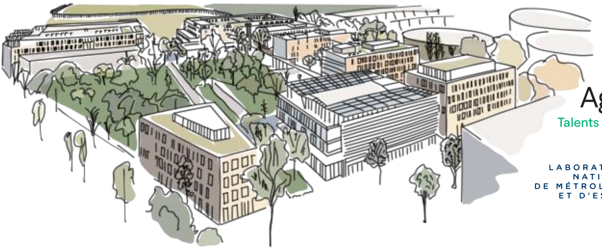


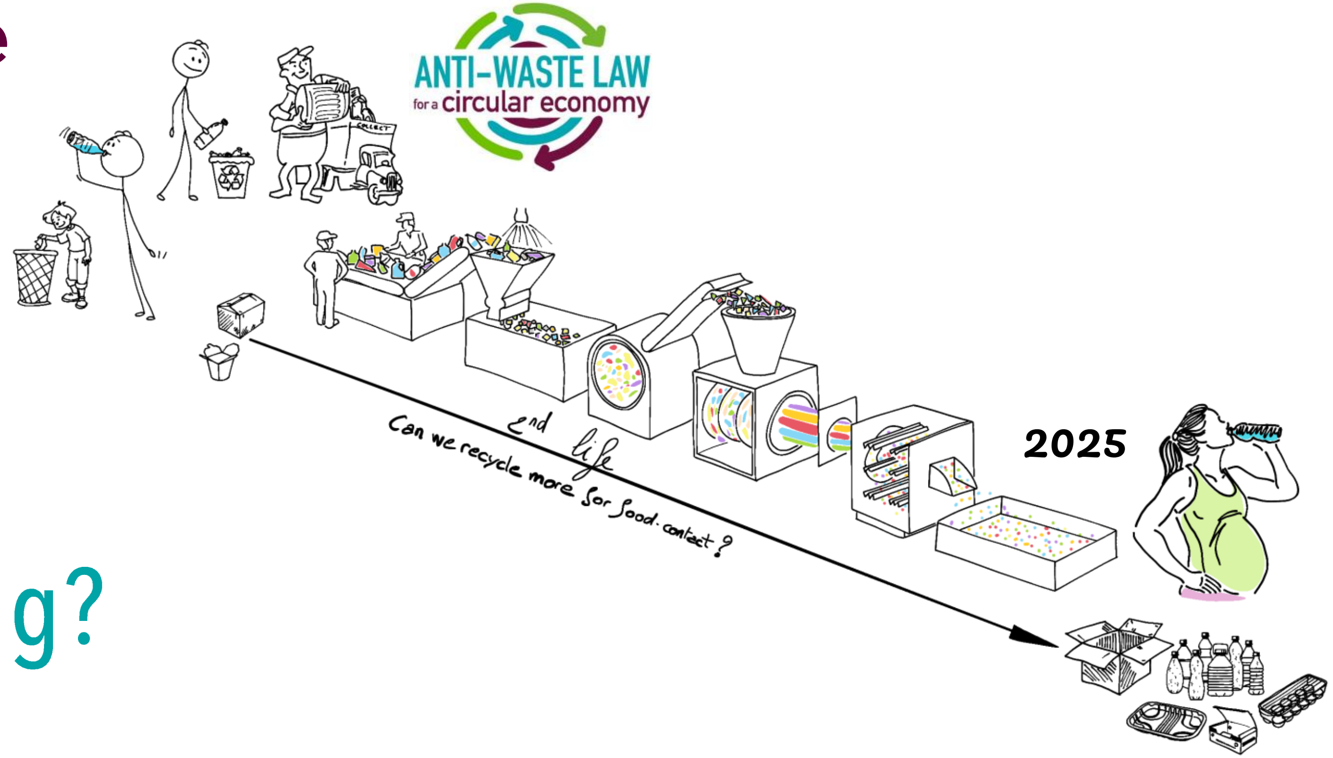
INRAE Department Food, Bioproducts and Waste

AgroParisTech Talents for a sustainable planet

Laboratoire National de Métrologie et d'Essais LNE

université PARIS-SACLAY

Last revision: 2022-05-27



Who we are?
What are we doing?

UMR 0782 SayFood Food & Bioproduct Engineering | UMT ACTIA 22.07 UMT SAFEMAT SAFETY OF PACKAGING

Olivier Vitrac, olivier.vitrac@agroparistech.fr, senior scientist at INRAE (https://www.inrae.fr/en)

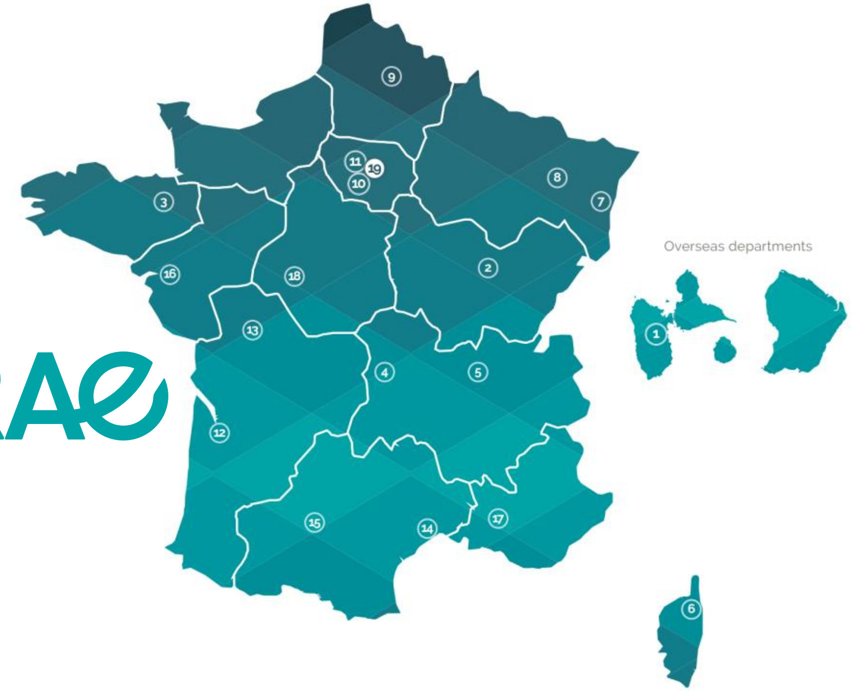
Phuong-Mai Nguyen, phuong-mai.nguyen@lne.fr, research engineer at LNE (https://www.lne.fr/en)

Hosting academic institutes

INRAE

National Research Institute for Agriculture, Food and the Environment (INRAE)

Staff: 12,000 – 200 laboratories - >1000 PhD students



https://www.inrae.fr/en

AgroParisTech

National Research Institute for Agriculture, Food and the Environment (INRAE)

Staff: 833 – 20 laboratories, 275 PhD students – 18,000 alumni

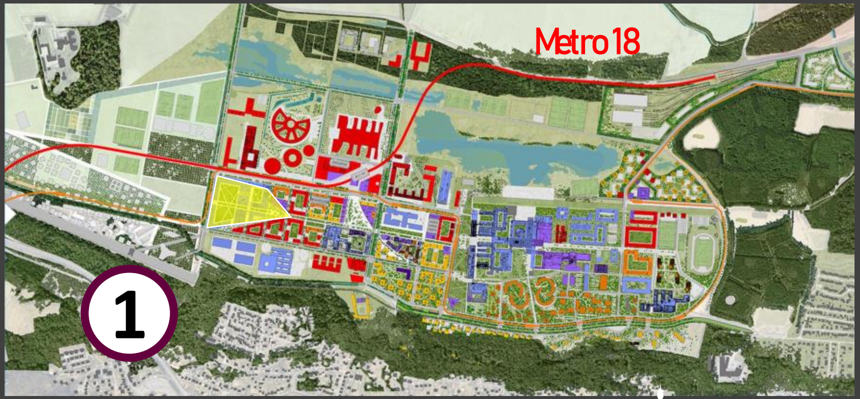
AgroParisTech
Talents for a sustainable planet

https://www.agroparistech.fr

INRAE AgroParisTech
Talents for a sustainable planet

UMR 0782

Joint Research Unit between INRAE and AgroParisTech – founding members of University Paris-Saclay



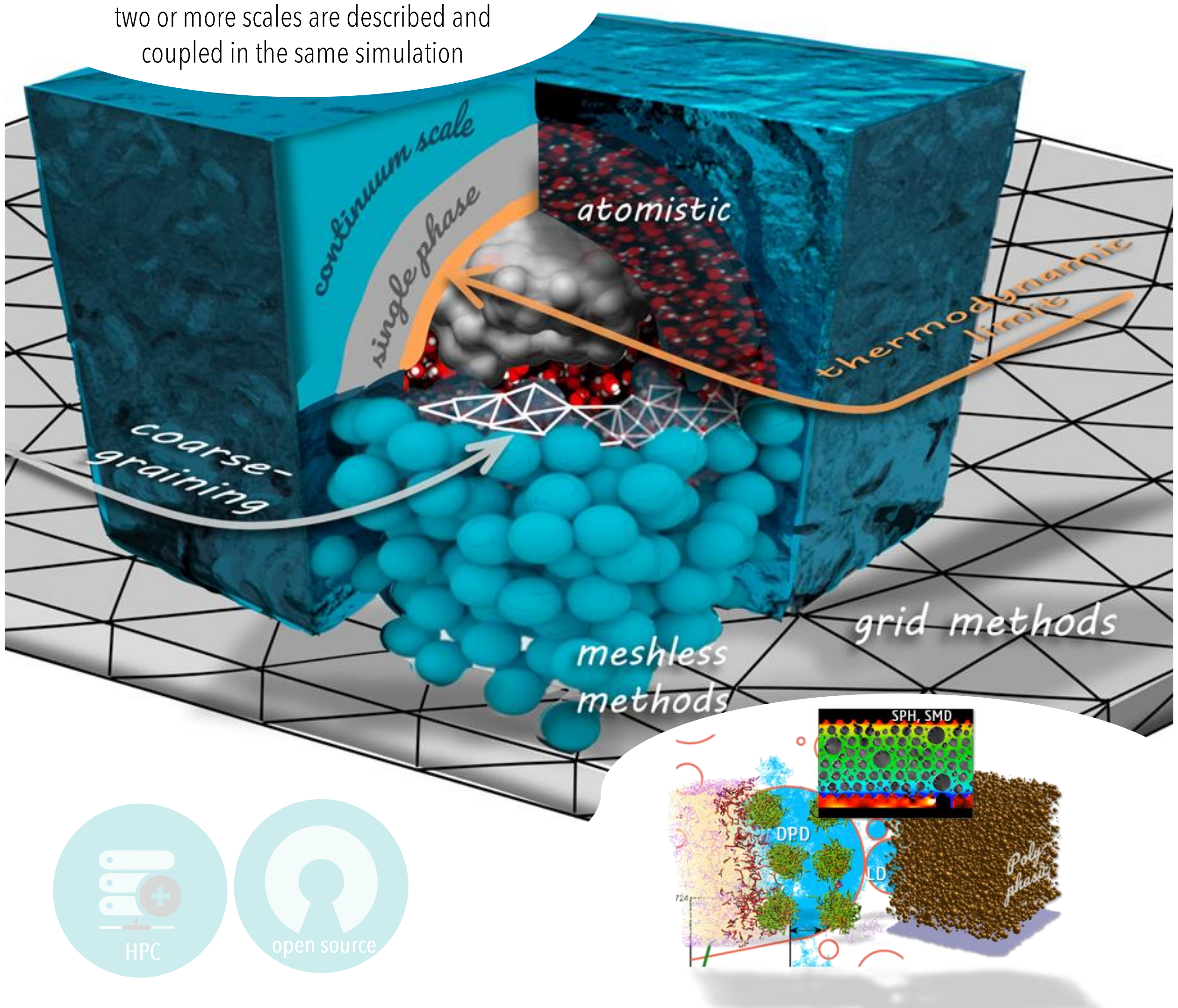
SayFood

Food & Bioproduct Engineering

https://www6.versailles-grignon.inrae.fr/umr-sayfood

SayFood group modeling and computational engineering research axis: Concurrent multiscale modeling

- Zoom in on details down to molecules within the same simulation (food, packaging)
- Breakthrough approaches: integration of chemical and structural information, image-based modeling, chemical reactions.
- Public-private partnership



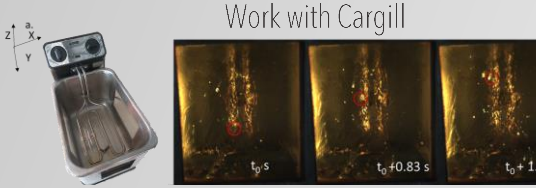
SayFood
Food & Bioproduct Engineering

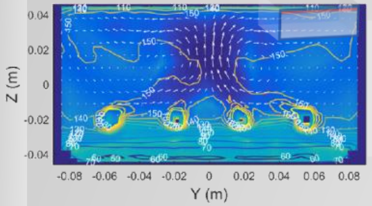
HPC

open source

Illustrations application to deep-frying

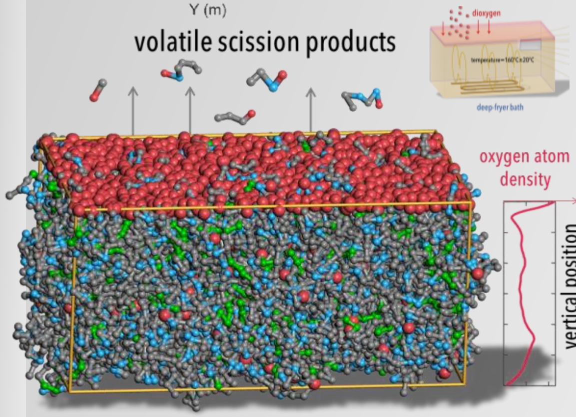
Work with Cargill



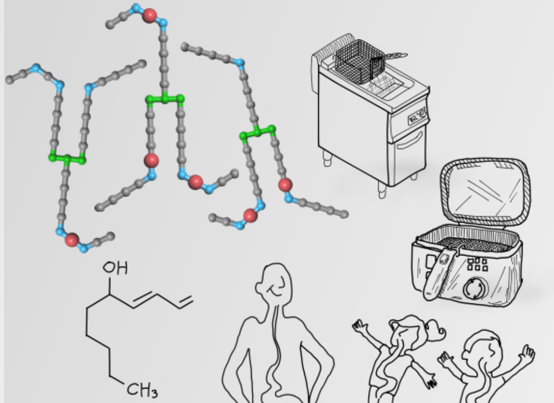


Physics of fluids 2021. 33: 085105 .

volatile scission products



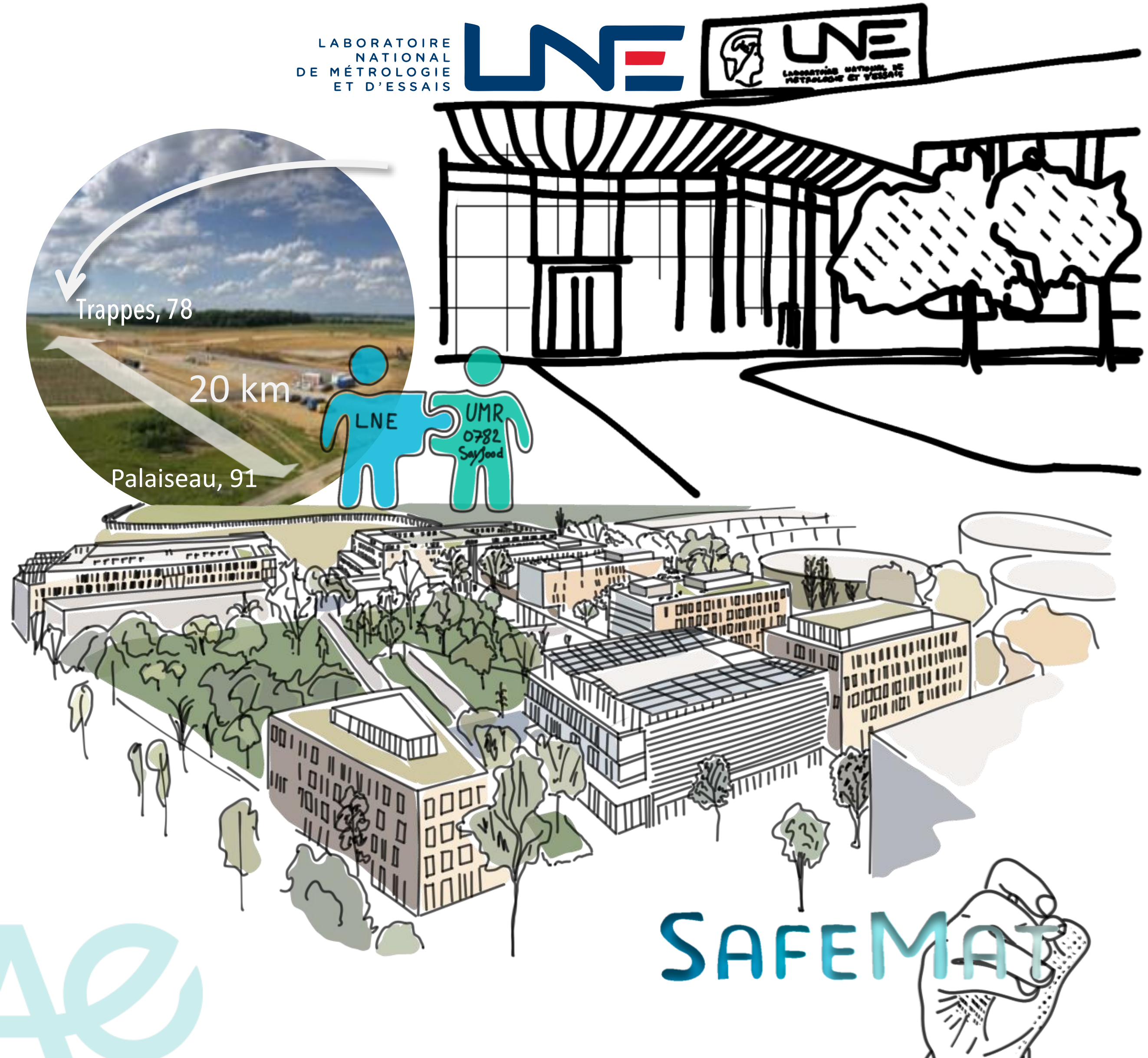
elementary volume at the extreme surface



A common laboratory between LNE and UMR SayFood

UMT ACTIA 22.07 SAFEMAT « Safe Materials for Food Contact »

UMT SAFEMAT SAFETY OF PACKAGING



- accredited by the French ministry of Agriculture and Food (since 2017)
- Competent organization for EFSA (for both LNE and INRAE) on food contact materials
- **LNE = national reference laboratory** for food contact materials
- Complementarity of means (computation, analytical chemistry), two groups of SayFood involved
- **24 persons (10 full-time eq.)**
- Administrative coordinator Jean-Mario Julien (LNE)
- Scientific coordinator **Olivier Vitrac (INRAE)**

LNE: MEASUREMENTS AND STANDARDS

LABORATOIRE NATIONAL DE MÉTROLOGIE ET D'ESSAIS

- **8 sites**

  France (Paris, Trappes, Saint-Denis, Nîmes, Saint-Etienne, Poitiers)

  USA (Washington DC)

  China (Hong Kong)

- **Resources**
  - ✓750 staff
  - ✓55,000 m^2 of laboratory space
  - ✓Extensive network of partners
  - ✓77.2 M€ revenue including 55,6 M€ sales
  - ✓25 M€ investment over last five years
  - ✓25% of budget allocated to R&D

LNE: EXTENSIVE SCIENTIFIC AND TECHNOLOGICAL EXPERTISE

Research

Tests and calibration

Technical assistance

Certification

Training Information

LABORATOIRE NATIONAL DE MÉTROLOGIE ET D'ESSAIS

UMT SAFEMAT

SHARED EQUIPMENTS AND PLATFORMS

UMT SAFEMAT SAFETY OF PACKAGING

Mass spectroscopy high resolution

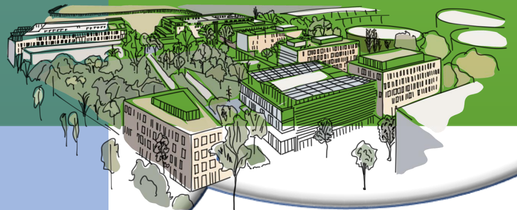
Spectroscopies NMR ^{1}H, FTIR-ATR, Fluo.

78

- High performance computer
- Multiphysics modeling
- Material characterization
- Permeability
- Chemometrics
- Risk analysis
- Databases
- Material processing
- Etc.

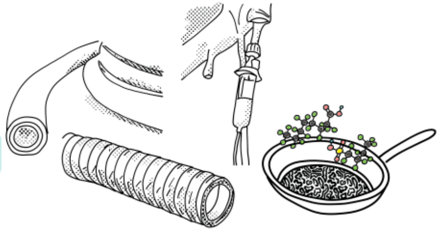
91

Molecular modeling
Thermodynamic characterization
GC-MS 2D
Chemical imaging (UV, RAMAN)
Mixer

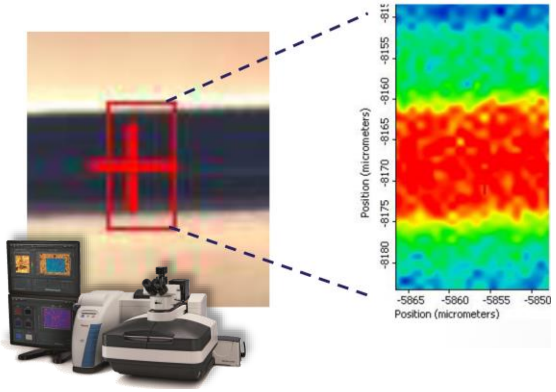


Analytical chemistry
Nanomaterial platform
Metrological platform CARMEN
Test benches (e.g., aging, flow test)

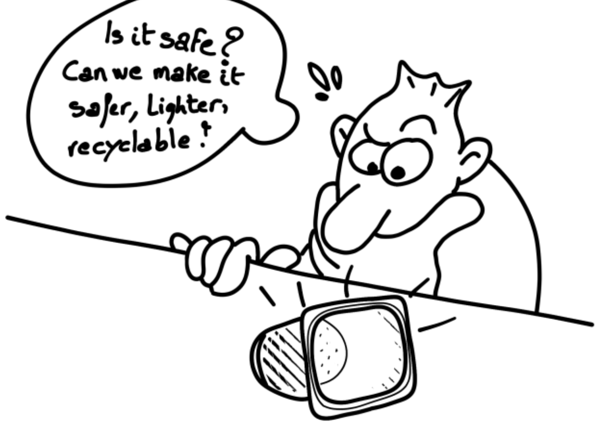
UMT CORE



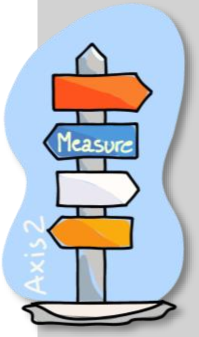
NMR ^{1}H



3 AXIS R&D (food industry, packaging)
PREDICT, MEASURE, DISSEMINATE & COMMUNICATE

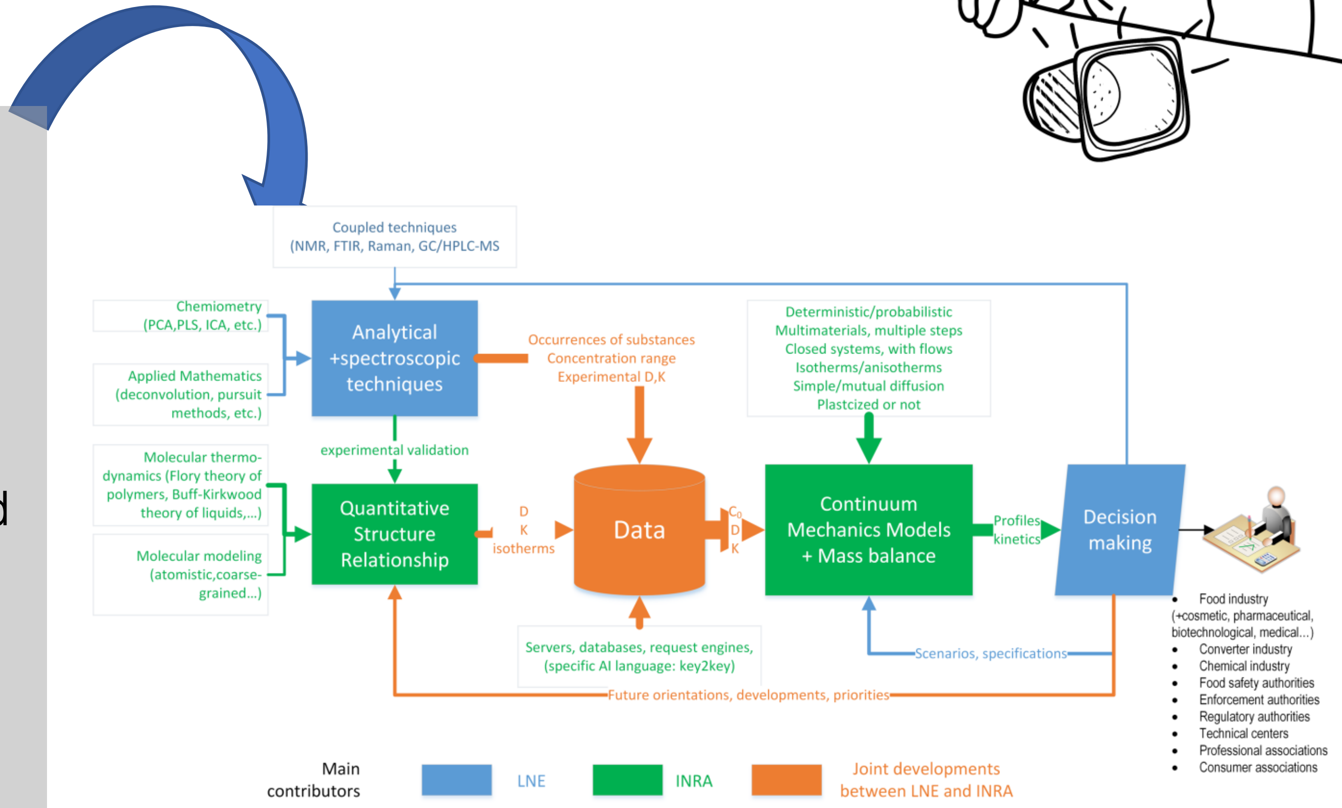


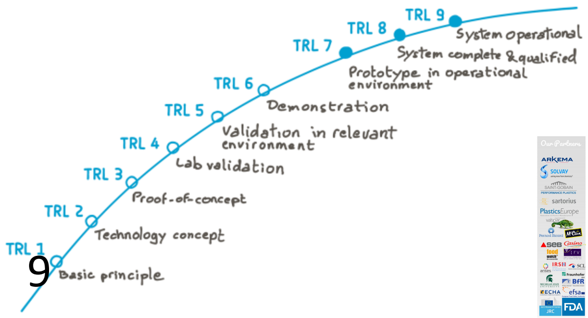
Consolidation and validation of knowledge on MOLECULAR PHENOMENA, contamination pathways, barrier properties, means of controlling them...



Develop ad-hoc **METROLOGY** of thermodynamic and transport properties, high throughput **ANALYTICAL CHEMISTRY**, ad-hoc test benches (flow, aging)

- **DISSEMINATION** to the industry of tools, safe design concepts of substances, materials, packaging





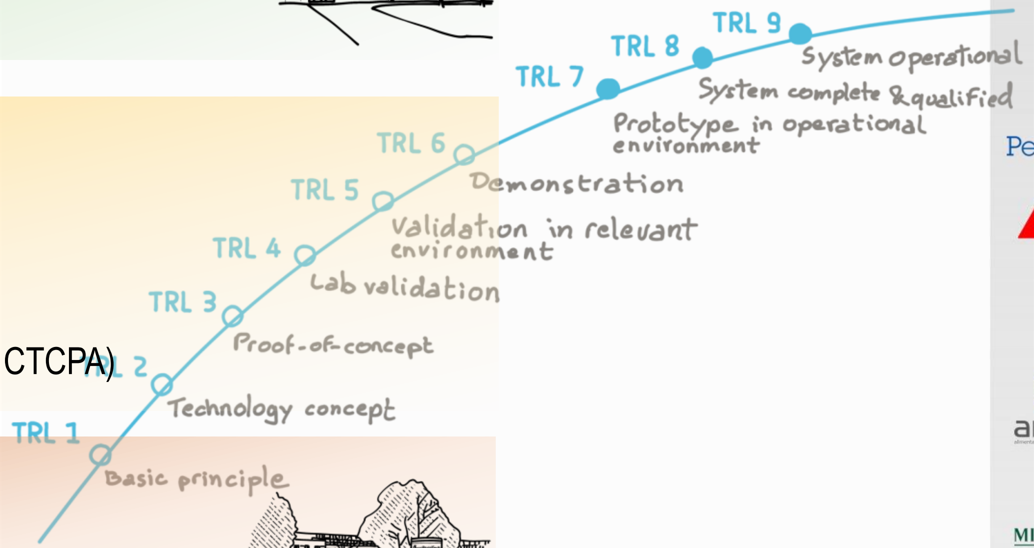
OUR STRATEGY

High TRL

- ✓ Services and training for food industry and distributors (LNE)
- ✓ H2020 program (ex. MyPack)
- ✓ ERASMUS+ program (e.g. FITNess)
- ✓ Collaboration agreement with the chemical industry
- ✓ Methodological transfer to related sectors (cosmetics, etc.)
- ✓ Synthesis works (in progress)
- ✓ Communications (MATBIM, ACS...)

Intermediate TRL

- ✓ Partnership research with CIFRE theses
- ✓ ANR FoodSafeBio Pack
- ✓ Calculation platform, database
- ✓ Interactions with other industrial technical centers (IPC, CTCPA)



Low TRL

- ✓ Theses on own funds (chemometrics, life cycle)
- ✓ Integration for part in CIFRE theses
- ✓ Collaboration with Fraunhofer, FDA
- ✓ Formalization of ASEM (Analysis of Systems at the Molecular Scale) concepts

Our Partners

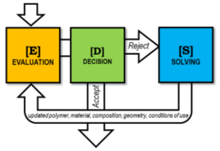
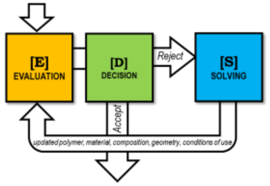
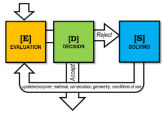
New 5 year project : Unit SAFEMAT 2.0

renewal period 2022-2026

LOI ANTI-GASPILLAGE pour une économie circulaire

UMT SAFEMAT SAFETY OF PACKAGING

Goals UMT 2.0

Public mission	Recycle	Reduce	Reuse
Support the evolution of European regulations + AGEC decrees		pas de contribution	
Supporting the substitution of materials			
Make the product safe and ensure the performance of the packaging			

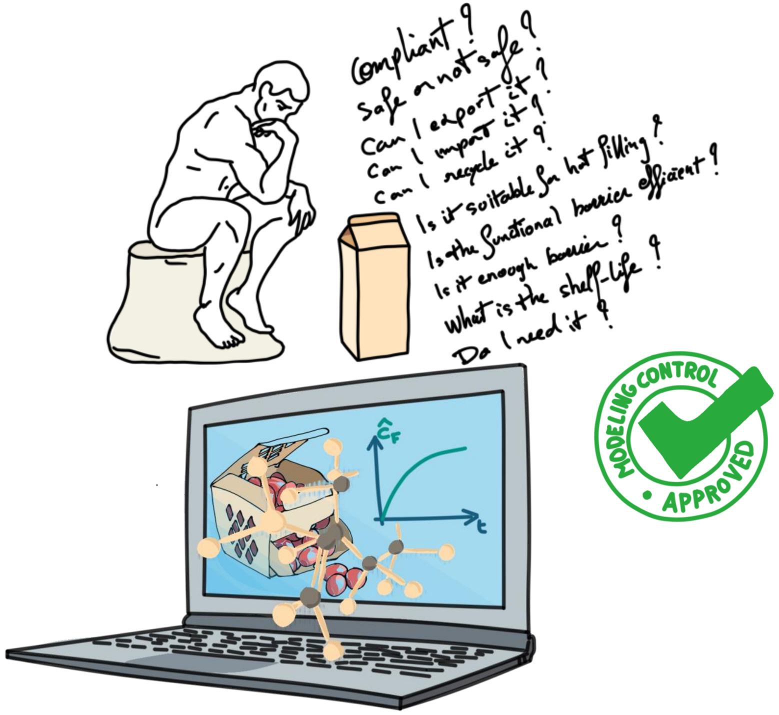
Objectives of the 3Rs Decree

5-year project built around 3 R&D axis (TRL 1-7)

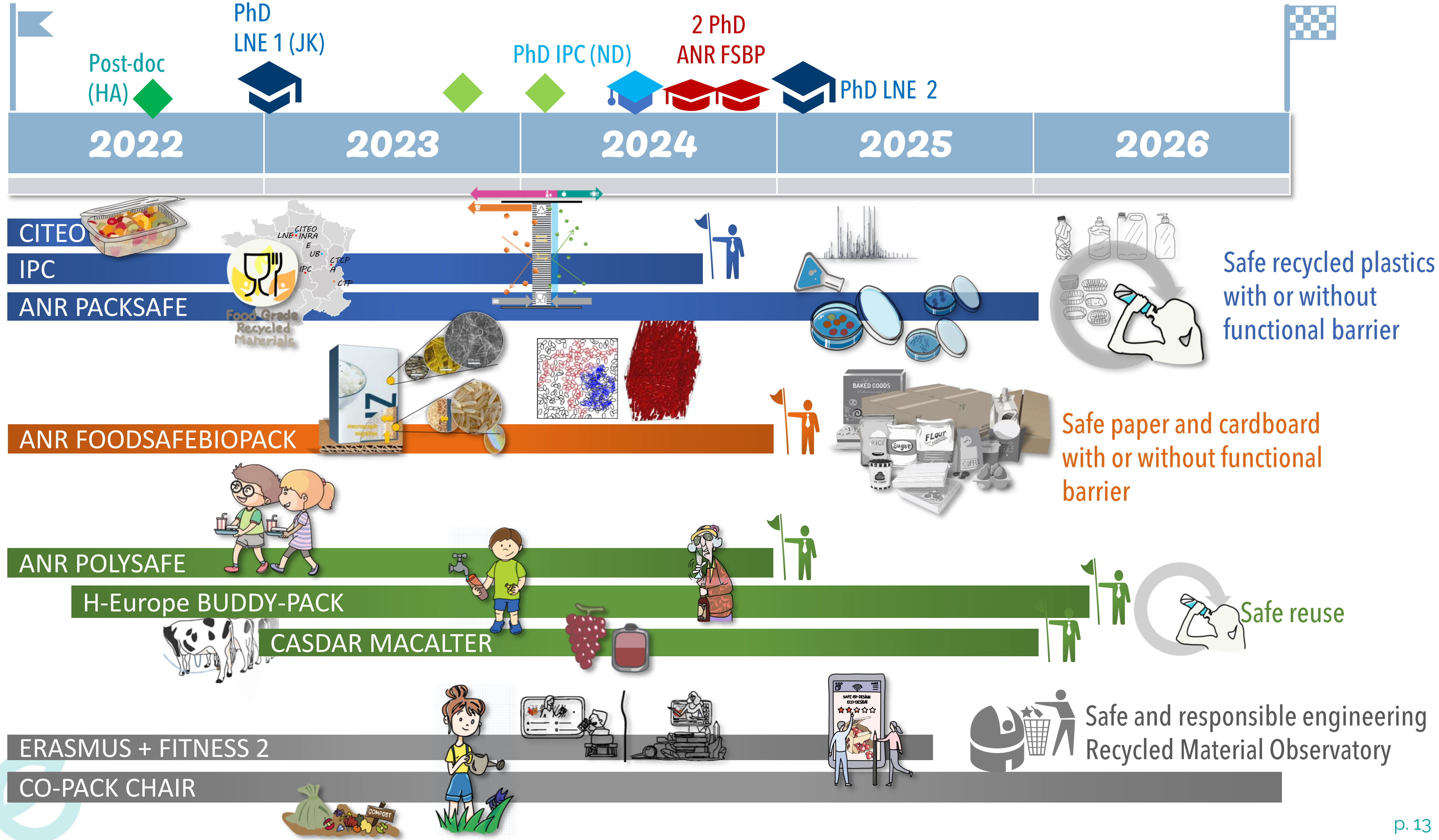
AXIS 1
FOOD GRADE RECYCLATES
(recognized)

AXIS 2
AGING OF RECYCLED MATERIALS, REUSED, REEMPLOYED, COMPOSTABLE
(to be built)

AXIS 3
ENGINEERING INTEGRATING THE COUPLE PACKAGING-PRODUCT
(to federate)



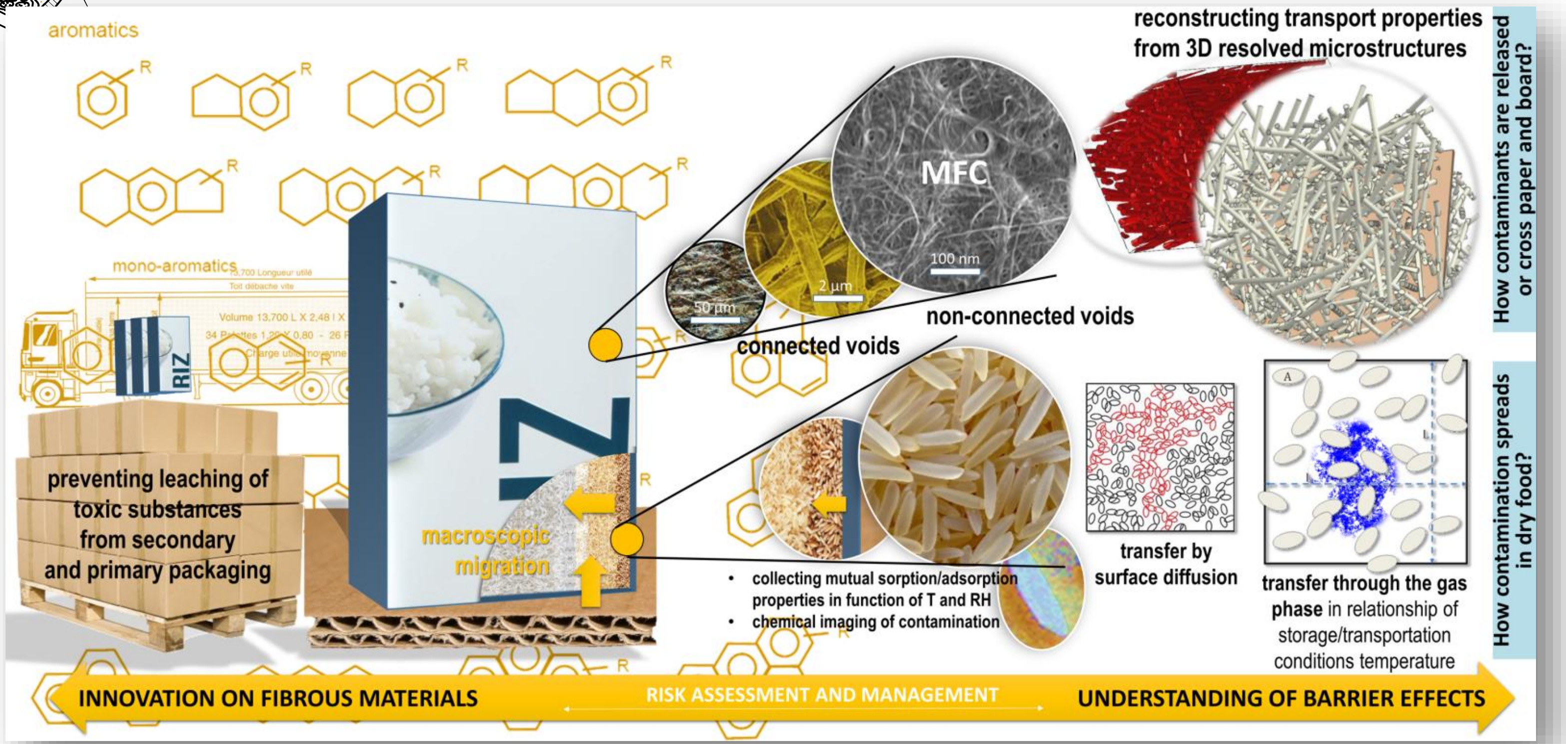
Mission of public interest, support the evolution of regulations, reconcile safety and performance



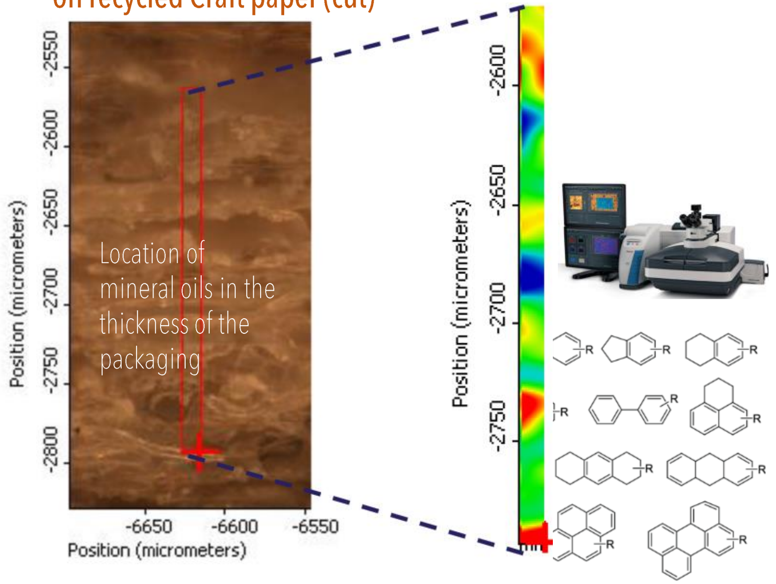
Post-doc (HA)
PhD LNE 1 (JK)
PhD IPC (ND)
2 PhD ANR FSBP
PhD LNE 2
2022
2023
2024
2025
2026
CITEO
IPC
ANR PACKSAFE
Food Grade Recycled Materials
Safe recycled plastics with or without functional barrier
ANR FOODSAFEBIOPACK
BAKED GOODS
RICE
Sugar
FLour
Safe paper and cardboard with or without functional barrier
ANR POLYSAFE
H-Europe BUDDY-PACK
CASDAR MACALTER
Safe reuse
ERASMUS + FITNESS 2
CO-PACK CHAIR
COMPOST
Safe and responsible engineering
Recycled Material Observatory

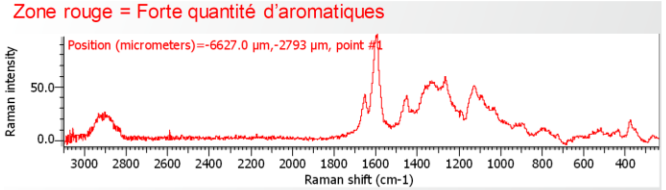
FoodSafe BioPack

(2021-2024, coord. O. Vitrac) – Illustration of the scientific approach

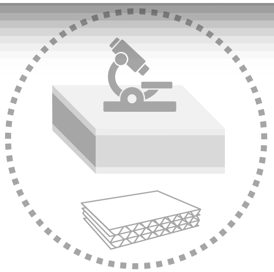


Chemical imaging (Raman) on recycled Craft paper (cut)





T1. Production of reference materials



T2. Characterization of materials and functional barriers

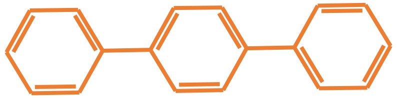
T3. Direct/indirect characterization of ores/sources

T4. Thermodynamic description of mass transfer

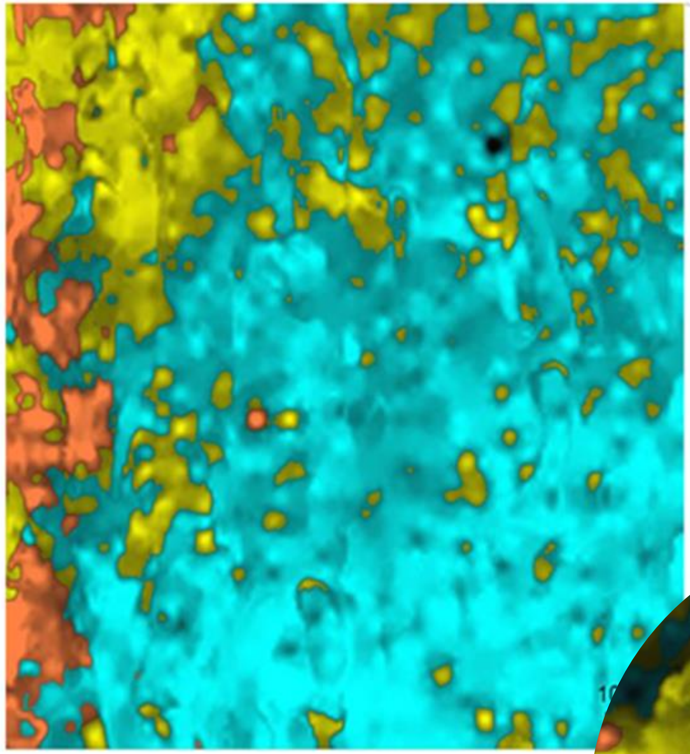
T5. Multiscale modeling / validation

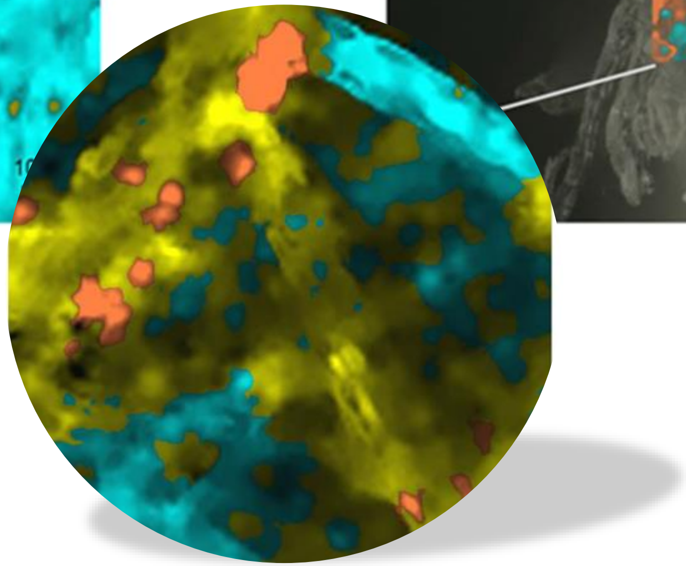
T6. Risk assessment and performance optimization

Chemical imaging – Raman spectroscopy on paper

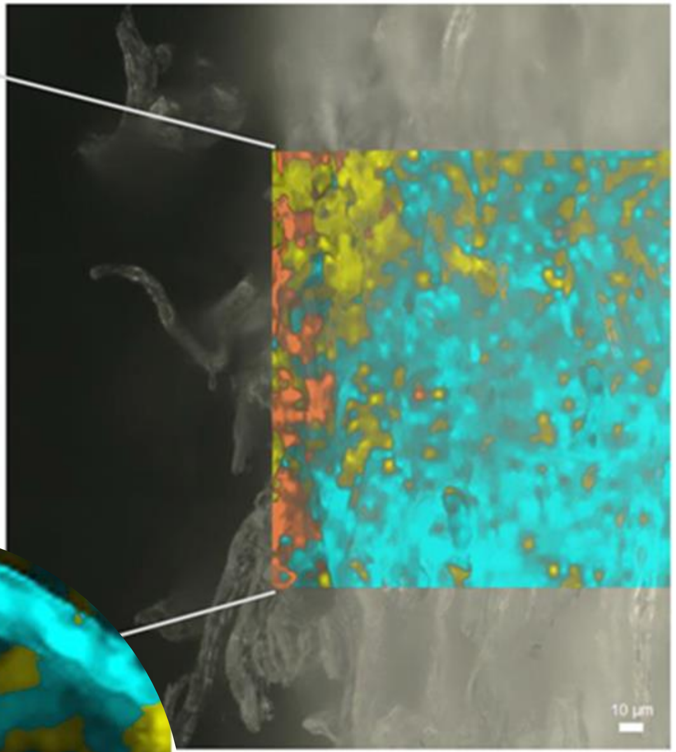


Raman image of p-terphenyl/cellulose

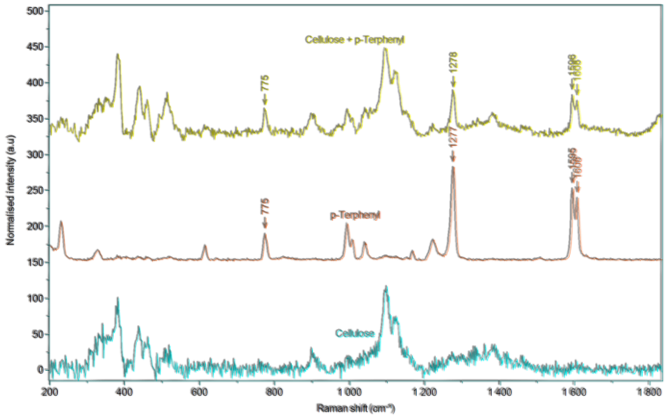




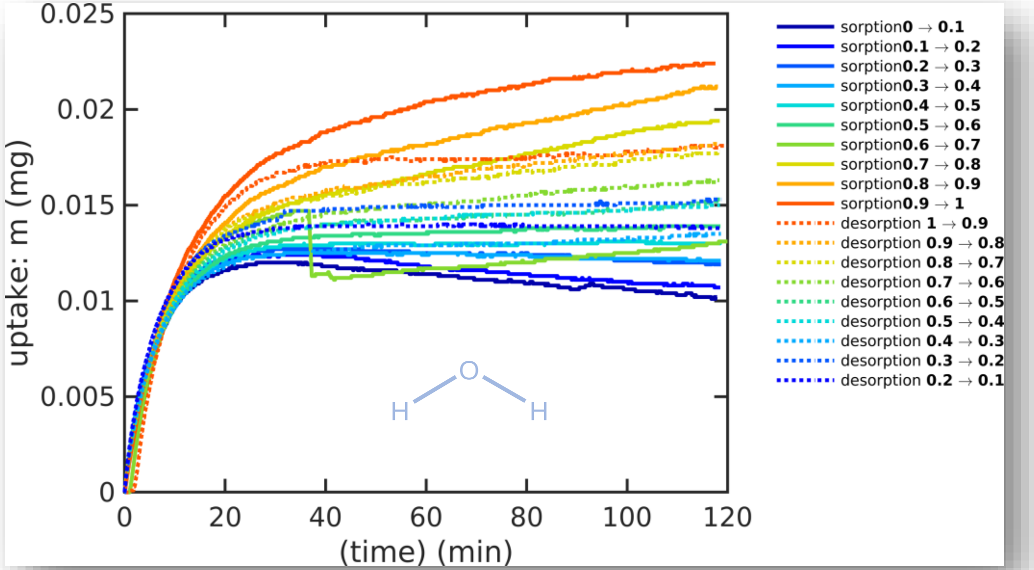
Overlay of Raman image on video image



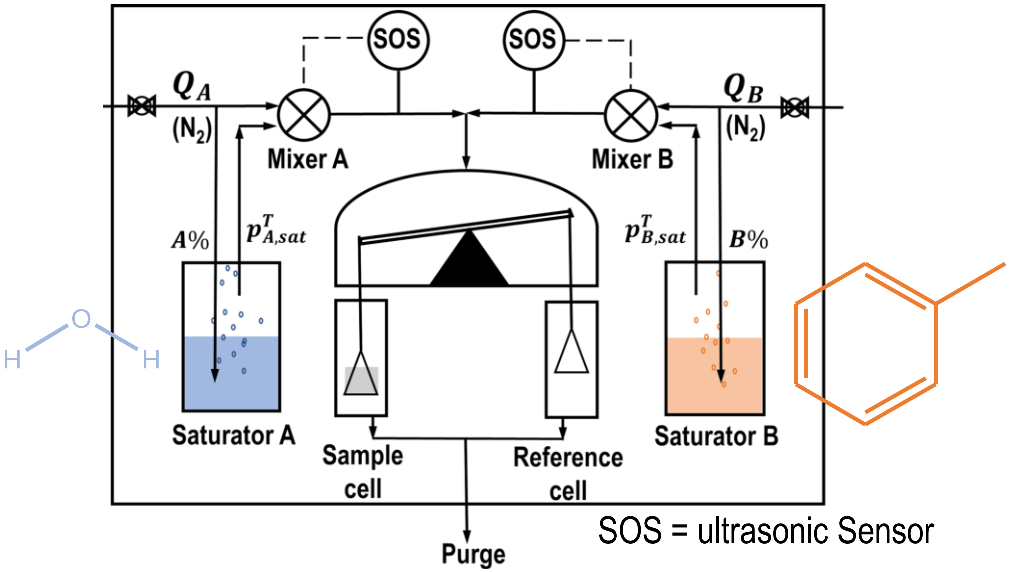
Reference spectra from raman image

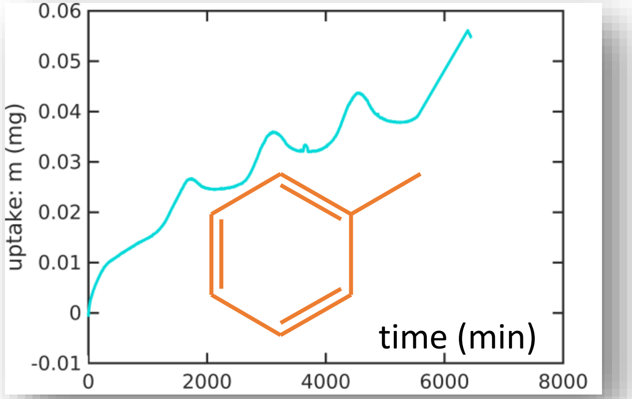


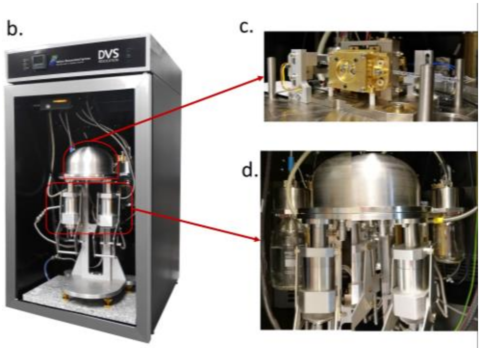
Thermodynamic measurements (e.g. 25 µm thick - PET)



Automatic microbalance





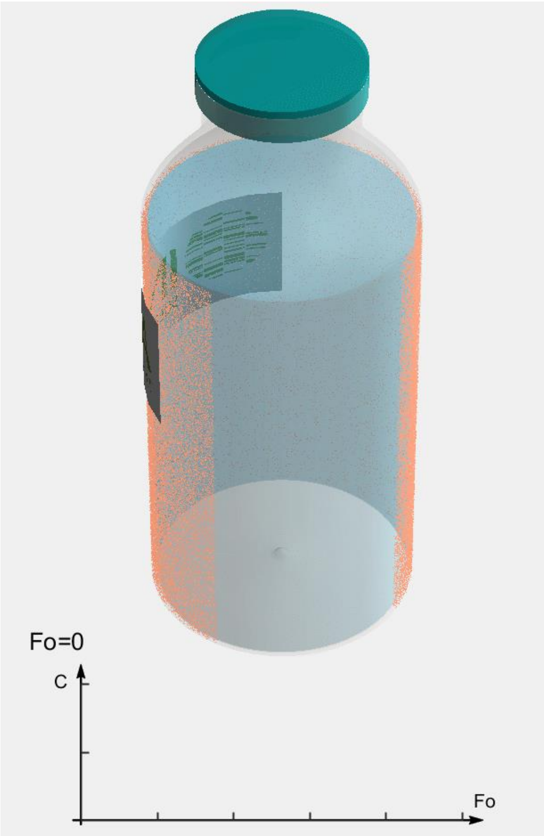


FUNCTIONAL BARRIERS

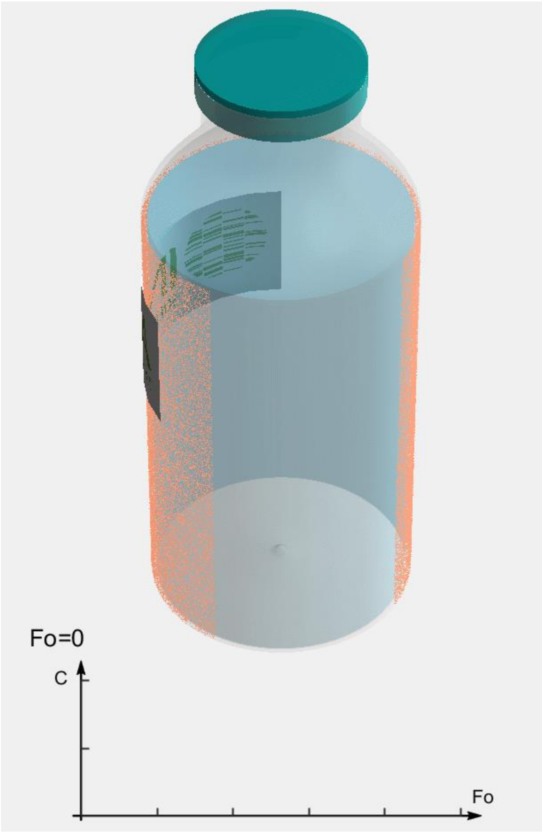
Polymer with high cohesive energy and dense, and recyclable: EVOH…

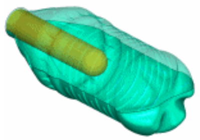
Plasma treatments (SiOx), other technologies (MFC)

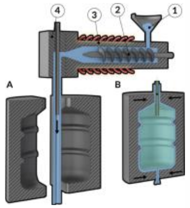
monolayer

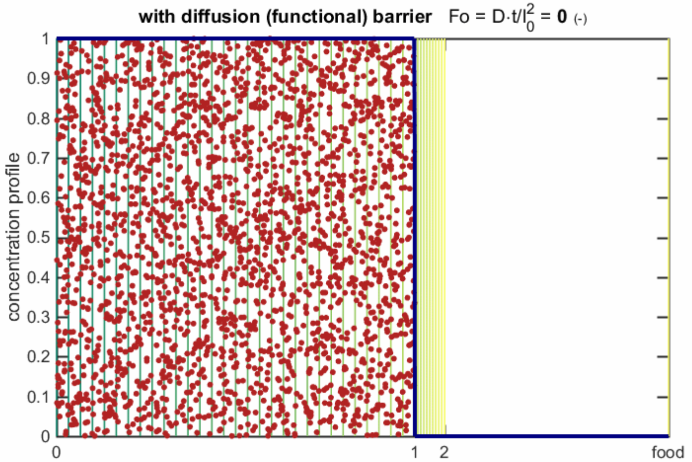


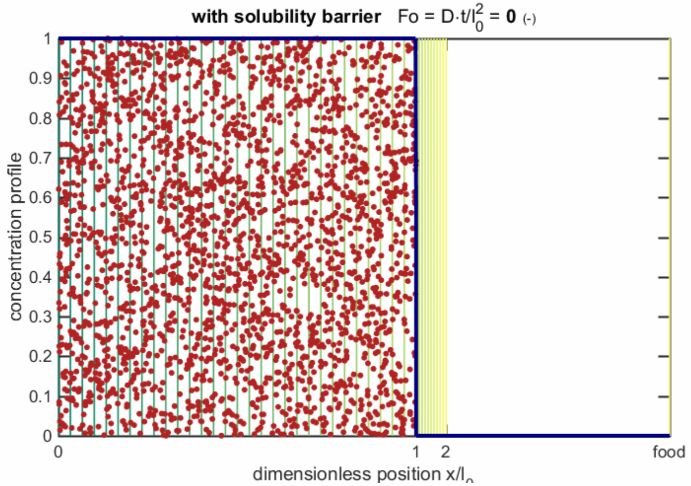
with barrier to diffusion

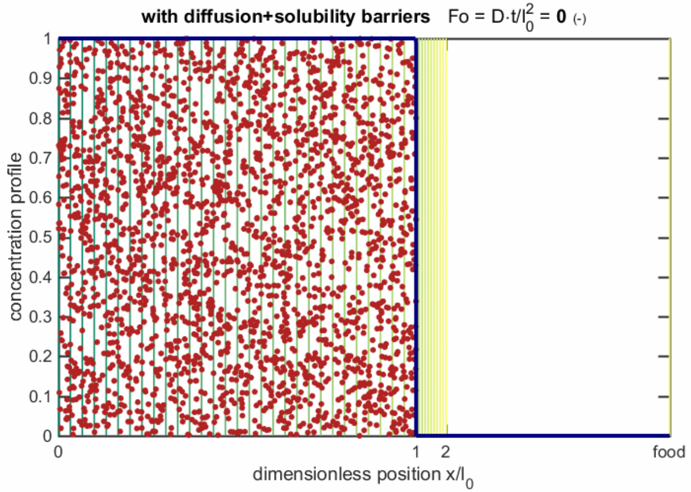






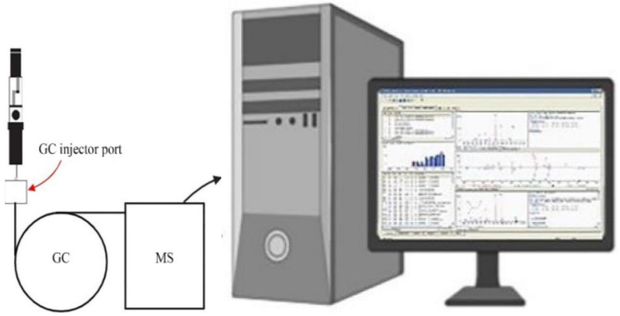


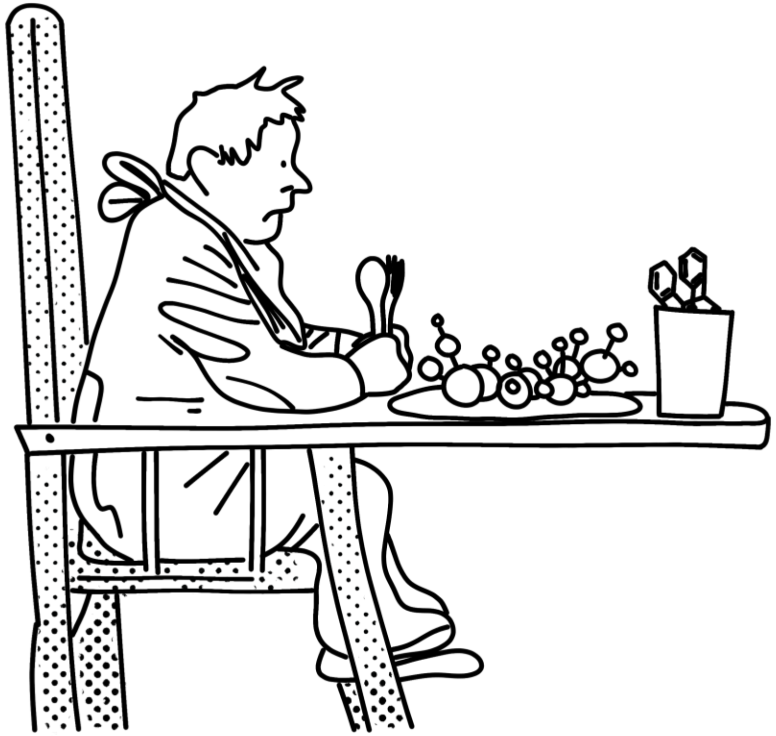




Revisiting the principles of safety assessment

Looking for viable strategies

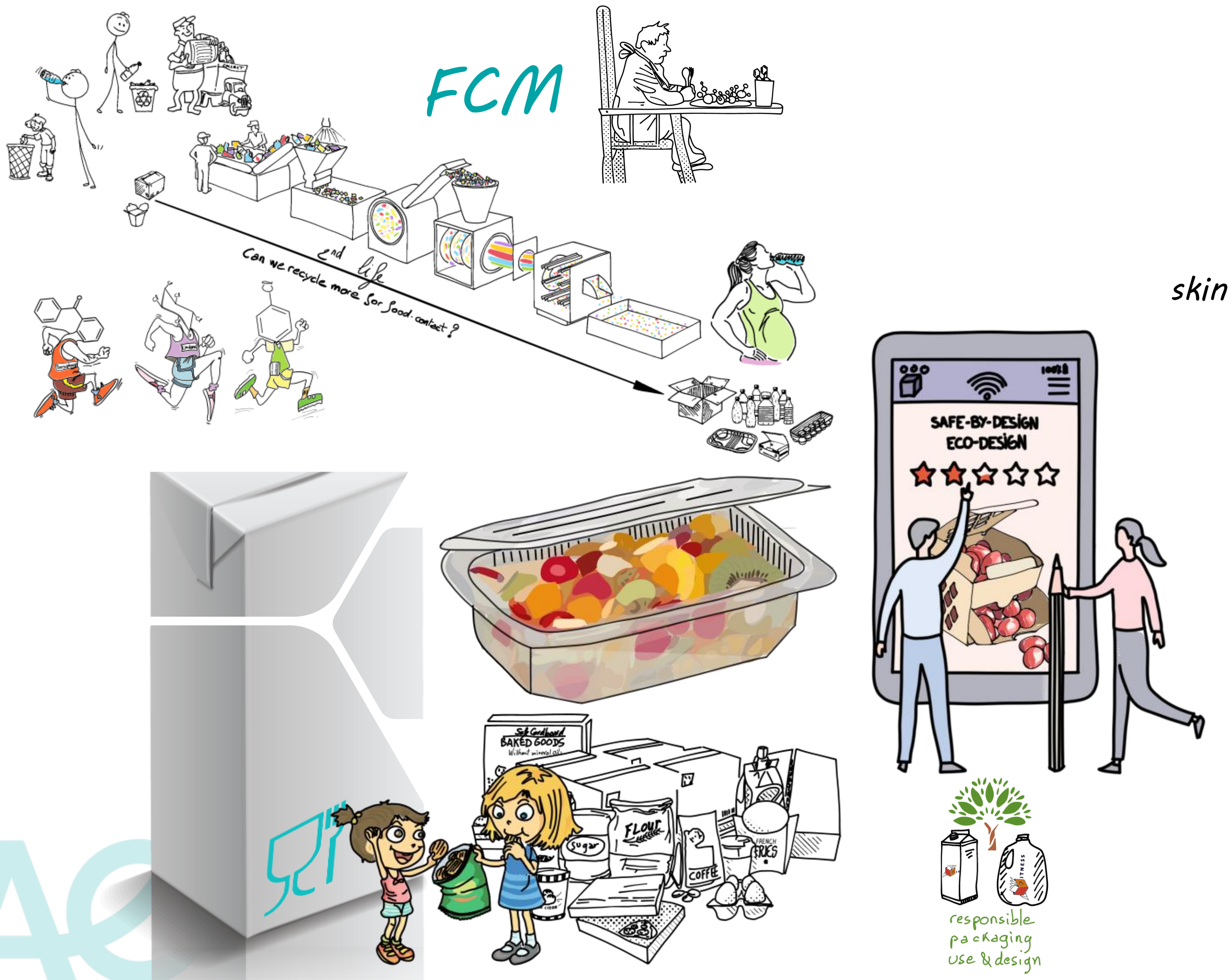


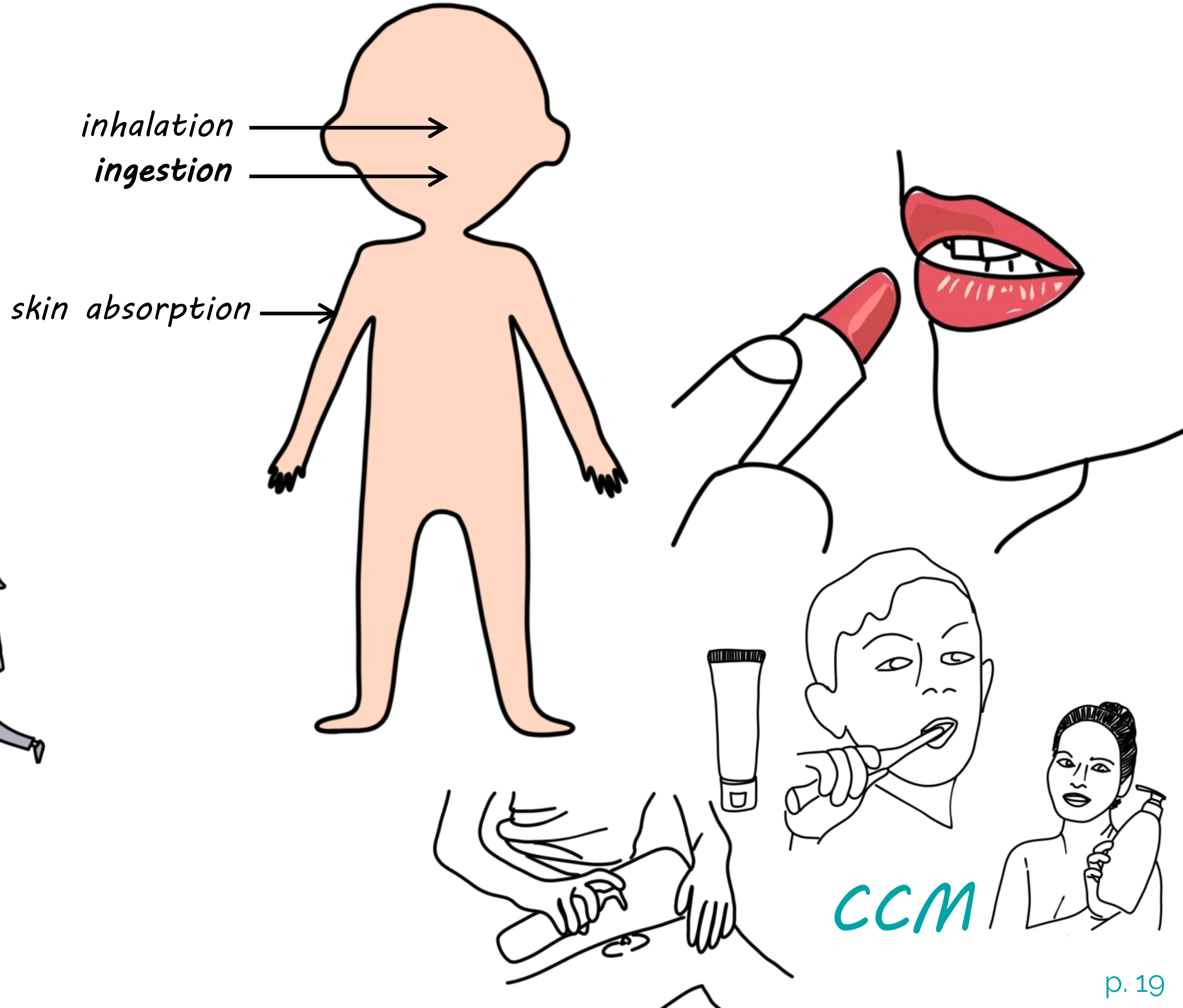


- **Traceability of sourcing, managing cross-contamination** during collection, sorting and recycling
- **Risk assessment and management of unknown chemicals (NIAS)** via consumer exposure
- **Unknown acceptable thresholds** (acute toxicity, endocrine disruptors, cocktail effects)
- **The aging of materials** needs to be considered
- **Functional barrier?** virgin/recycled/decontaminated? which solution? How to evaluate them? Which service life?
- **Evaluating migration / exposure** below the detection limit
- **Migration modeling** is the only viable approach but which contamination level to consider?

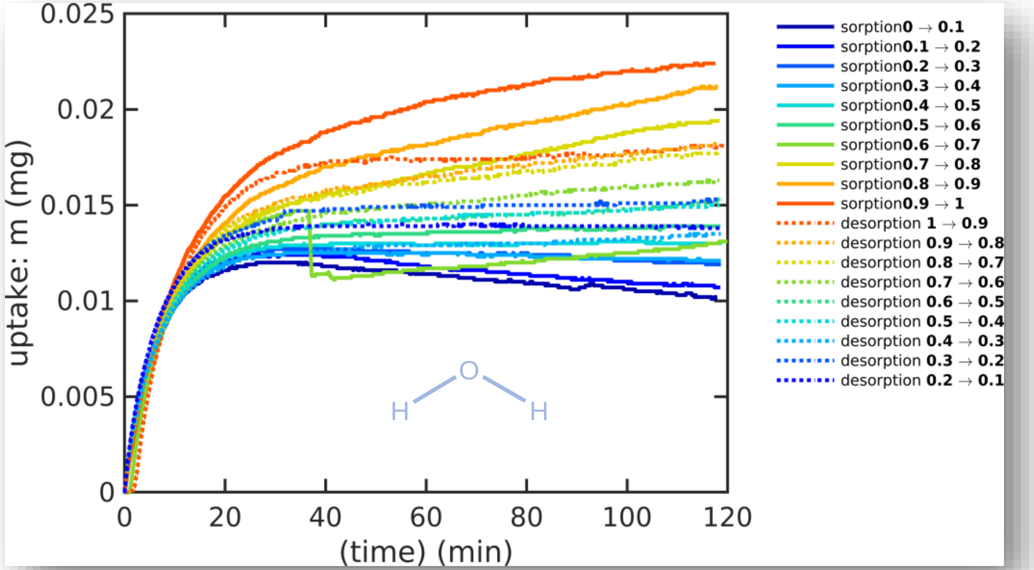
BEYOND FOOD CONTACT

The EU regulation (EC) 1223/2009 of cosmetic products refers to the framework regulation (EC) 1935/2004 of food contact materials (FCM) to manage the risk of contamination of cosmetic contact materials (CCM)

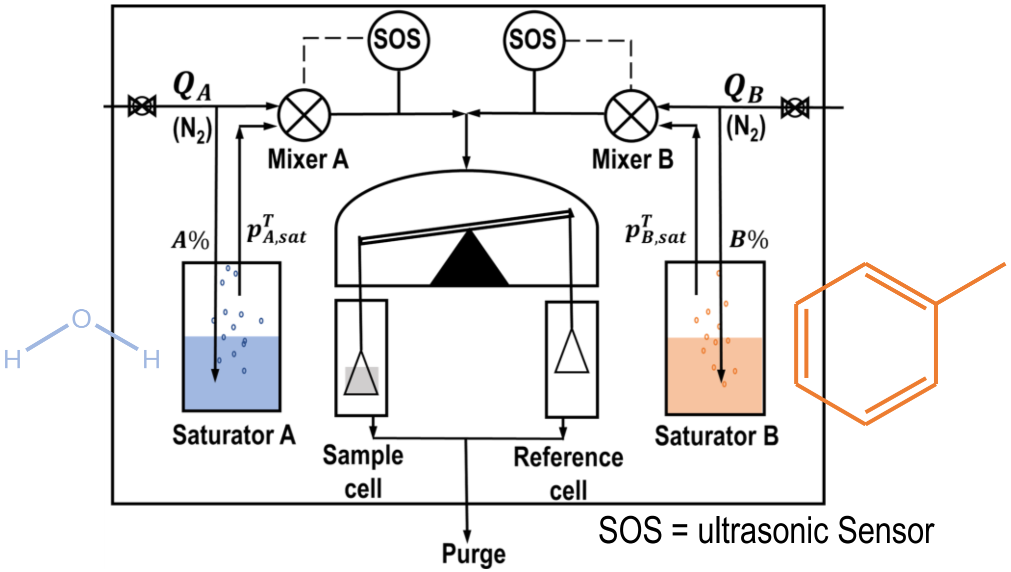


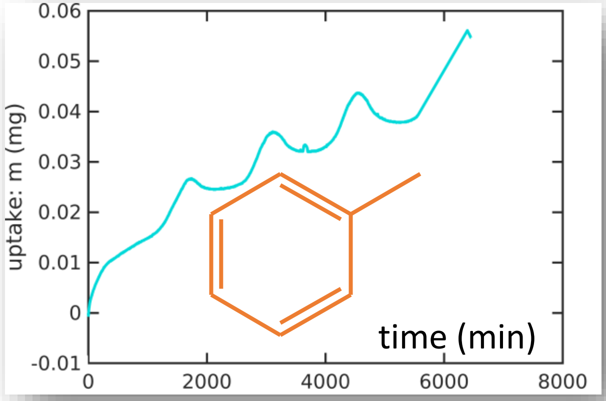


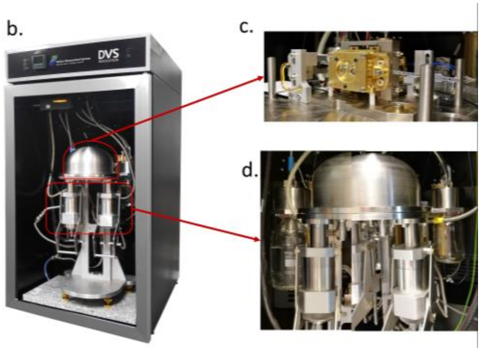
Thermodynamic measurements (e.g. 25 µm thick - PET)



Automatic microbalance

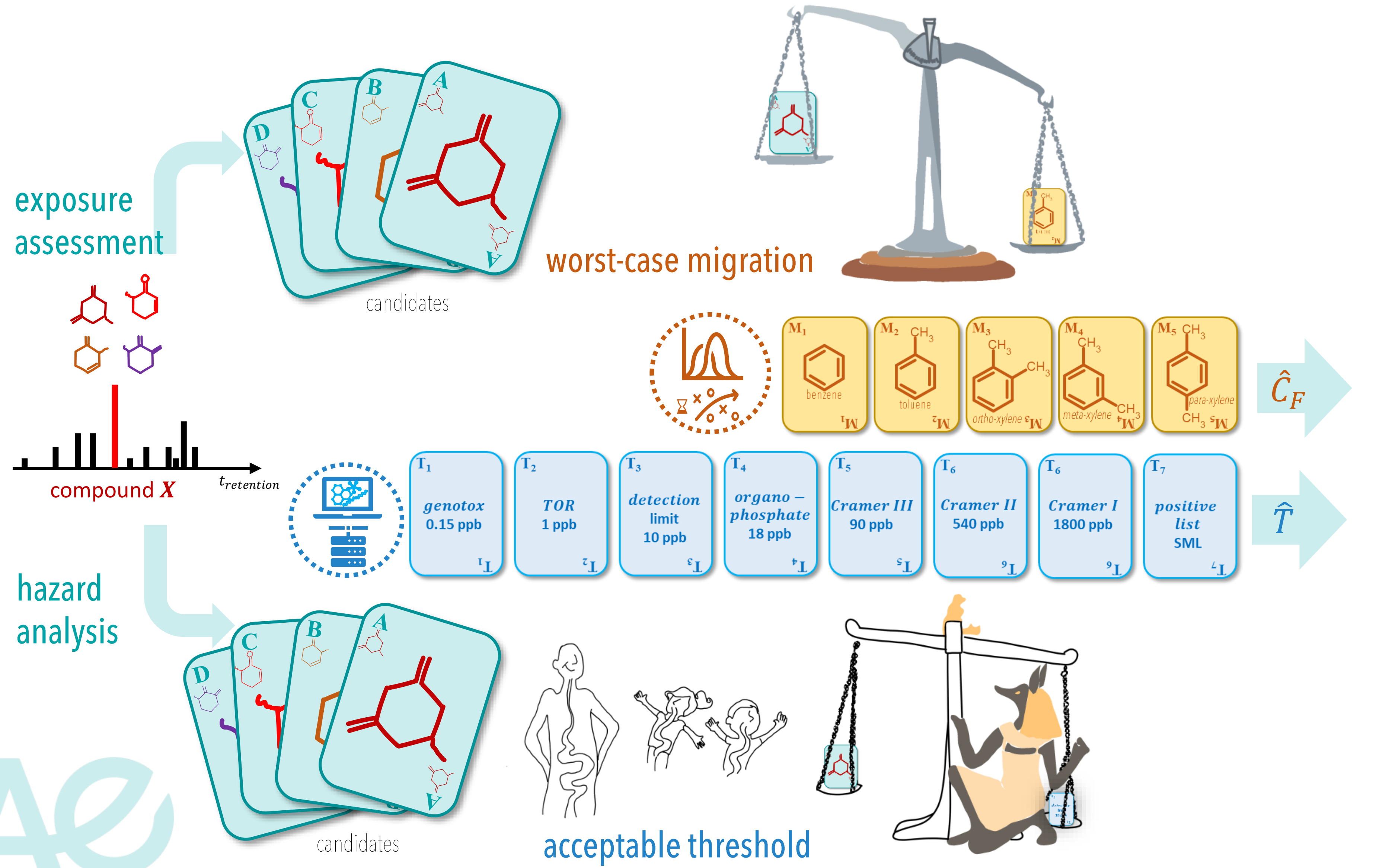


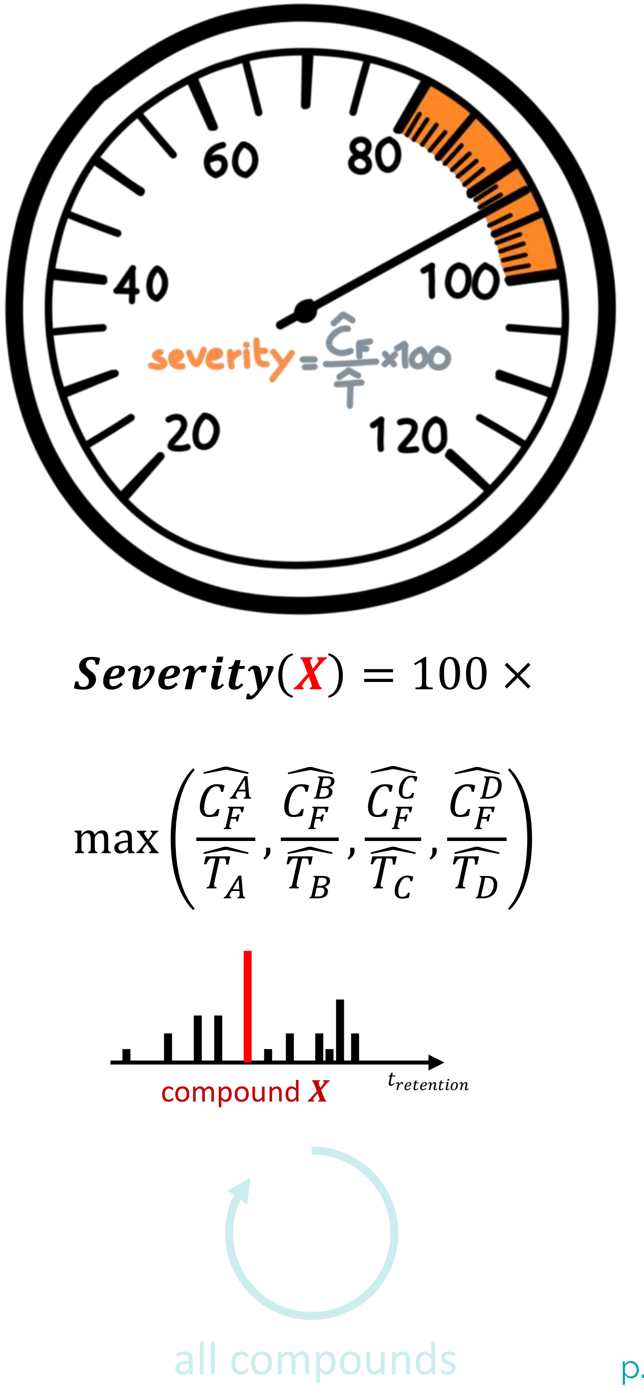


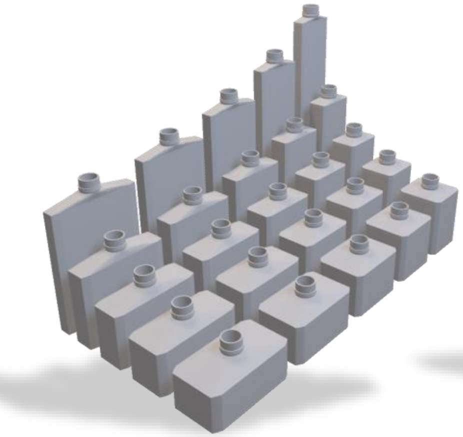


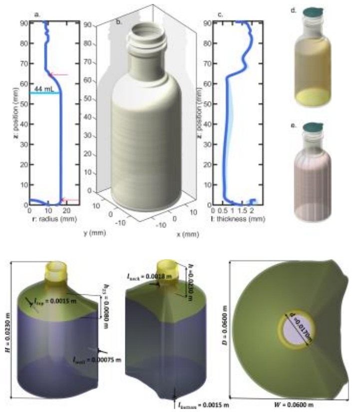
The challenge of NIAS

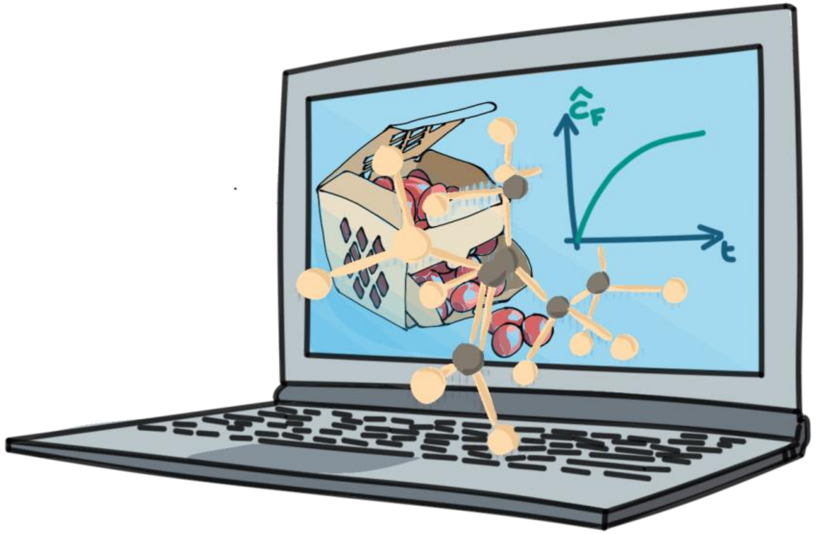
Propagating uncertainty with the risk that no decision can be reached





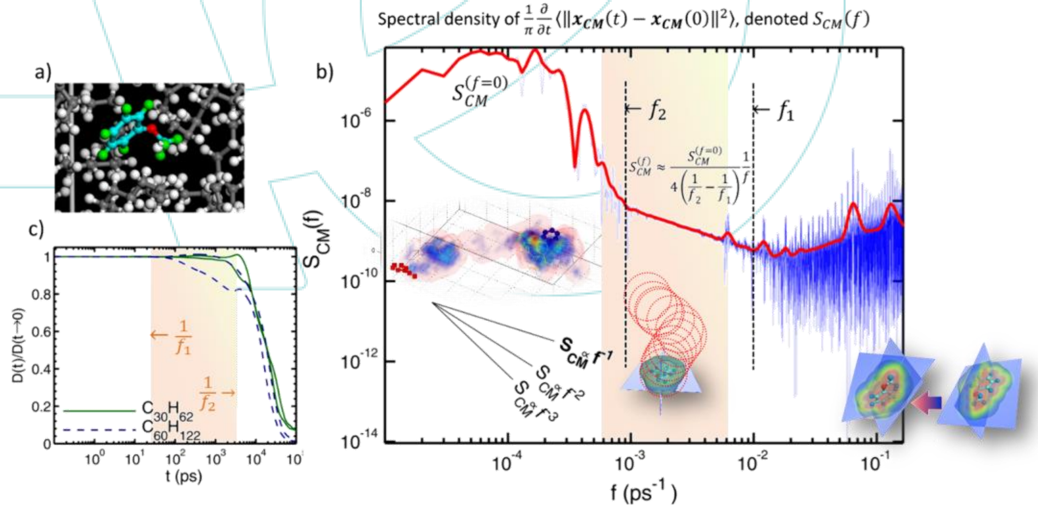


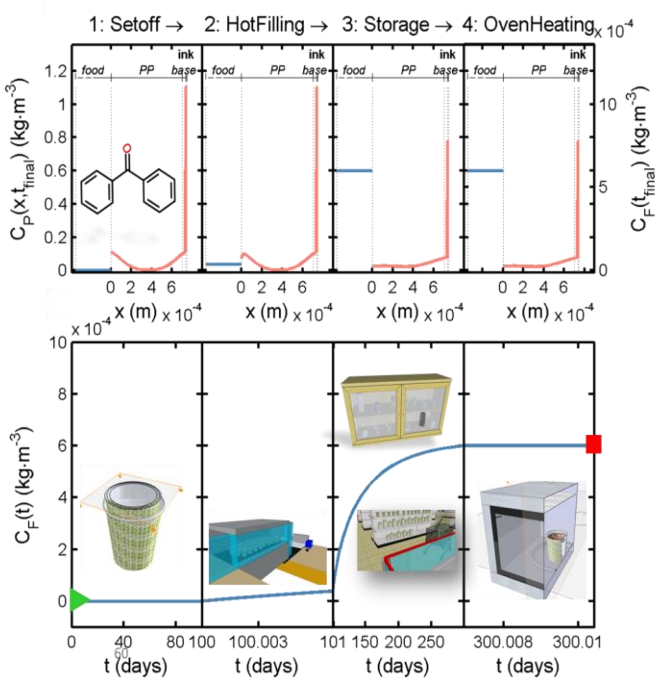


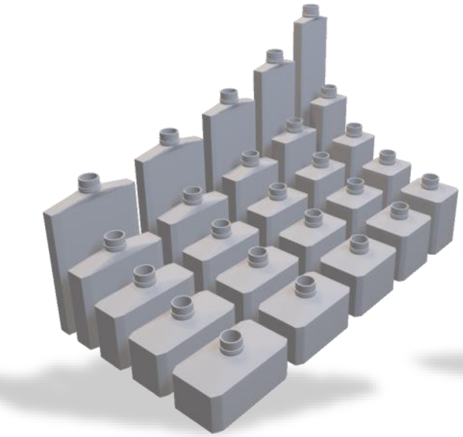


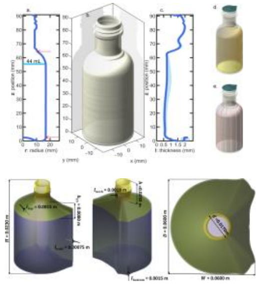
Migration modeling and computational engineering

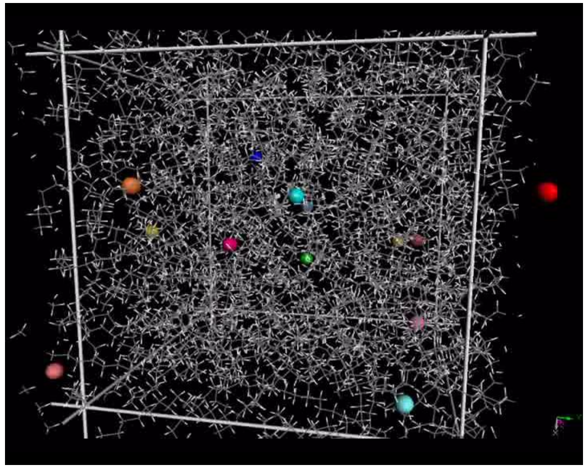
OUR WAY OUT

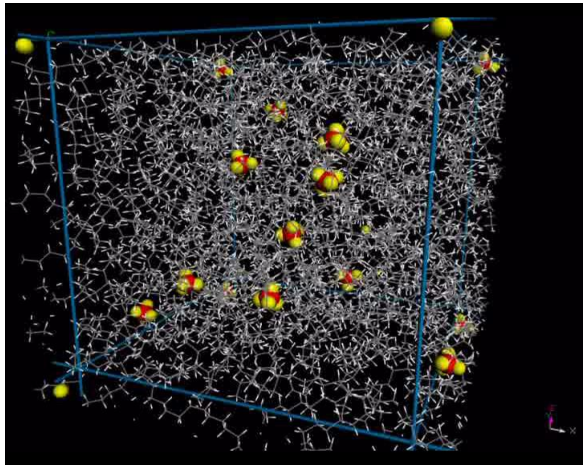






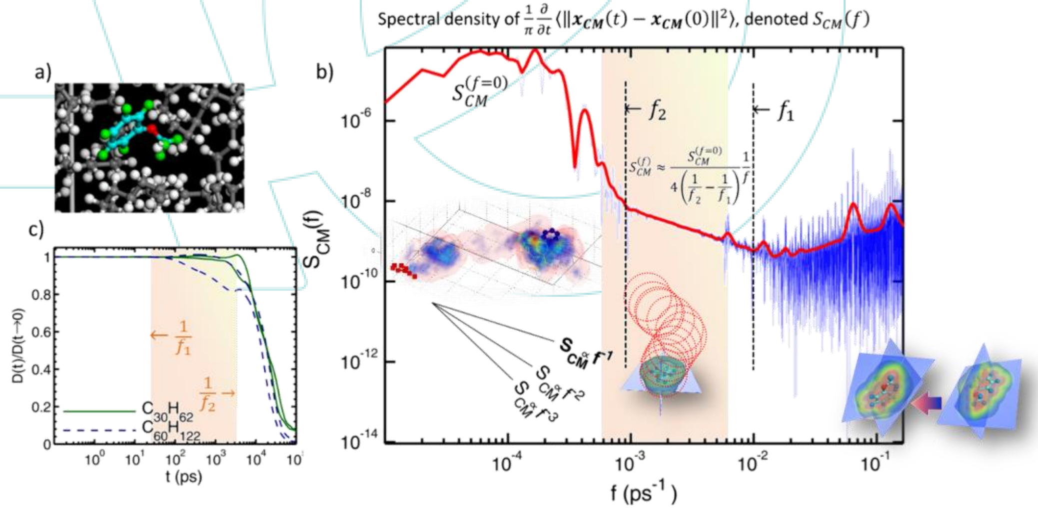


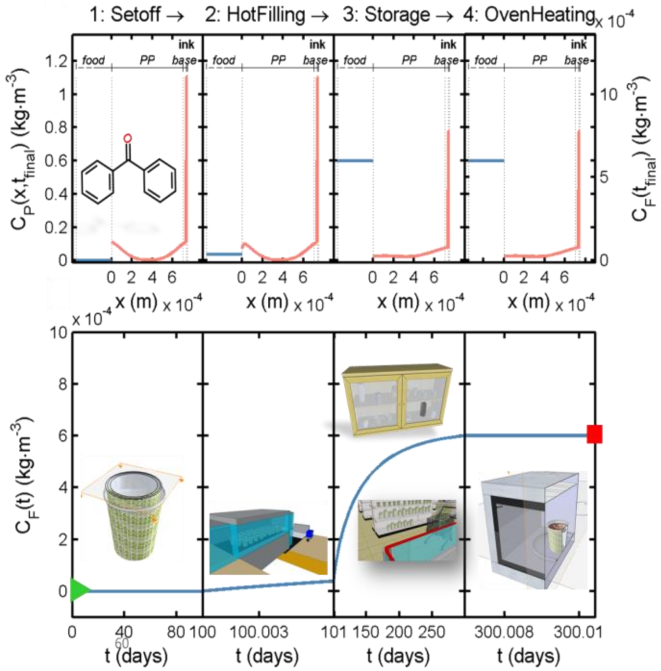


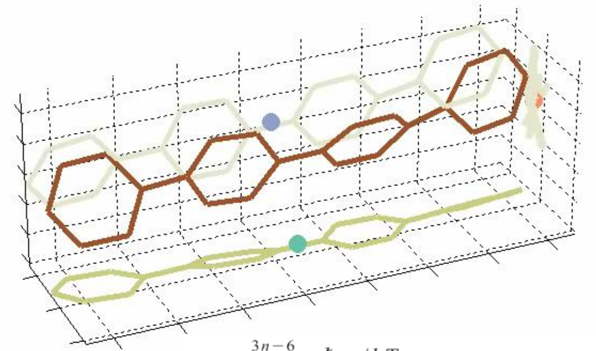


Migration modeling and computational engineering

OUR WAY OUT







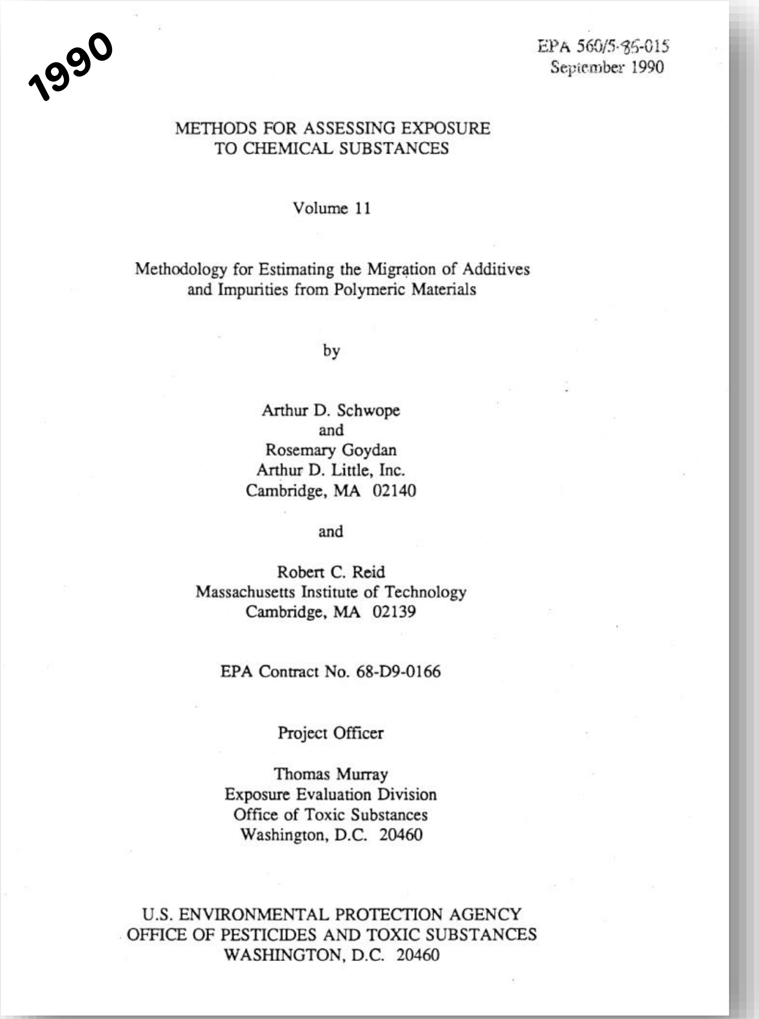
$$S_{ho}=k\sum_{i}^{3n-6}\frac{\hbar\omega_i/kT}{e^{\hbar\omega_i/kT}-1}-\ln(1-e^{-\hbar\omega_i/kT})$$

Migration modeling is well accepted in the US, Europe and China

Revisions and to extensions to non-plastic materials are pending

US guidance

Methodology for Estimating the Migration of Additives and Impurities from Polymeric Materials


1990

EPA 560/5-85-015
September 1990

METHODS FOR ASSESSING EXPOSURE TO CHEMICAL SUBSTANCES

Volume 11

Methodology for Estimating the Migration of Additives and Impurities from Polymeric Materials

by

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EPA Contract No. 68-D9-0166

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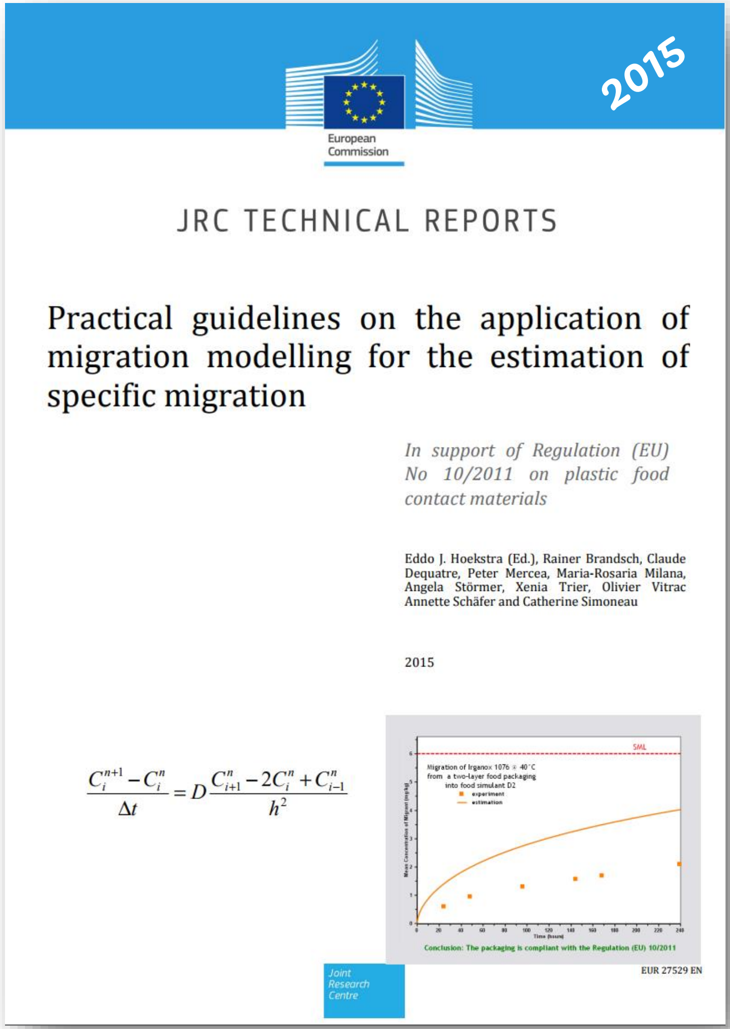
OFFICE OF PESTICIDES AND TOXIC SUBSTANCES
WASHINGTON, D.C. 20460

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


2015

European Commission

JRC TECHNICAL REPORTS

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

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

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

2015

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

Conclusion: The packaging is compliant with the Regulation (EU) 10/2011

EUR 27529 EN

Joint Research Centre

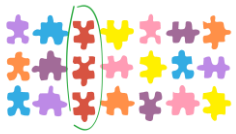
http://publications.jrc.ec.europa.eu/repository/handle/JRC98028

Europe guidance

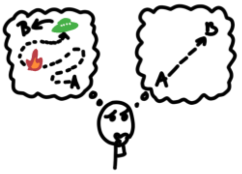
The five principles of migration modeling

- *The first principle* ("**conservatism**") is that modeling and related calculations should overestimate the real migration or contamination.

- *The second principle* ("**reliability**") implies that the foreseen mass transfer pathways and substances obey well-described mechanisms, accepted conditions (e.g., uniform distribution), and proper implementation in software.



- *The third principle* ("**consistency**") is that inputs in the model are known or guessed in a way that fulfills the requirements of the first principle.



- *The fourth principle* ("**parsimony**") states that sophisticated and refined scenarios should be considered only when simpler ones cannot demonstrate compliance or safety.

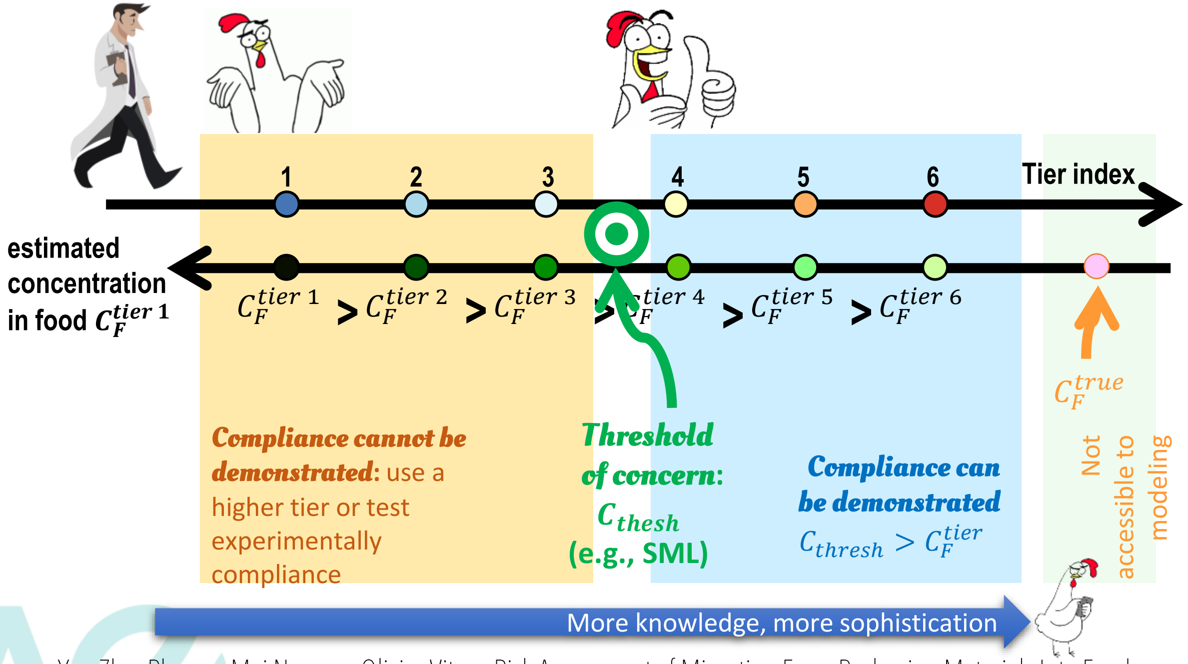
- *The fifth and final principle* ("**proportionality**") is that non-compliance cannot be demonstrated by calculation.

Parsimony vs. sophistication

During the last decade migration modeling became high throughput, multiscale and connected to chemometric approaches

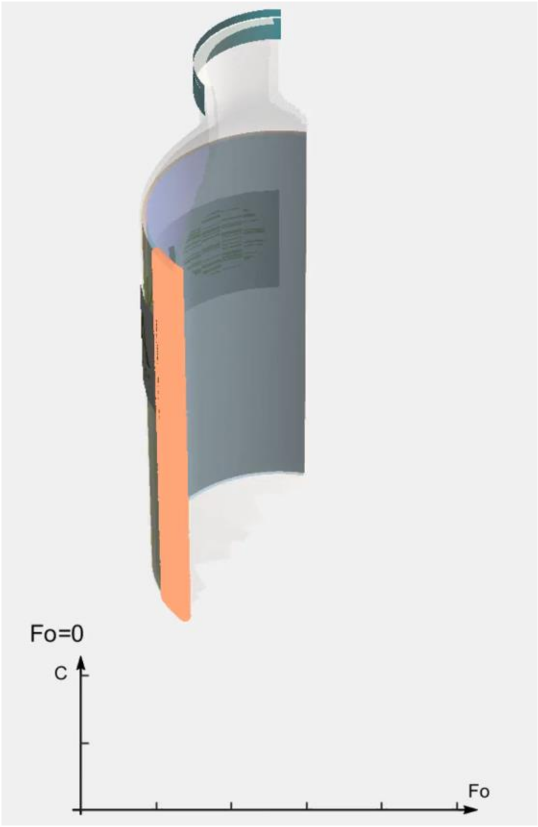
What is the goal?

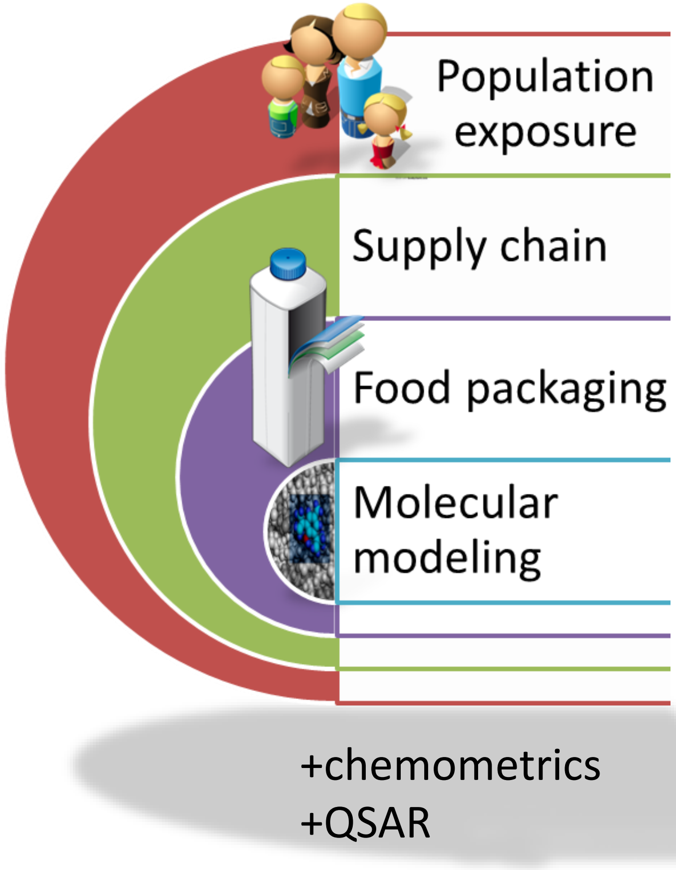
The art of migration modeling consists in building a sequence of scenarios so that the last scenario provides a value lower than the threshold of concern while being large than the real concentration (unknown).



Yan Zhu, Phuong-Mai Nguyen, Olivier Vitrac, Risk Assessment of Migration From Packaging Materials Into Food, Reference Module in Food Science, Elsevier, 2019, https://doi.org/10.1016/B978-0-08-100596-5.22501-8.

Multiscale modeling

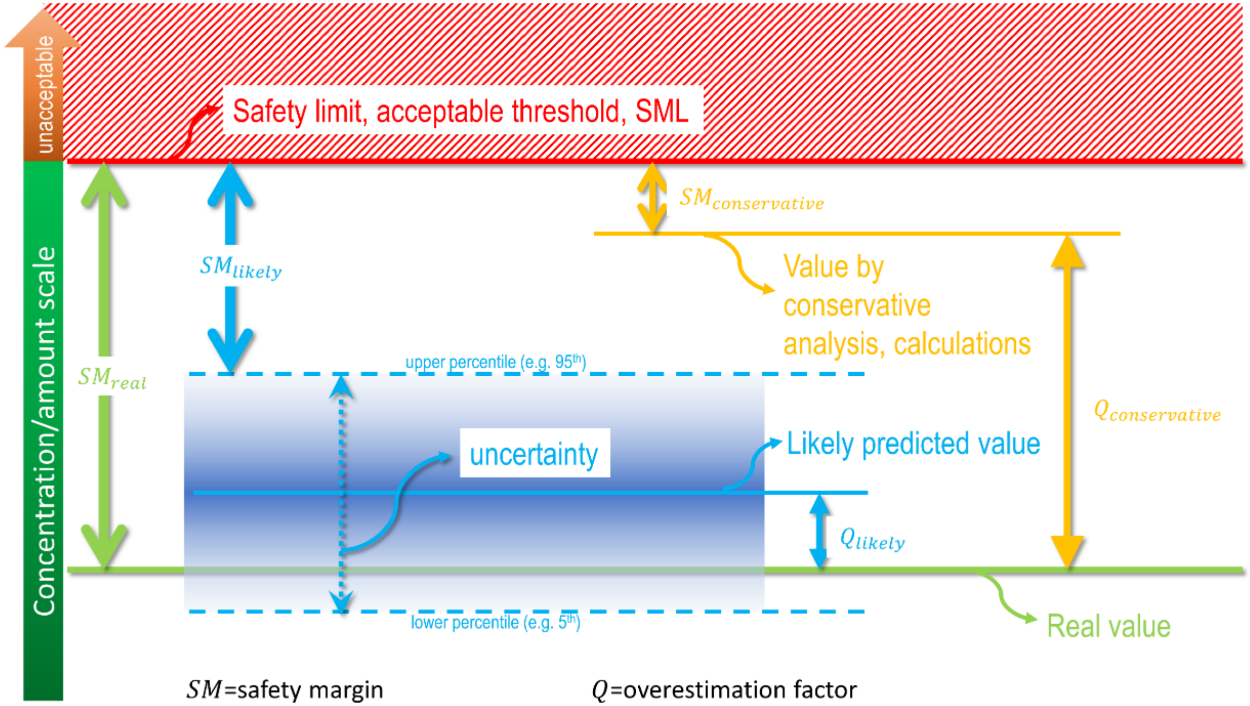


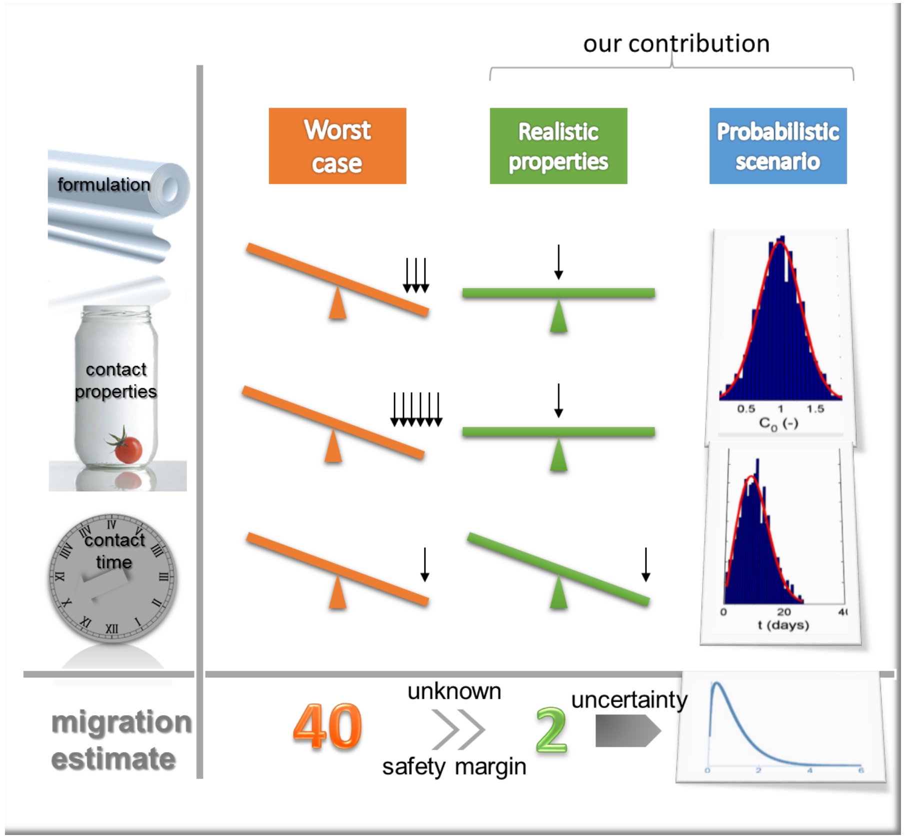


How to manage uncertainty ?

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.

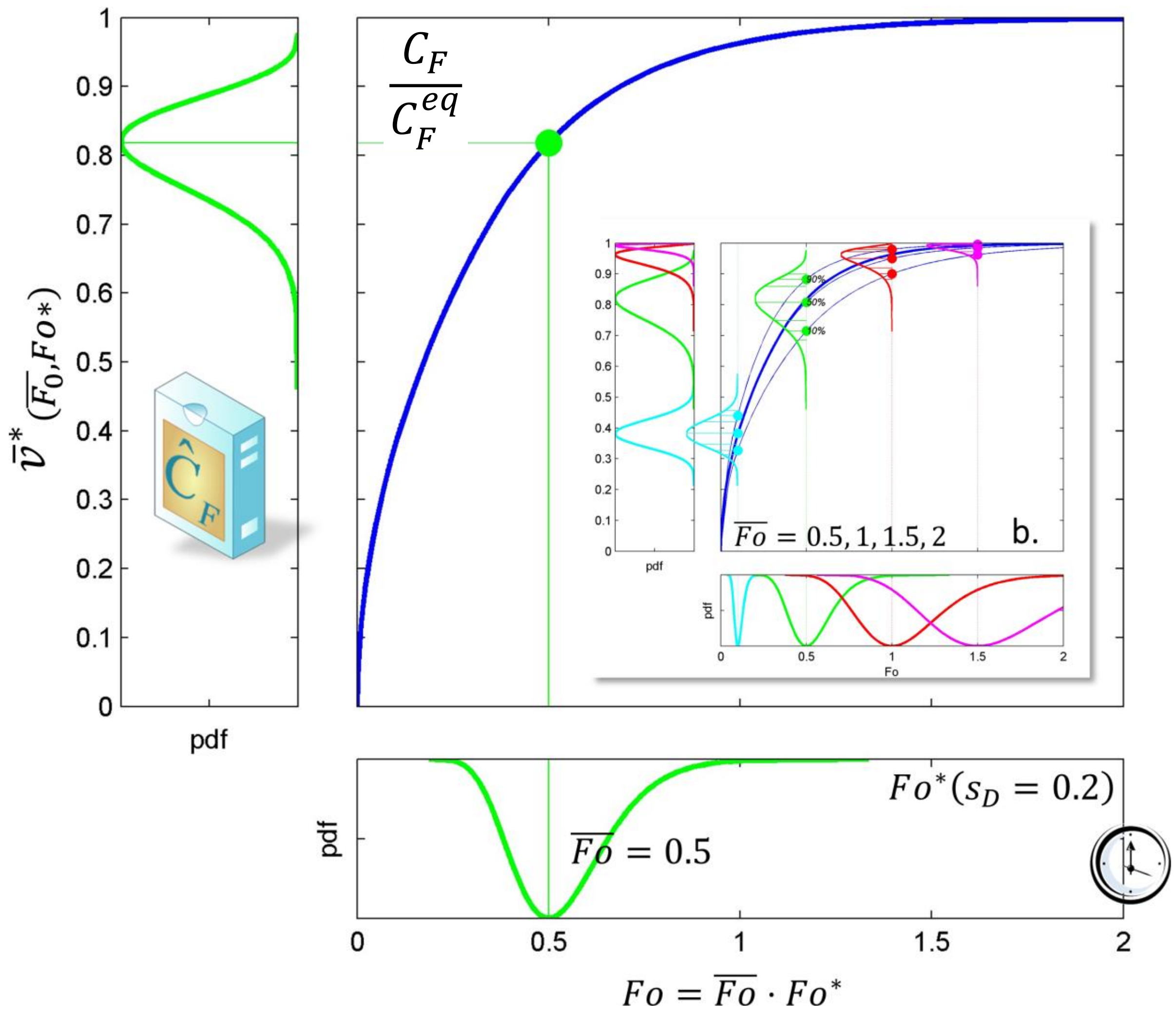
Probabilistic modeling

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.

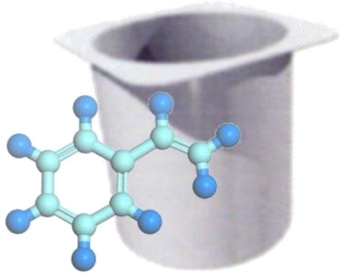
$$f_{\bar{v}^*}(v) = \sum_{k=1}^{p} f_{Fo}\left(\bar{v}^{*-1}\Big|_{Fo\in Y_k}(v)\right)\left|\frac{d}{dv}\bar{v}^{*-1}\Big|_{Fo\in Y_k}(v)\right|^{-1}$$

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.**

Styrene from yoghurt pots: an example of forecast

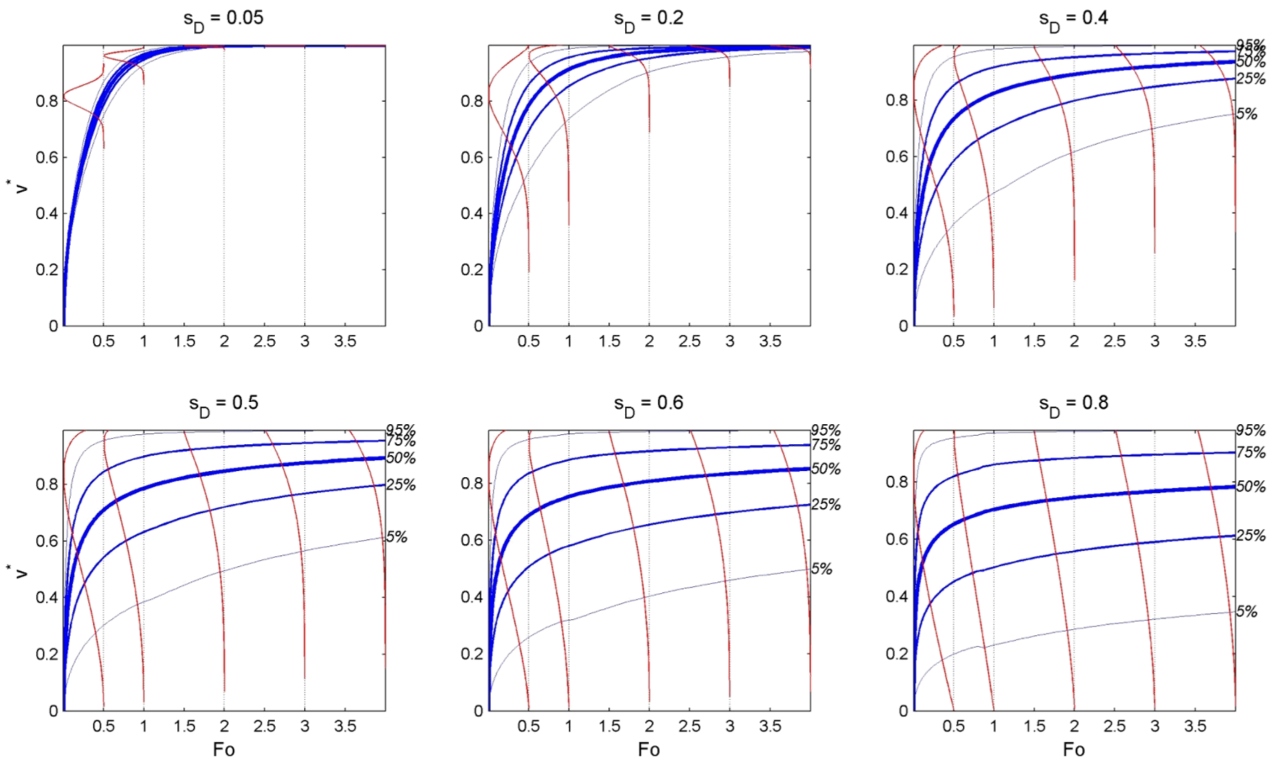


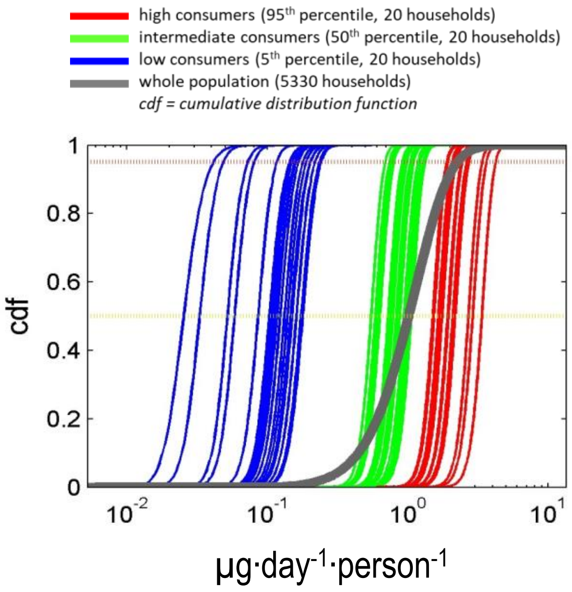
$$\underset{\text{product scale}}{p_r\left(C \le x\right)} = f\begin{pmatrix}\text{food, packaging, migrants} \\ \text{storage cond., uncertainty}\end{pmatrix}$$

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

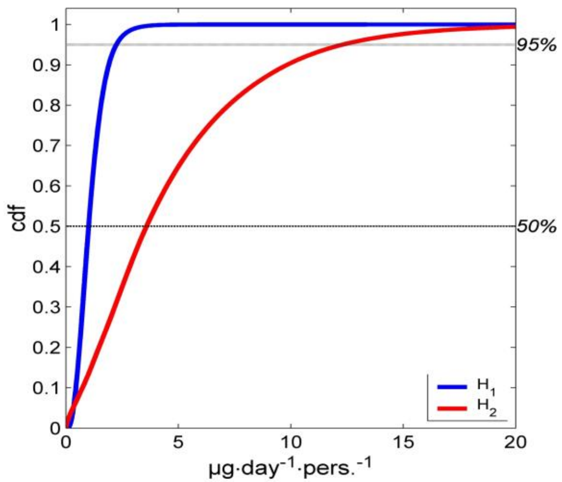
$$E_k = \frac{c_0 \cdot \overline{v}_\infty^*}{365 \cdot P_k} \cdot \sum_{i=1}^{N_k} \overline{v}_i^*\left(Fo_i, Bi, K, L\right)$$

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



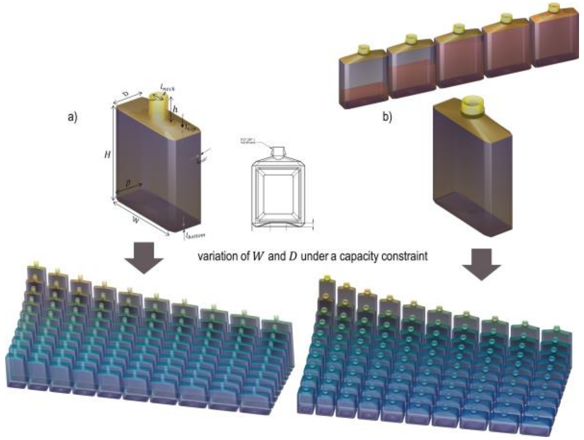


2 physico-chemical scenarios



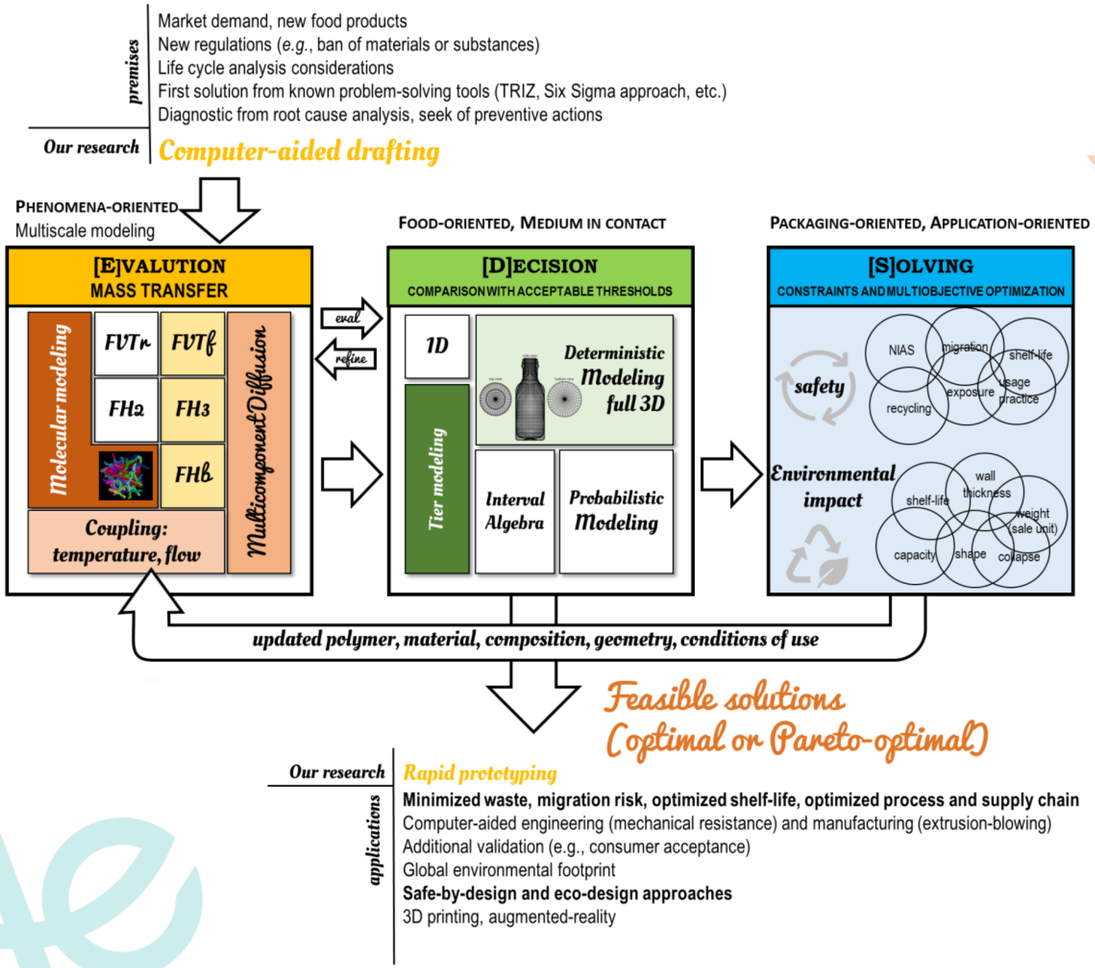
O. Vitrac and J.-C. Leblanc, *Food Additives and Contaminants Part a-Chemistry Analysis Control Exposure & Risk Assessment* ***2007, 24, 194-215.***

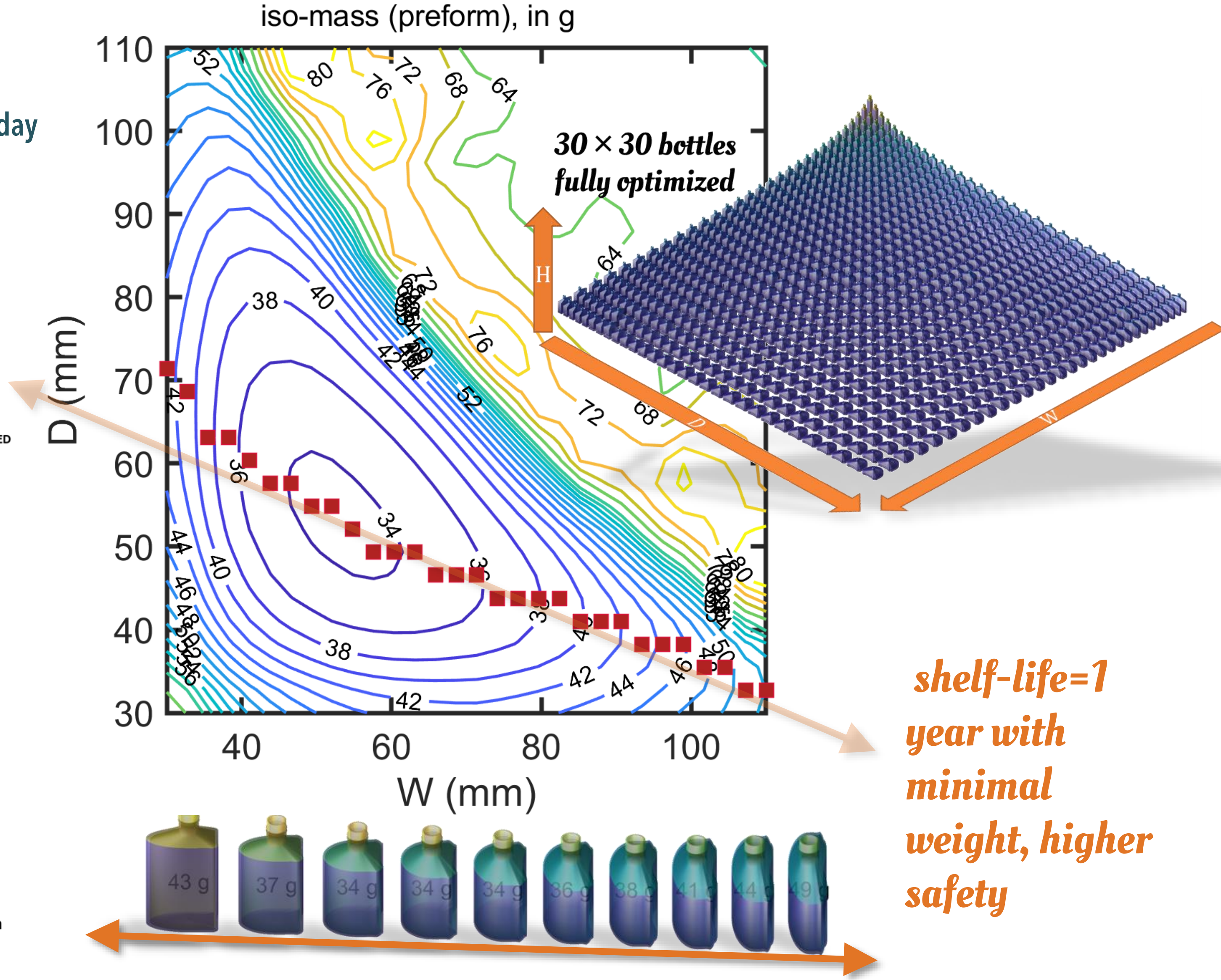
Integrated engineering



Example: redesign of PET bottle for alcoholic beverages (optimized shape, recycled content, reduced weight, improved shell-life)

3D prototype printed the same day



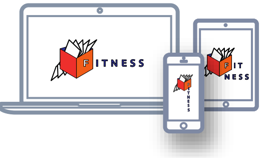


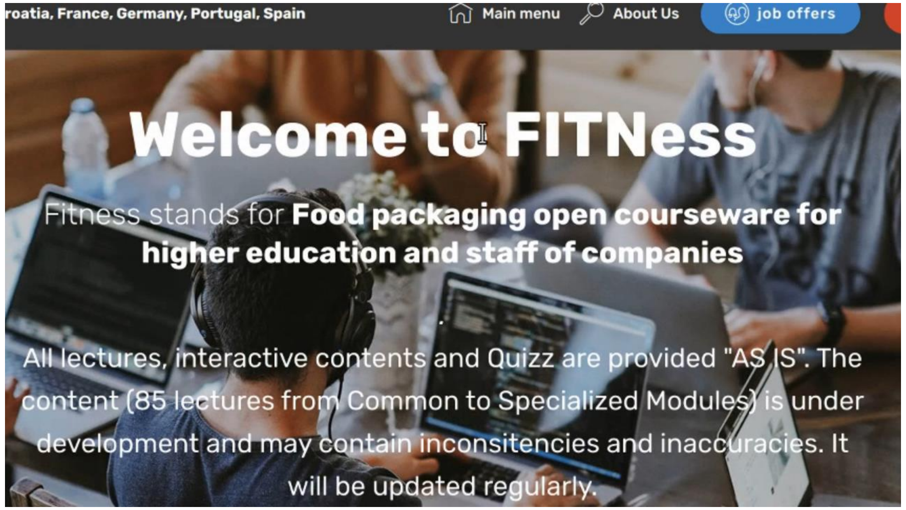
Zhu, Y., Guillemat, B., et Vitrac, O. (2019). Rational Design of Packaging: Toward Safer and Ecodesigned Food Packaging Systems. *Frontiers in Chemistry, 7(349).*

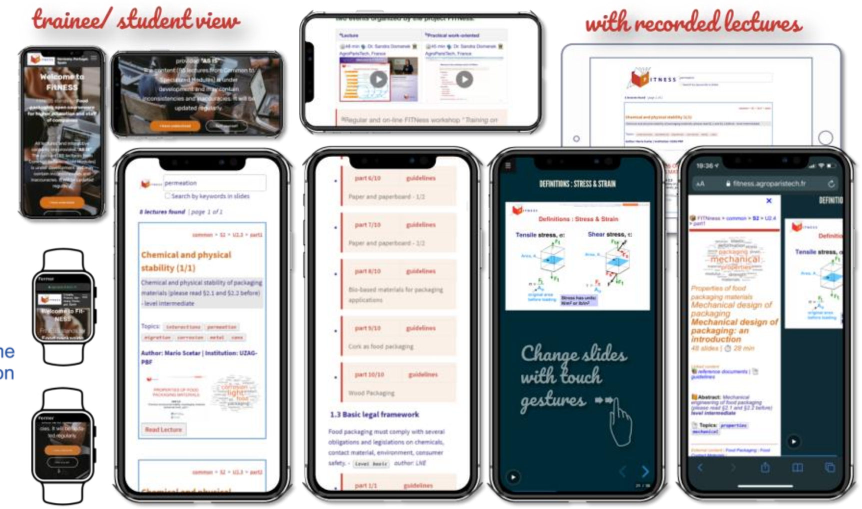
EDUCATION

Three months online curriculum on packaging design

https://fitness.agroparistech.fr/







BONNE PRATIQUE

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