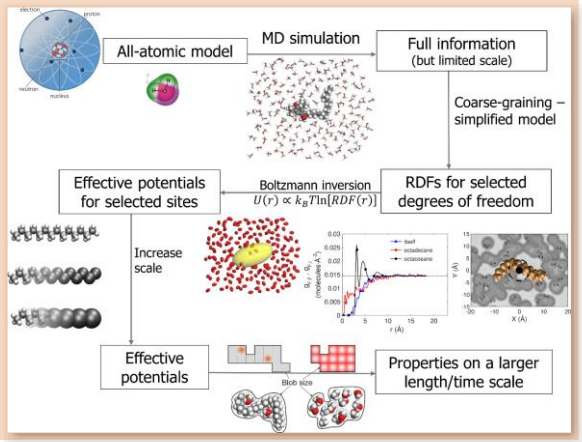
$F = 0$ for $T > T_{gm}$

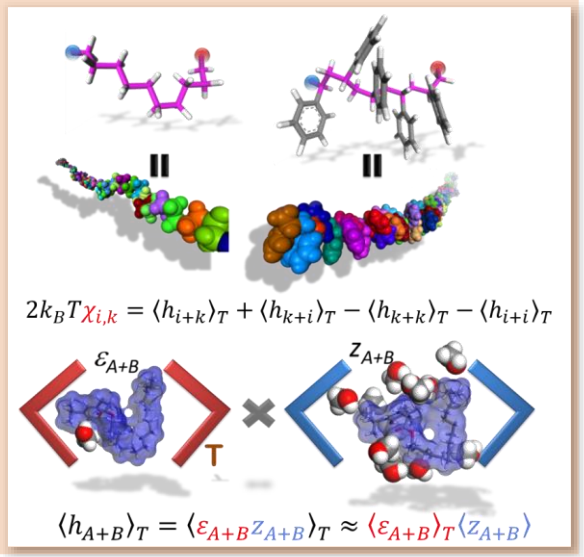
$$T_{gm} = T_{g2} - A \cdot w_1$$

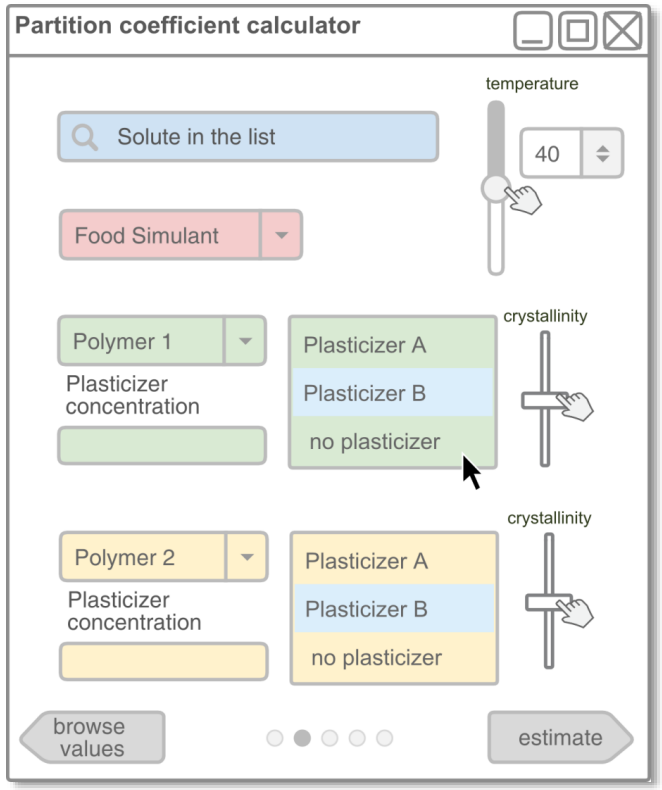
$$A = \frac{-\mathrm{d}T_{gm}}{\mathrm{d}w_1}$$

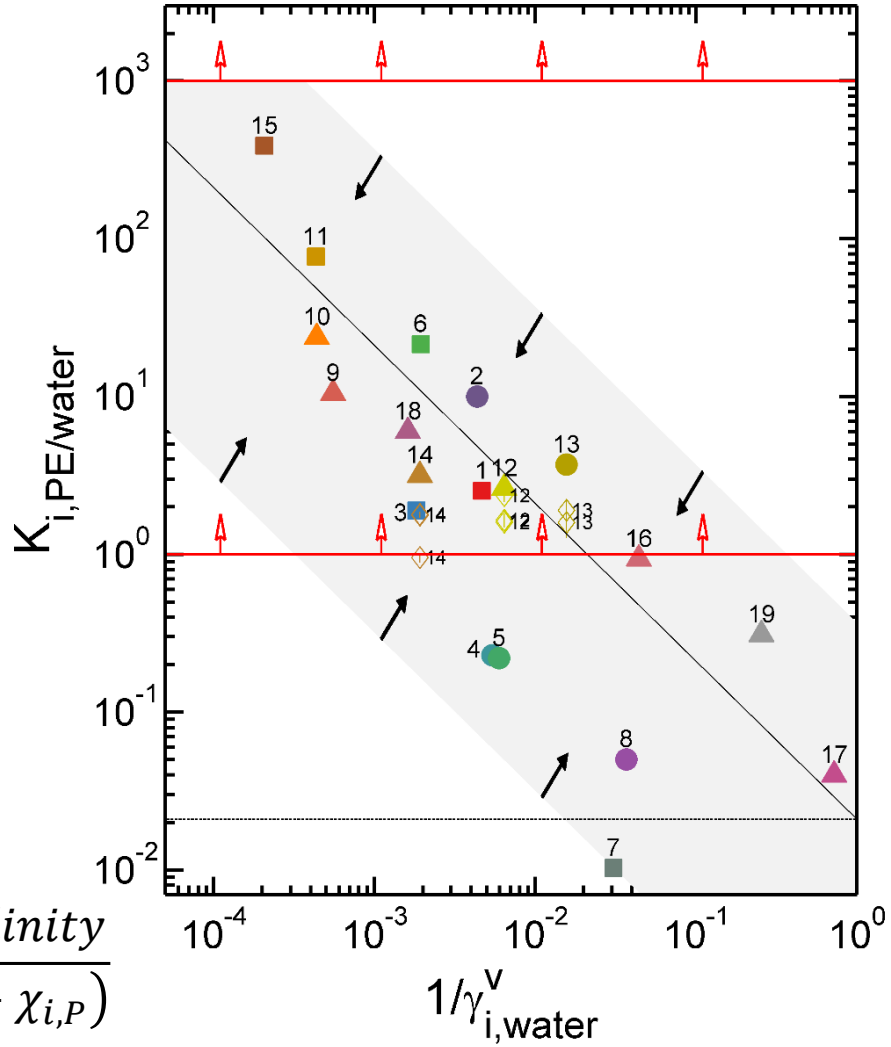
APPROACHES DEVELOPED FOR THE INDUSTRY

OVERVIEW









$$K_{i,P/F}^{semi-crystalline} \approx \frac{1 - crystallinity}{\phi_{i,F}^{sat}\exp\left(1+\chi_{i,P}\right)}$$

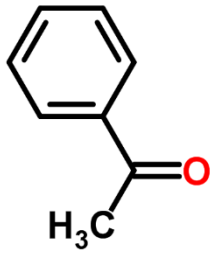
$$\left\{\mu_{i,k}^{excess}\right\}_{k=P,F} = \ln\gamma_{i,k}^{v} = \left(1-\frac{1}{r_k}\right)\phi_k + \chi_{i,k}\phi_k^2$$

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

INRA SCIENCE & IMPACT

PARTITION COEFFICIENTS WITH AIR

OVERVIEW




```
>> 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
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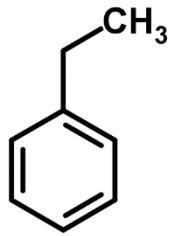


```
>> FMECAKairP ethylbenzene
LOAD_CHEMSPIDER    extraction of ChemSpiderID=7219 ('ethylbenzene') completed in 11.9 s
LOAD_CHEMISPIDER: updated cache
       7219.mat      21-sept.-2015 21:42:34      107.1 kBytes   C:\Data\Olivier\INRA\Codes\MS\cache.ChemSpider
CHEMSPIDER reuses cached data for 'ethylbenzene'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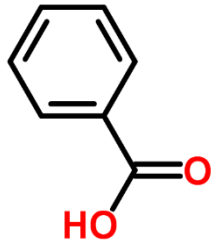
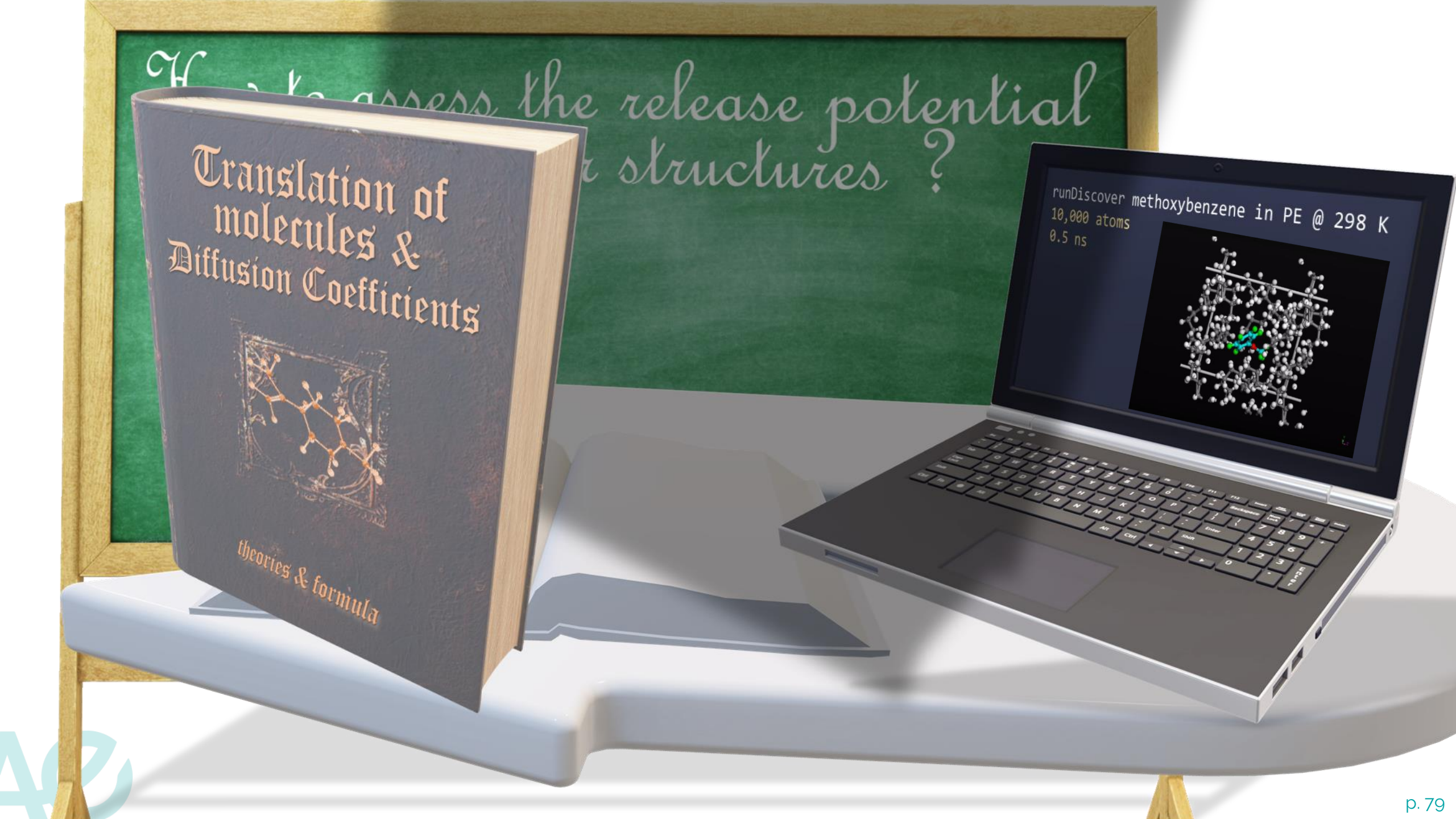
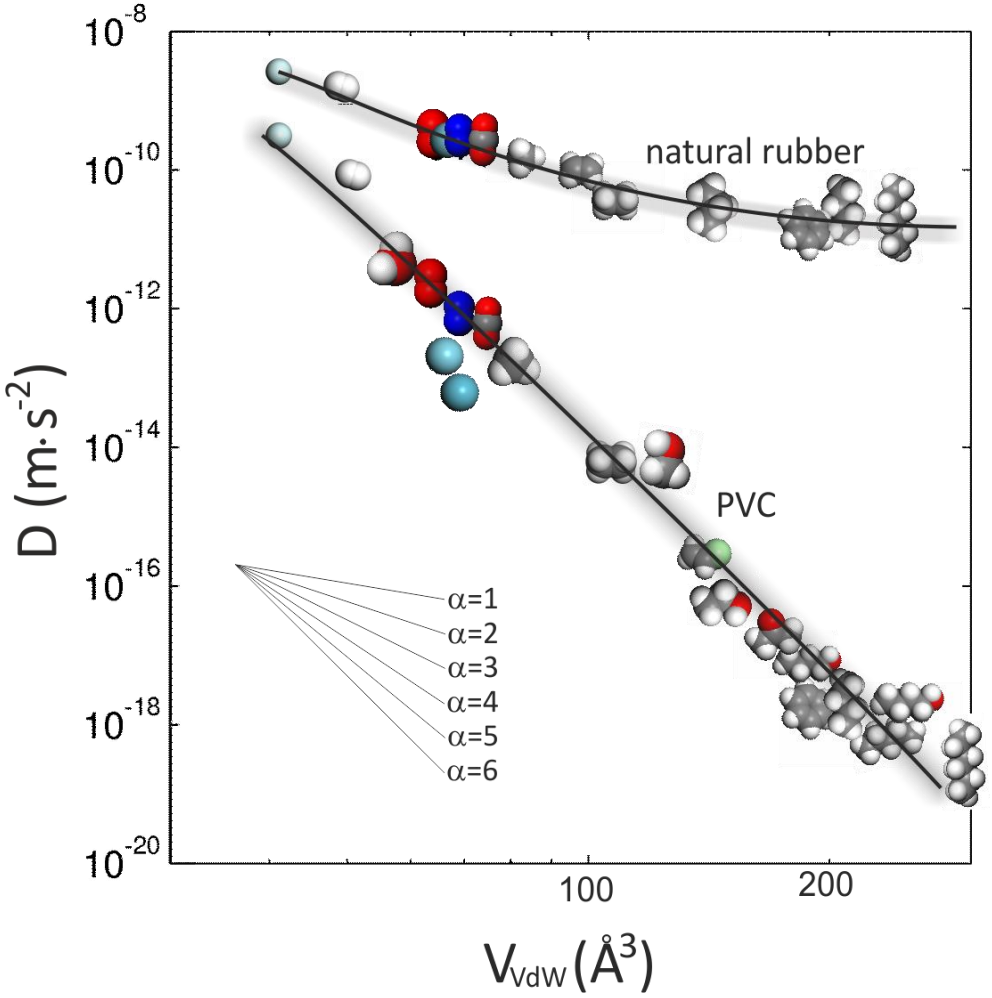


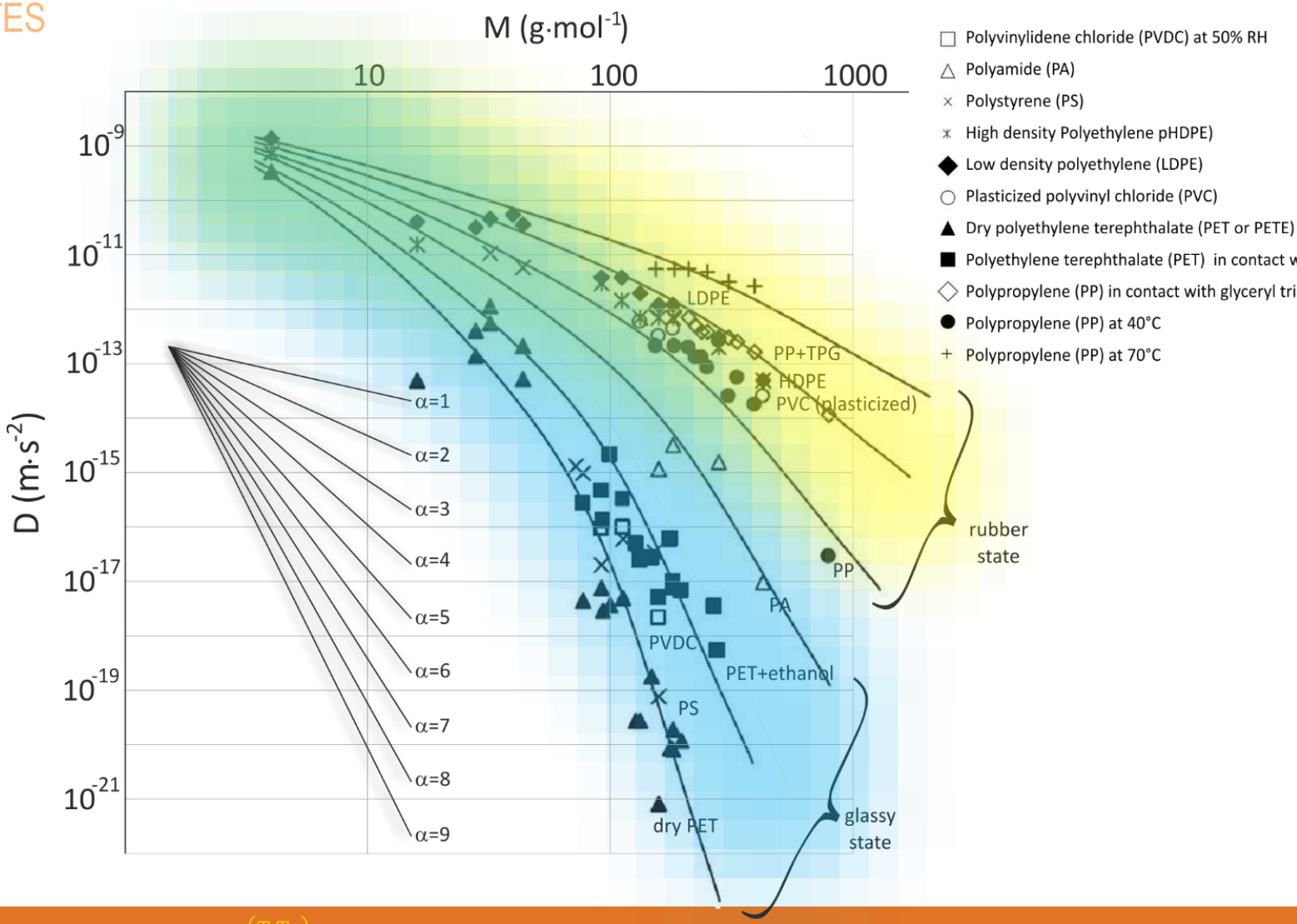

```
>> FMECAKairP 'benzoic acid'
LOAD_CHEMSPIDER    extraction of ChemSpiderID=238 ('benzoic acid') completed in 5.746 s
LOAD_CHEMISPIDER: updated cache
       238.mat 21-sept.-2015 21:45:01      41.2 kBytes   C:\Data\Olivier\INRA\Codes\MS\cache.ChemSpider
CHEMSPIDER reuses cached data for 'benzoic acid'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


Translation of molecules & Diffusion Coefficients
theories & formula
runDiscover methoxybenzene in PE @ 298 K
10,000 atoms
0.5 ns

MAIN EFFECTS ACTING ON DIFFUSION COEFFICIENTS

POLYMER T_g, SOLUTE VOLUME FOR RIGID SOLUTES

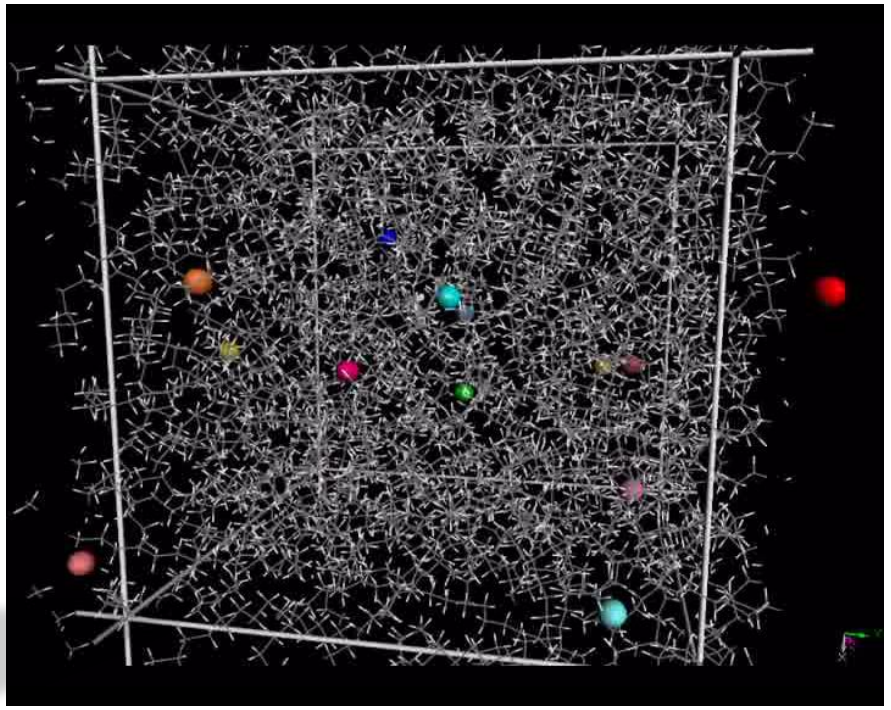


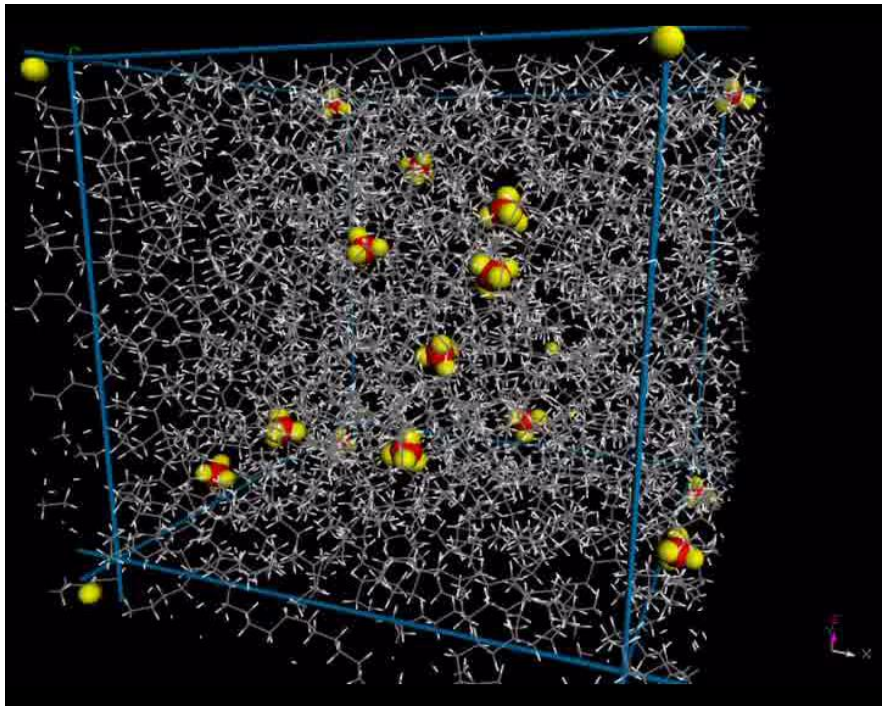


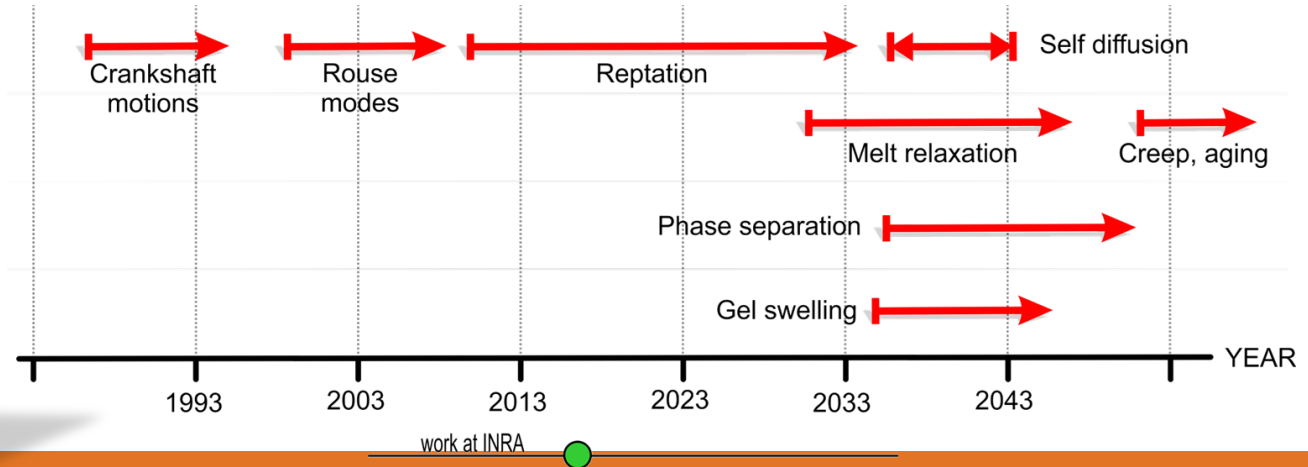
$$\frac{D(M,T)}{D(M_0,T)} \propto \left(\frac{M}{M_0}\right)^{-\alpha(T,T_g)}$$

Fang X, Vitrac O. *Critical Reviews in Food Science and Nutrition. 2017;**57:275-312***

A. R. Berens, Pure Appl. Chem., **1981**, 53, 365



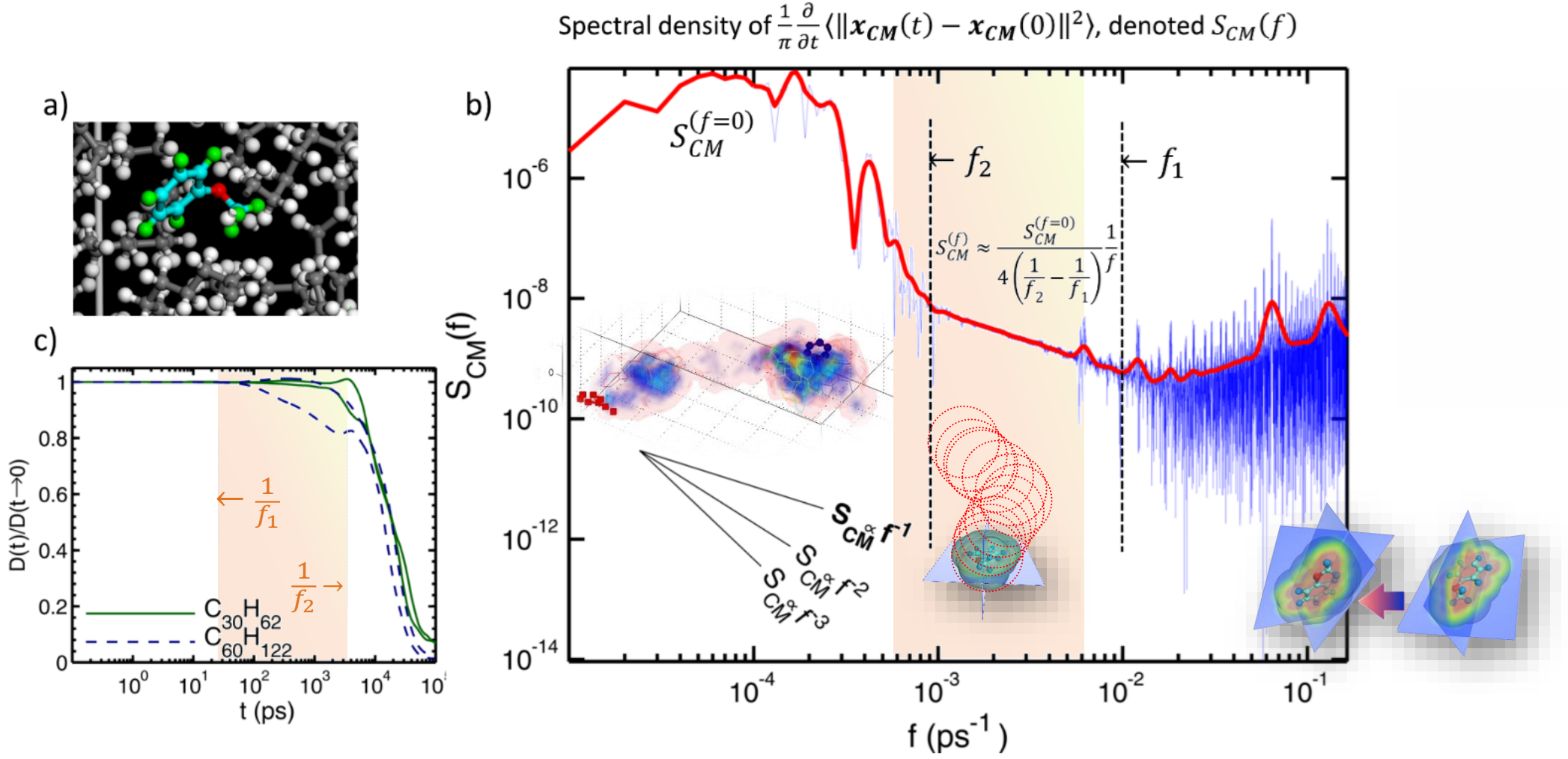




$$D \approx \frac{1}{6}\frac{\partial}{\partial t}\left\langle \left(x_{CM}(t) - x_{CM}(0)\right)^2 \right\rangle$$

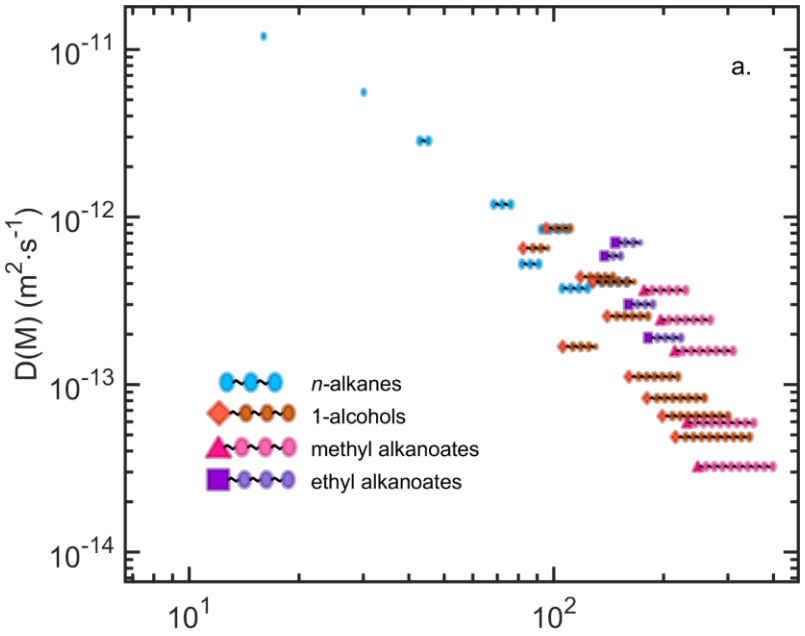
HOW RANDOM WALKS EMERGE FROM THERMAL VIBRATIONS

MOLECULAR DYNAMICS SIMULATION OF METHOXYBENZENE IN AMORPHOUS POLYETHYLENE AT 298 K

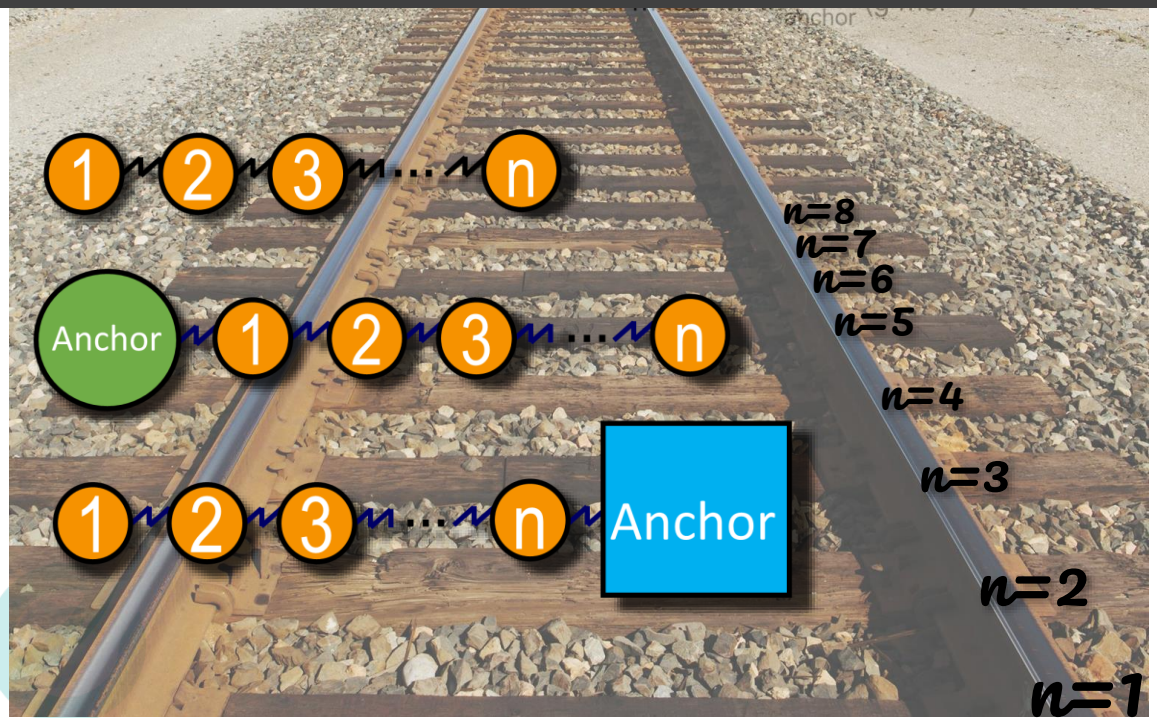


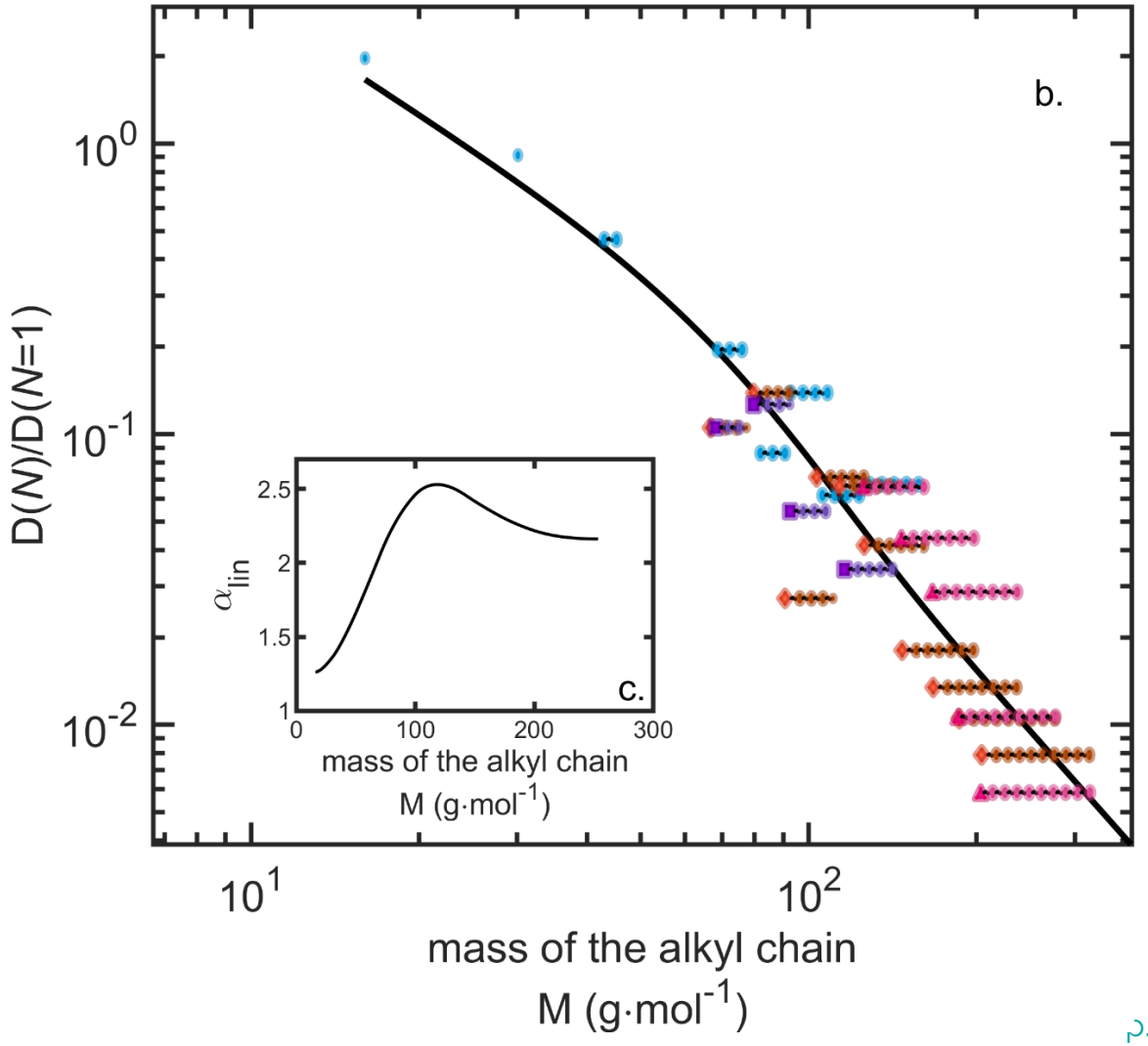
$$D \approx \frac{1}{6}\frac{\partial}{\partial t}\left\langle\left(\boldsymbol{x_{CM}}(t)-\boldsymbol{x_{CM}}(0)\right)^2\right\rangle$$

Diffusivities in LDPE @298K



$$\frac{D(M_a + M, T)}{D(M_a + M_0, T)} \propto \left(\frac{M}{M_0}\right)^{-\alpha(T,T_g)}$$

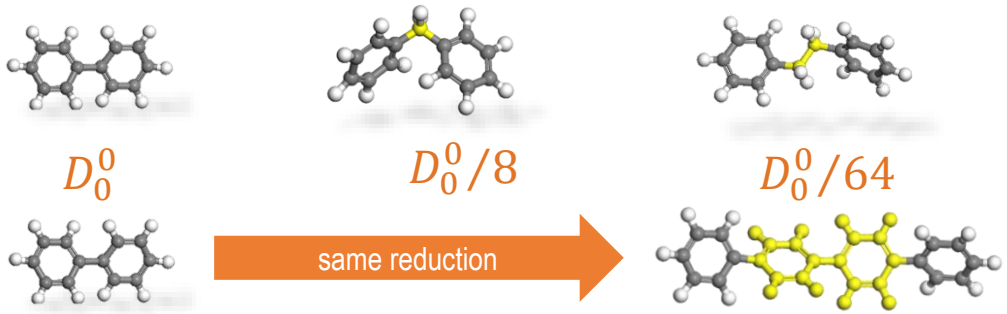


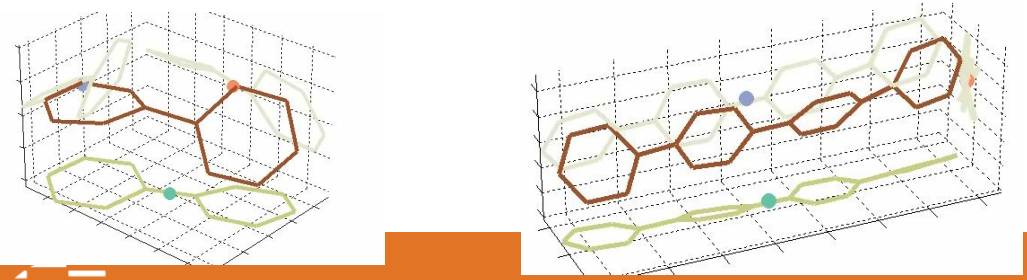


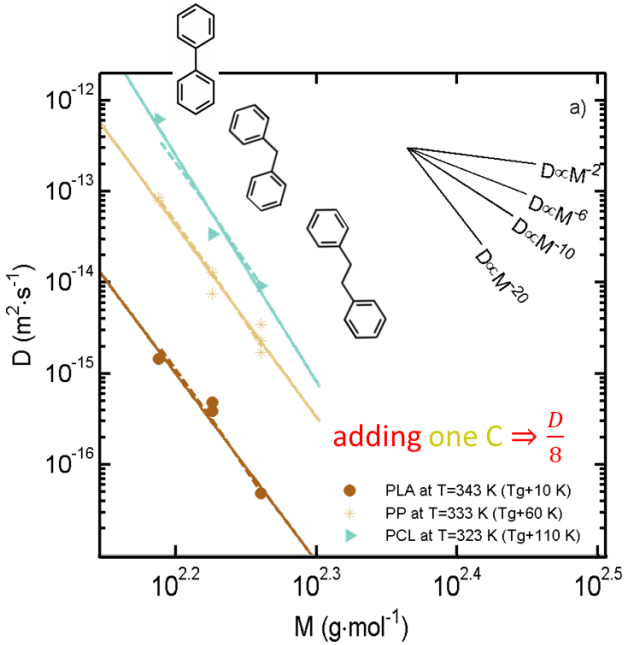
MAIN EFFECTS ACTING ON DIFFUSION COEFFICIENTS

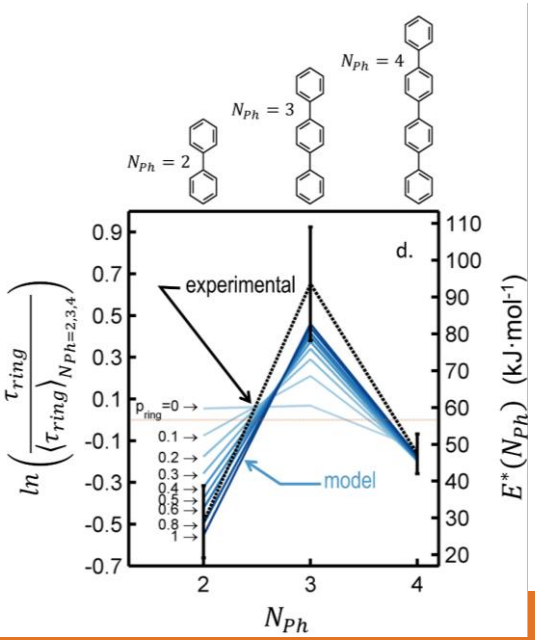
SOLUTE FLEXIBILITY, CHAIN LENGTH

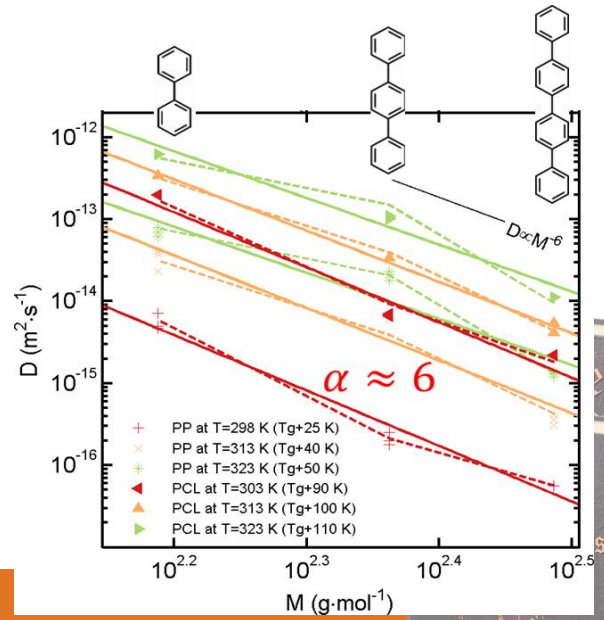
$$D(M,T,T_g) = D_0 \exp\left(-\frac{E_a{}^{blob}}{RT}\right) \times \exp\left(-\frac{E^{*(M)} - E^*_{blob}}{RT}\right)\left(\frac{M}{M_{blob}}\right)^{-\alpha(T,T_g)}$$

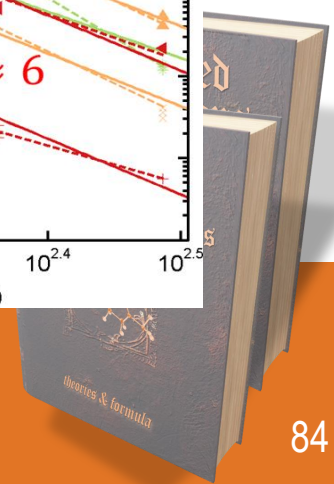








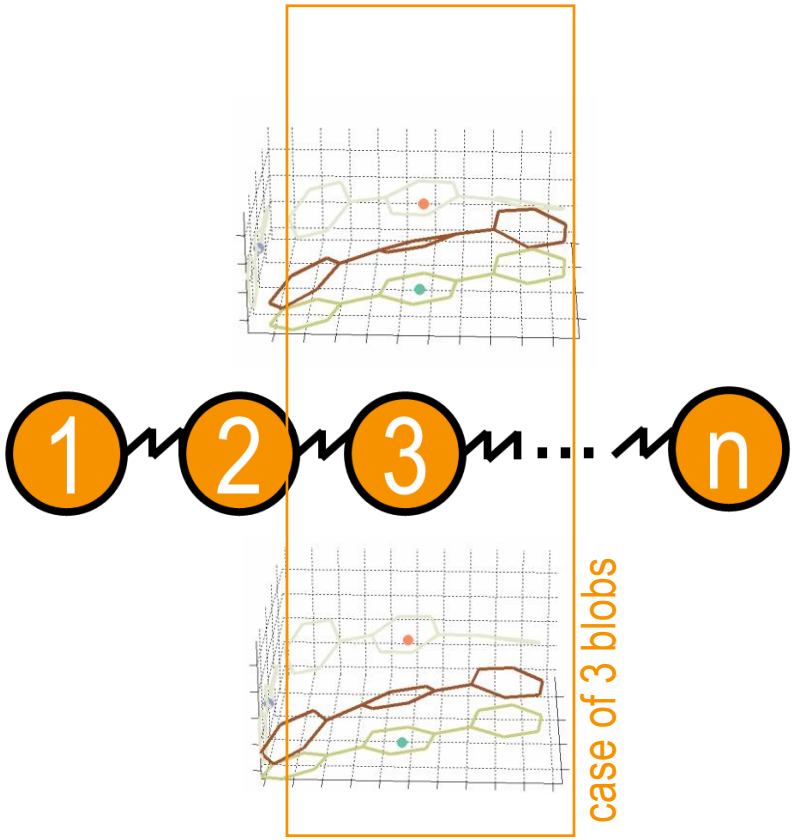


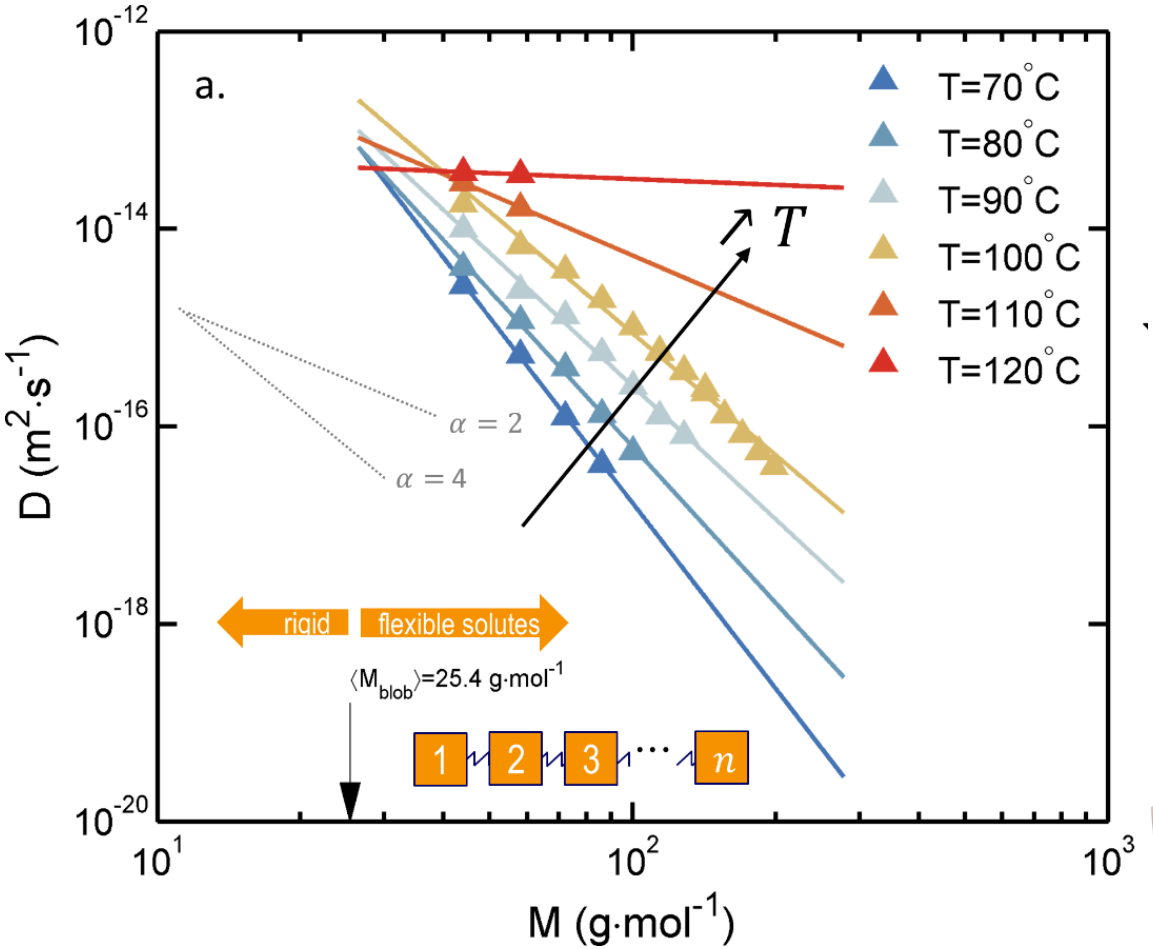


Macromolecules 2013, **46**(3), 874-888

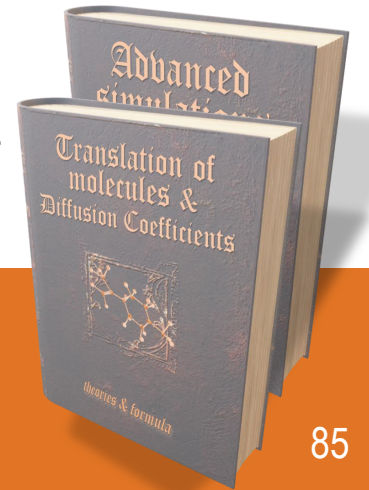
EFFECTS OF SOLUTE LENGTH DEPENDS ON TEMPERATURE

AROMATIC & LINEAR SOLUTES





n-alkanes in PET (T_g=81°C)

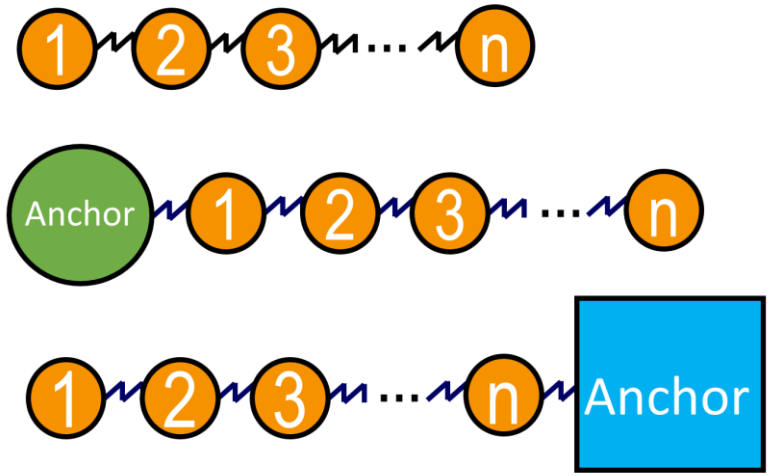


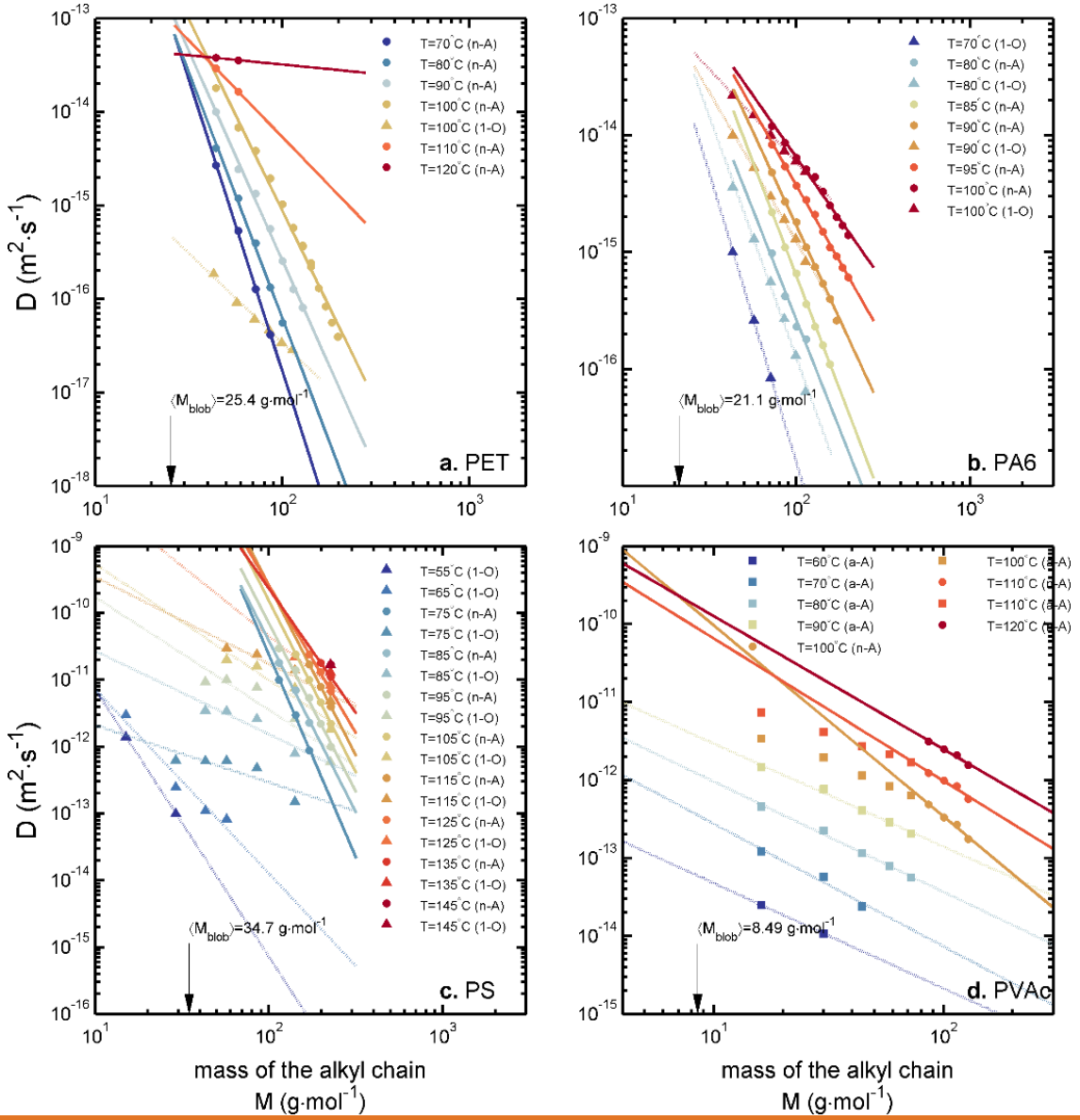
Y. Zhu, F. Welle, O. Vitrac, *Soft-Matter* ***2019, 15, 8912.***

EXTENSIONS TO ANCHORS

SCALING EXPONENTS IN PET, PA6, PS, PVAC

$$\frac{D(M,T)}{D(M_0,T)} \propto \left(\frac{M}{M_0}\right)^{-\alpha(T,T_g)}$$





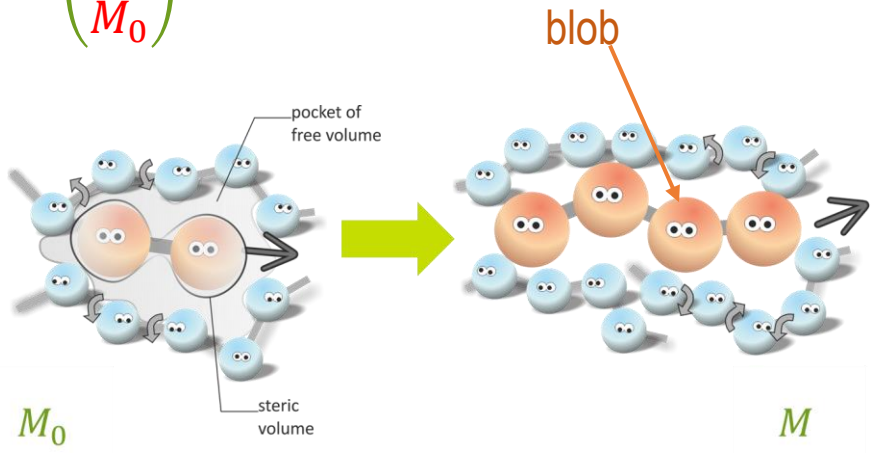
Scaling of diffusion for *n-alkanes, 1-alcohols, alkyl acetates* in undocumented polymers (PET, PA6) and well-known ones (PS, PVAc)

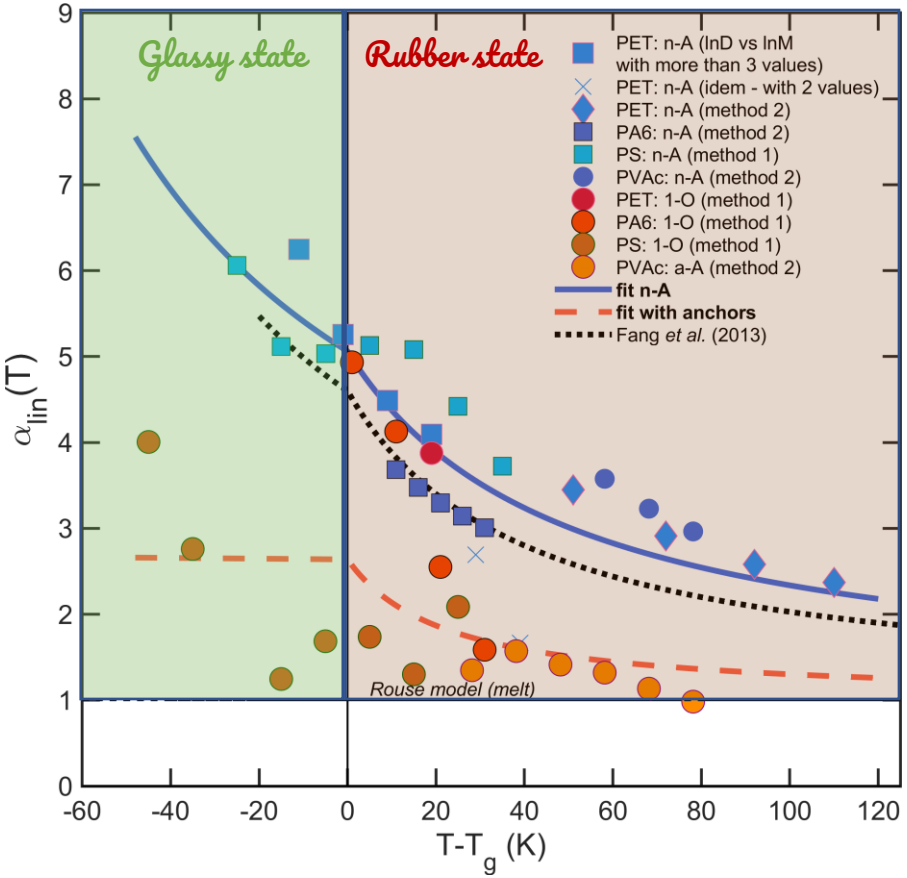
Y. Zhu, F. Welle, O. Vitrac, *Soft-Matter* ***2019, 15, 8912.***

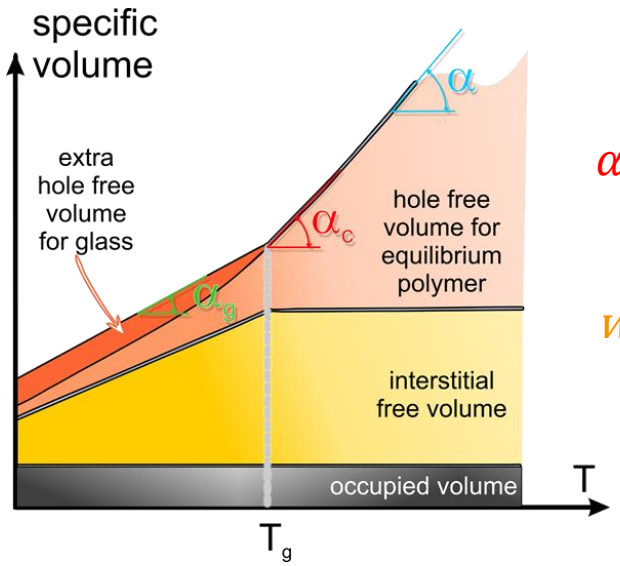
EXTENDED FREE VOLUME THEORY

UNIVERSAL SCALING EXPONENTS

$$\frac{D(M,T)}{D(M_0,T)} \propto \left(\frac{M}{M_0}\right)^{-\alpha_{lin}(T,T_g)}$$

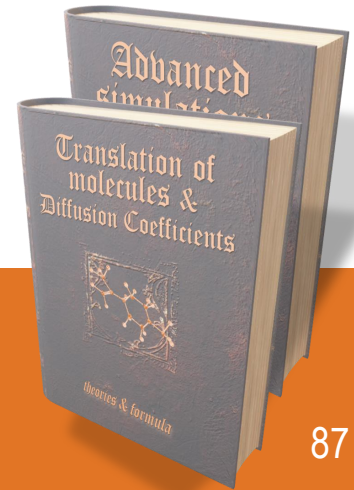






$$\alpha_{lin}(T,T_g) = 1 + \frac{K_\alpha}{r(T-T_g)+K_\beta}$$

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

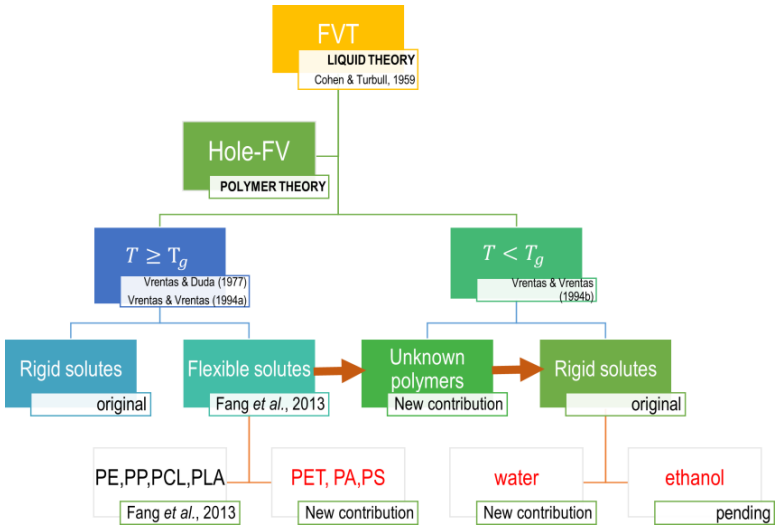


Y. Zhu, F. Welle, O. Vitrac, *Soft-Matter* **2019, 15, 8912.**

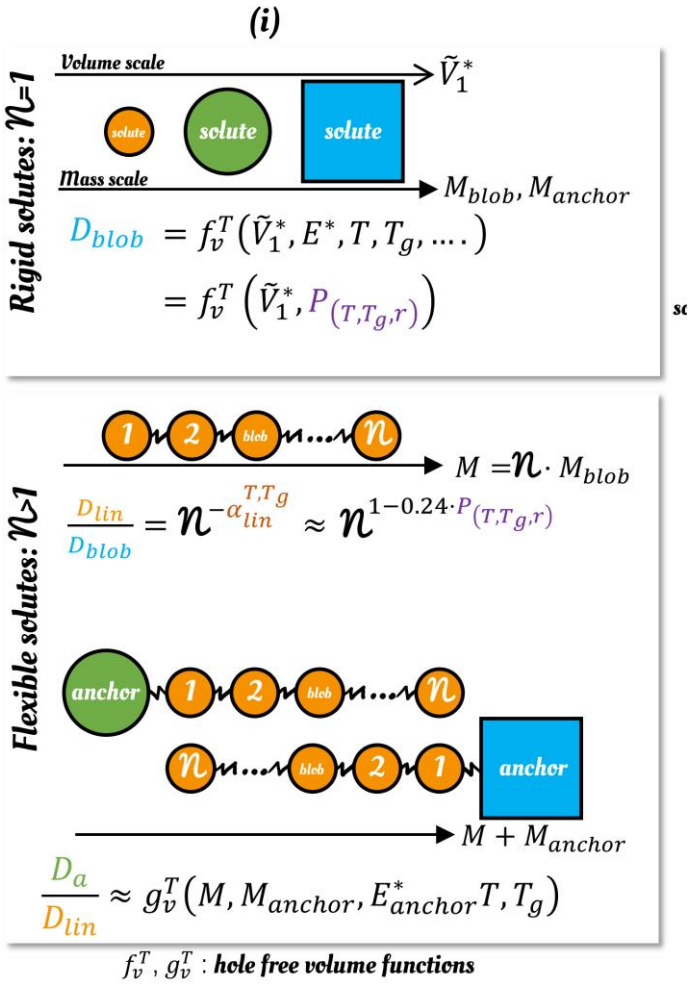
Fang *et al*. *Macromolecules*. 2013;46:874-88

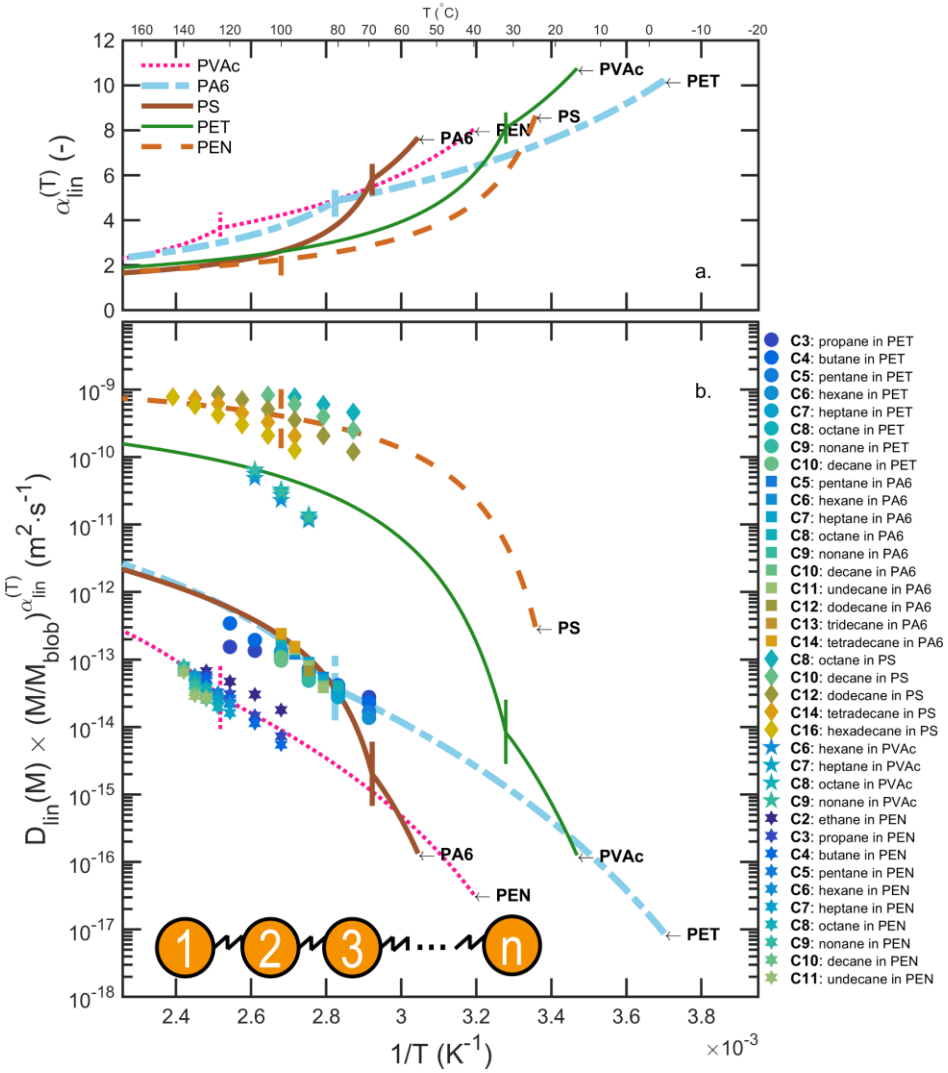
PREDICTIONS WIHTOUT FITTING FOR LINEAR SOLUTES

n-alkanes in PET, PA6, PS, PVAc



$$P(T,T_g) = \frac{\alpha_{lin}(T,T_g) + \beta_{lin}}{a_{lin}(T,T_g)}$$



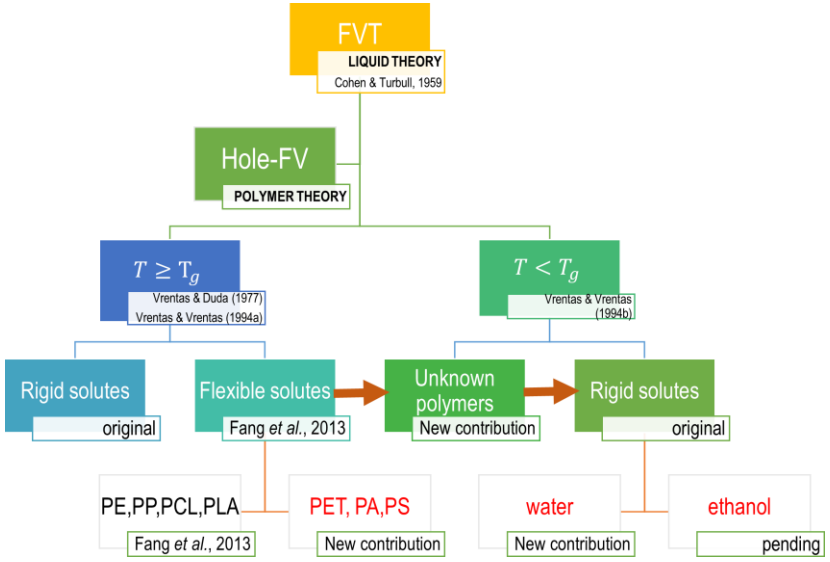


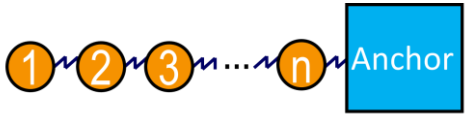
Y. Zhu, F. Welle, O. Vitrac, Soft-Matter 2019, 15, 8912.

$$D(M,T,T_g) = D_0(M_{blob}) \exp\left(-\frac{E^*(M_{blob})}{RT}\right) \exp\left(-\tilde{V}_1^*(M_{blob}) P(T,T_g)\right) \left(\frac{M}{M_{blob}}\right)^{-\alpha_{lin}(T,T_g)}$$

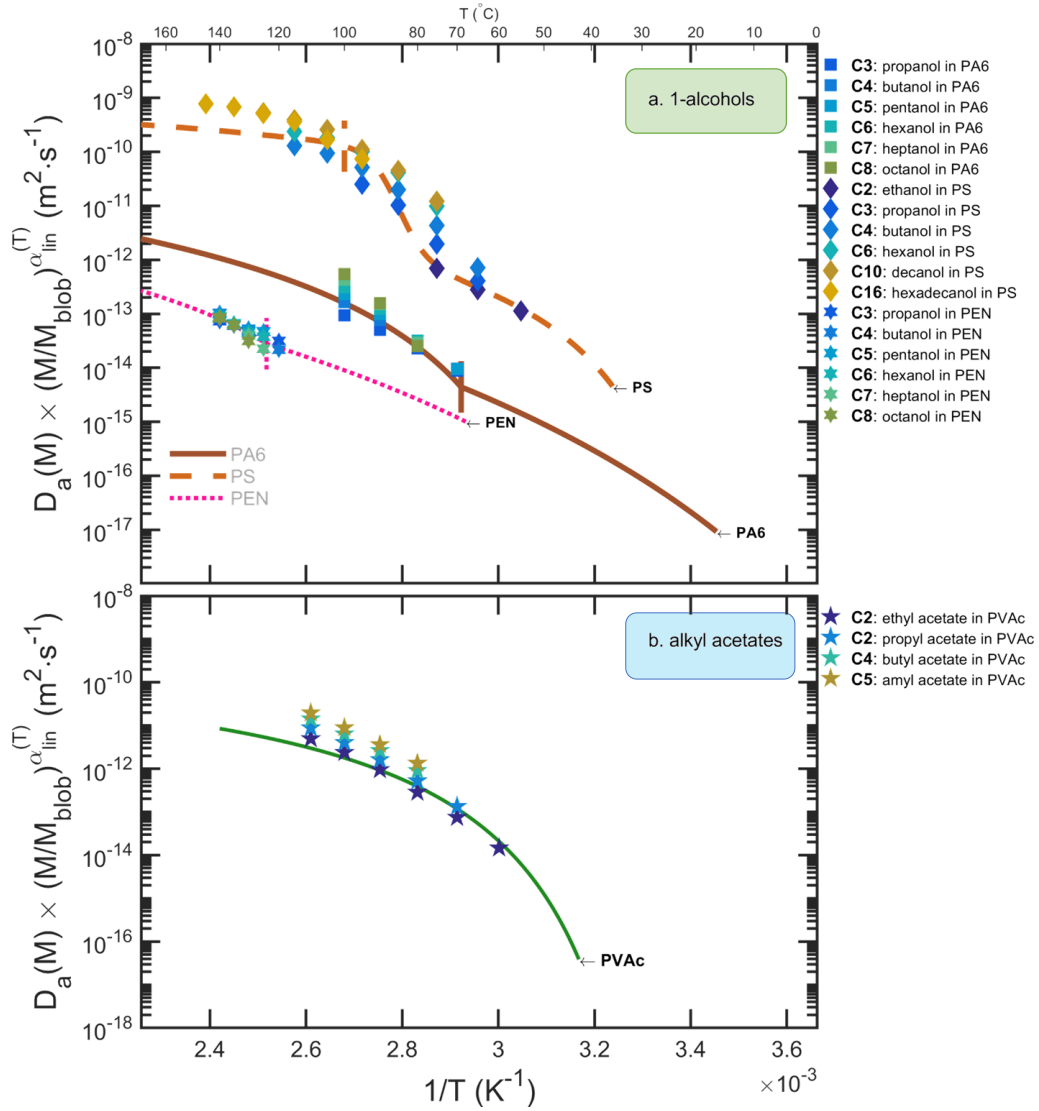
PREDICTIONS WIHTOUT FITTING FOR LINEAR SOLUTES WITH ANCHORS

1-alcohols and alkyl acetates in PA6, PS, PVAc





$$P(T,T_g) = \frac{\alpha_{lin}(T,T_g) + \beta_{lin}}{a_{lin}(T,T_g)}$$

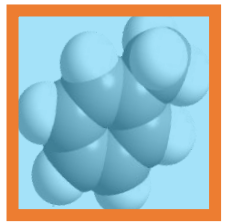


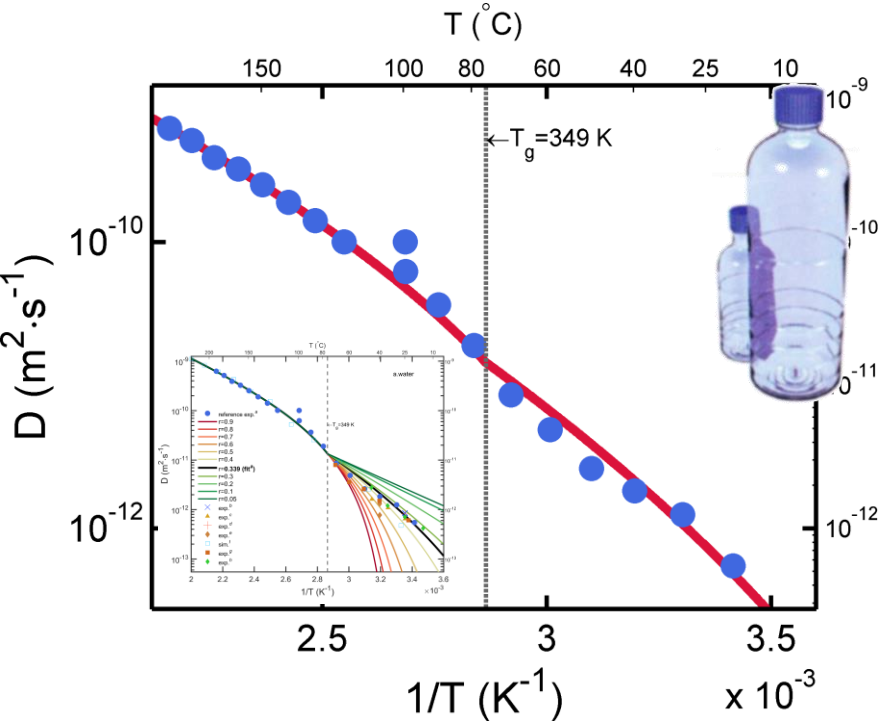
Y. Zhu, F. Welle, O. Vitrac, Soft-Matter 2019, 15, 8912.

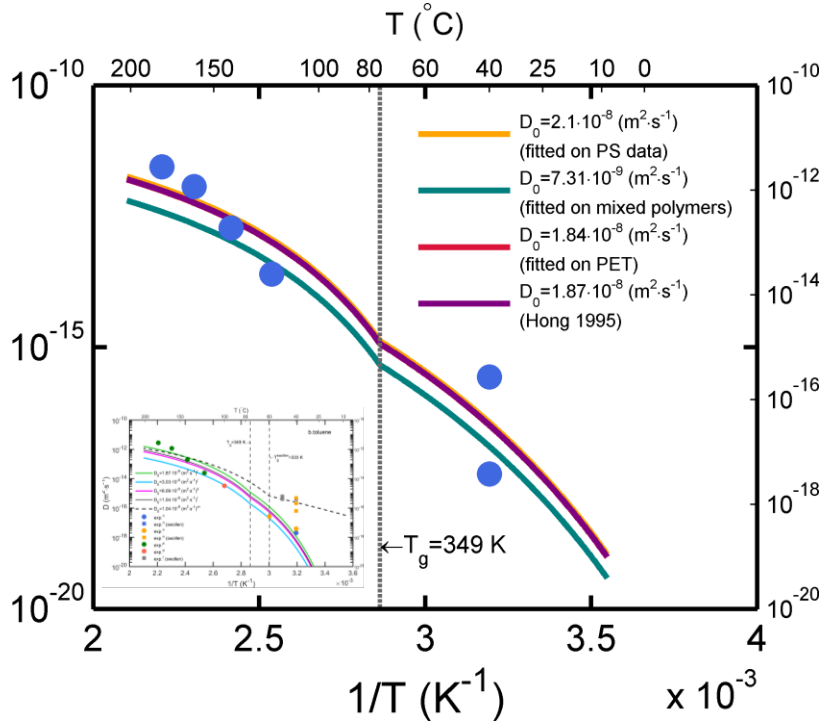
$$D_a(M,T) \approx \exp\left(-\frac{M_{anchor}}{M_{anchor}+M}\frac{E_a^{anchor}(T)}{RT}\right)\left(\left(\frac{M_{anchor}}{M}+1\right)\left(\frac{M_{anchor}+M}{M_{anchor}+M_{blob}}\right)^{\frac{M_{anchor}}{M}}\right)^{-\alpha_{lin}(T)} D(M,T)$$

PREDICTIONS WIHTOUT FITTING FOR RIGID SOLUTES

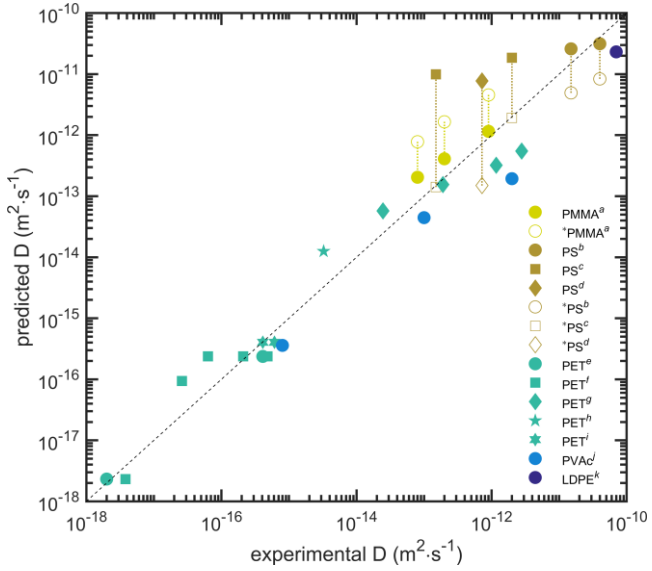
water, toluene in PET







toluene in other polymers



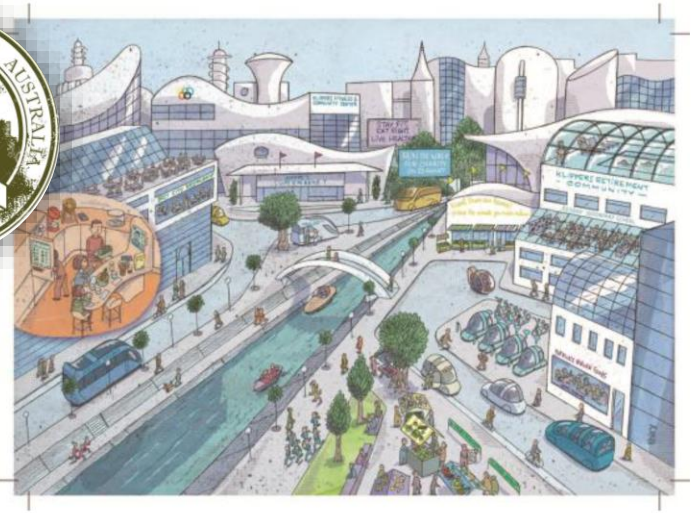
Y. Zhu, F. Welle, O. Vitrac, Soft-Matter 2019, 15, 8912.

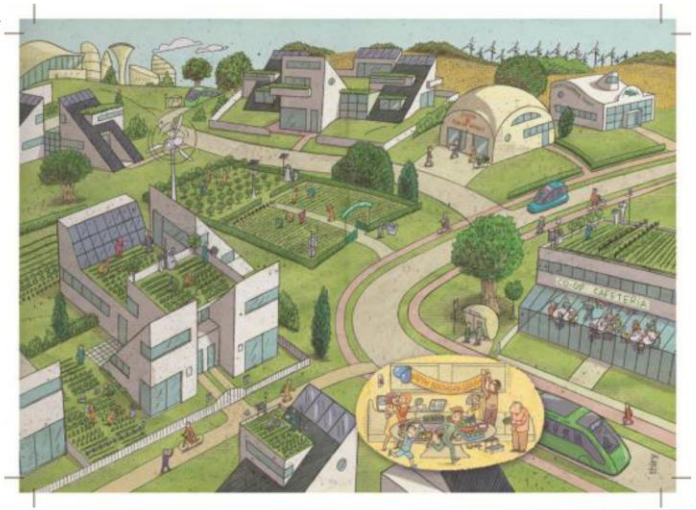
$$D(\xi, T, T_g) \approx D_0(\xi) \exp\left(-\frac{E^*(\xi)}{RT}\right) \exp\left[-\frac{\xi}{0.24}\left(2 + \frac{K_\alpha}{r(T - T_g) + K_\beta}\right)\right]$$

Conclusions & Perspectives

PARIS SMART CITY 2050
Vincent Callebaut Architectures, 2015

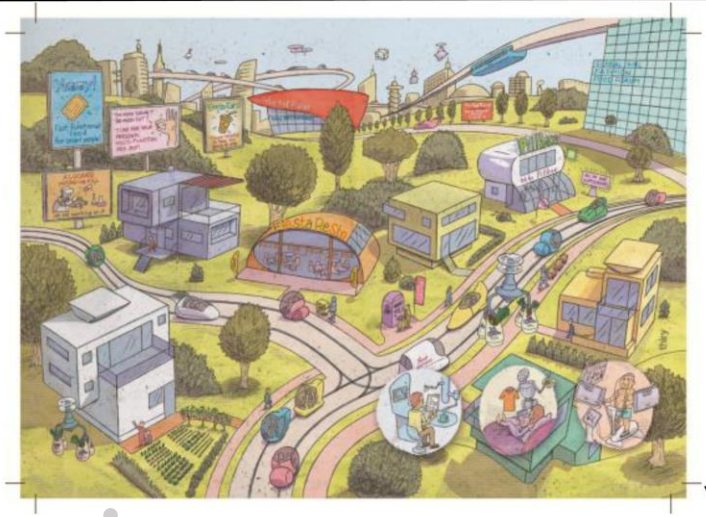
Strong community spirit (sustainable, safety and quality)





Low agriculture commodity and food price

High agriculture commodity and food price

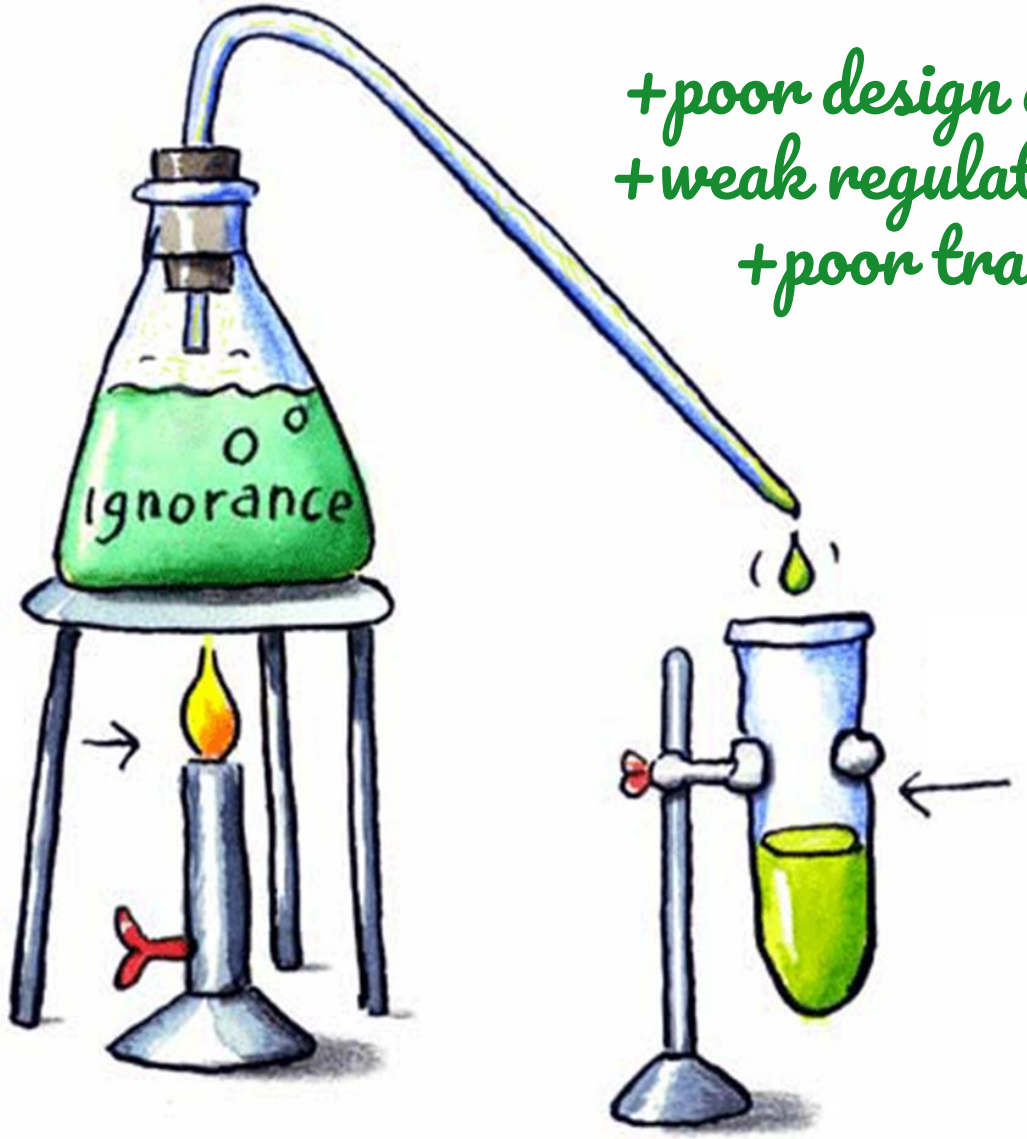


Credits: European Commission, JRC

Individualistic society (individual rights and initiatives valued)

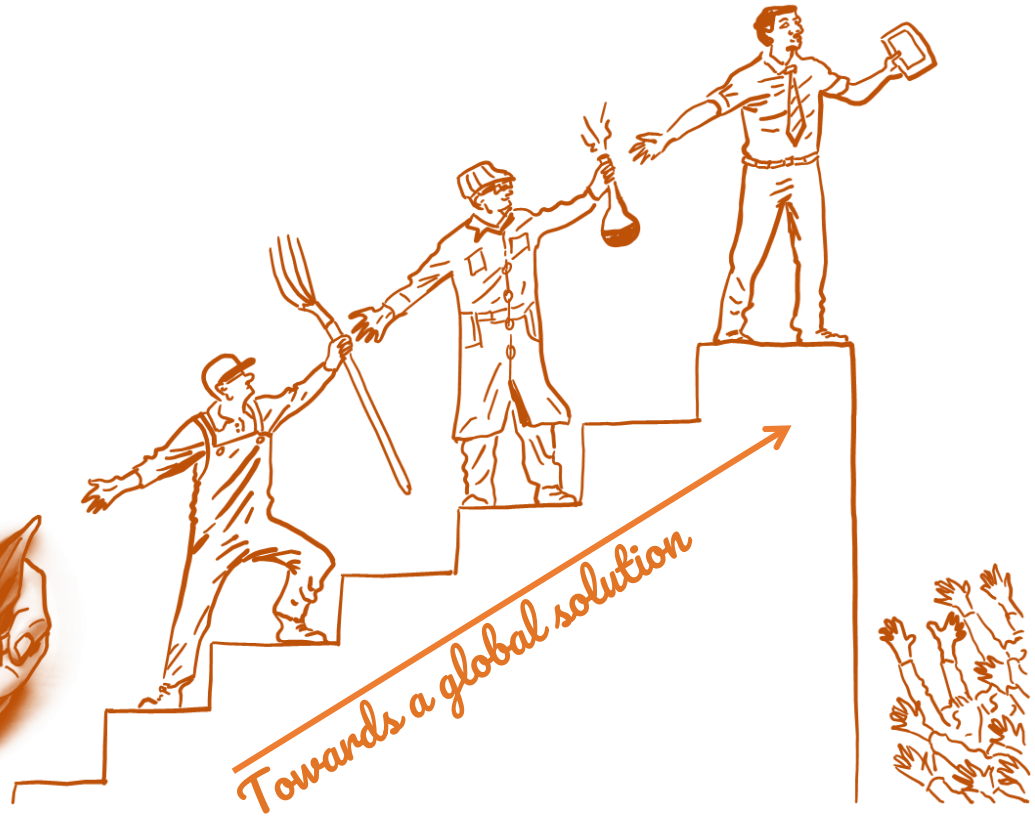
Think BIG with modeling

Let's the food engineer contributes to building the future.



+poor design and GMP
+weak regulation rules
+poor training

=Risk of Contamination + Environmental impact

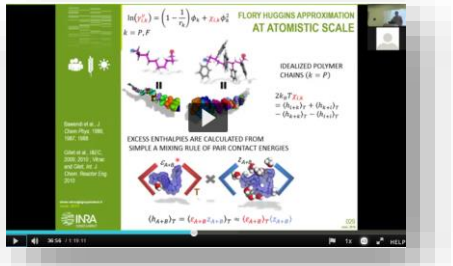


$$ignorance = \frac{IT}{WHAT\ ABOUT\ IT}$$

AgroParisTech

- This lecture: http://modmol.agroparistech.fr/masterEU/

THE SCHOOL OF PACKAGING
MICHIGAN STATE UNIVERSITY



- 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+solutes+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

- RISK ASSESSMENT:
  https://www.youtube.com/watch?v=7LMnc4czpuY

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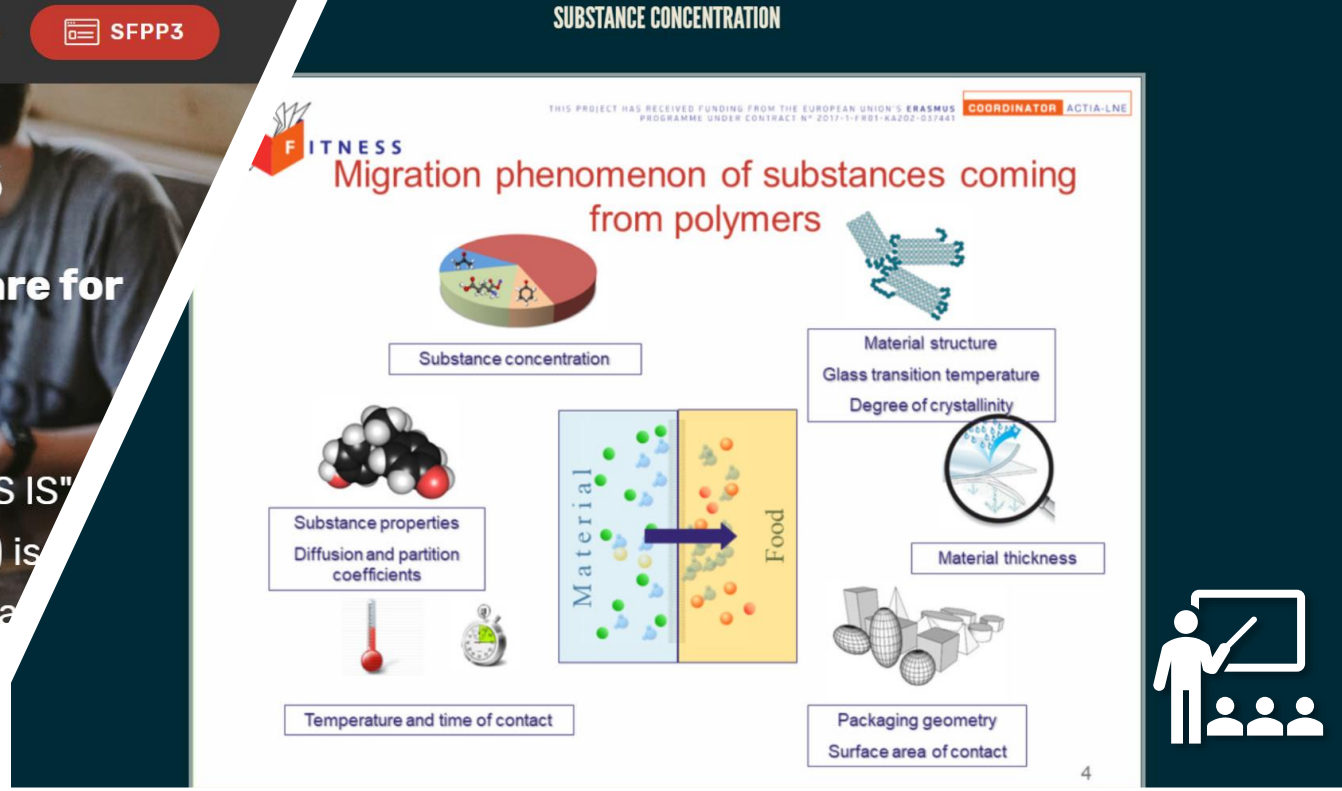
Online lectures

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



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part 1/1	references	extra	casestudies	howto	solutions

Session 4. Mass transfer in food packaging - Unit 4.2. Migration modeling in m onomaterial s

4.3 Modelling for multi-materials, multi-steps process

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

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part 1/1	references	extra	casestudies	howto	solutions