Large scale modeling of food systems: from molecules to food quality and safety

Olivier Vitrac, Yan Zhu, Phuong-Mai Nguyen, Gilles Trystram
olivier.vitrac@agroparistech.fr

UMR 1145 GENIAL

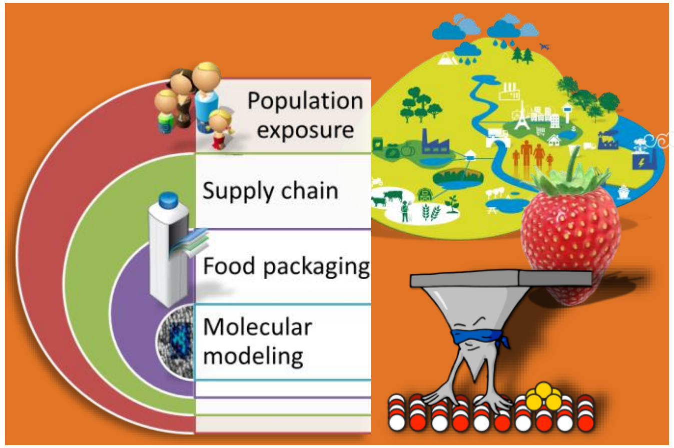
INRA
UMR 1145, Food Processing and Engineering
UMT SafeMat "Safe Materials"
AgroParisTech site de Massy, France

ICEF13
INTERNATIONAL CONGRESS ON ENGINEERING AND FOOD
MELBOURNE, AUSTRALIA
23-26 SEPTEMBER 2019
Engineering Innovations for Food Supply Chains
www.icef13.com

INRA SCIENCE & IMPACT

université PARIS-SACLAY

O. Vitrac and M. Touffet, in: Encyclopedia of Food Security and Sustainability. 1st Edition., Elsevier, Amsterdam, NL, 2018, pp. 434-453.



IT IS FAST, FASTER THAN EXPERIMENTS
(tailored methods)

RISK ASSESSMENT & MANAGEMENT

Responsible engineering

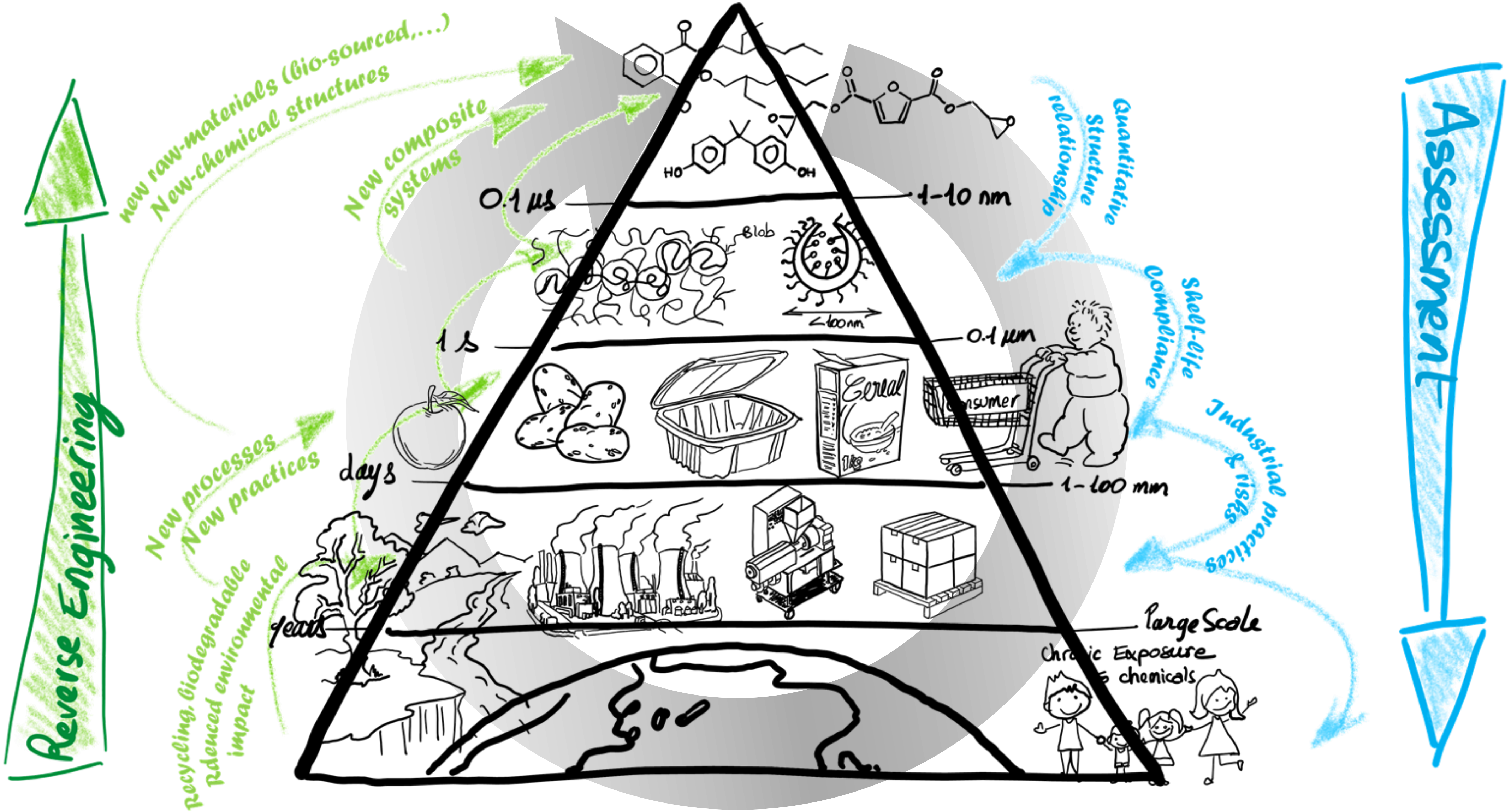
BREAK-TROUGH INNOVATION
(exploring alternatives)

Understanding
(coupling scales, computational microscope soft matter approaches)

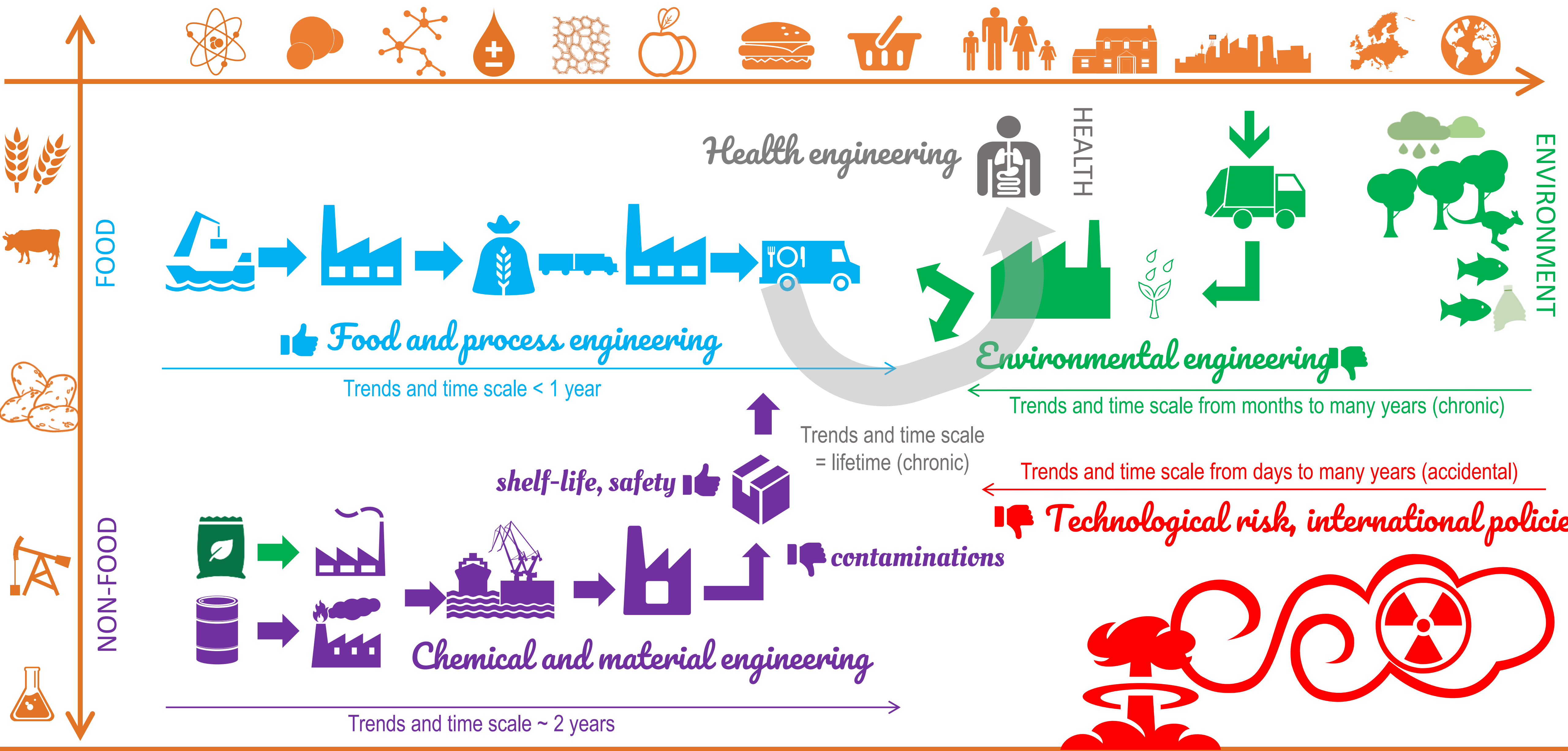
COMBINED WITH HIGH-THROUGHPUT EXPERIMENTS
(microcomputed Xray tomography, spectroscopy, etc.)

Foresight Modeling

Different shades of modeling



Large scale modeling = the new frontier



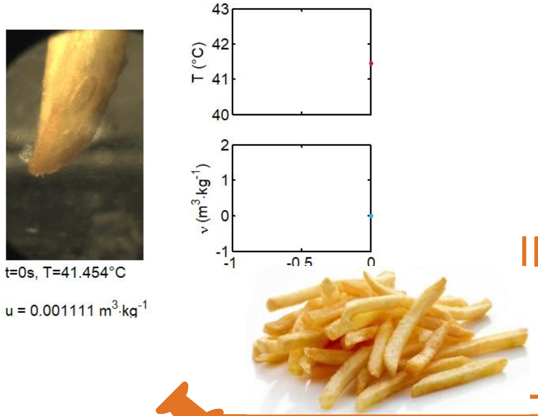
Health engineering
HEALTH
ENVIRONMENT
FOOD
NON-FOOD
Food and process engineering
Trends and time scale < 1 year
Environmental engineering
Trends and time scale from months to many years (chronic)
Trends and time scale
= lifetime (chronic)
shelf-life, safety
Trends and time scale from days to many years (accidental)
Technological risk, international policie
contaminations
Chemical and material engineering
Trends and time scale ~ 2 years

Inferring general rules from our own modeling experience:

prediction (the truth exist), forecast (likely future), foresight (only possibilities)

FOOD

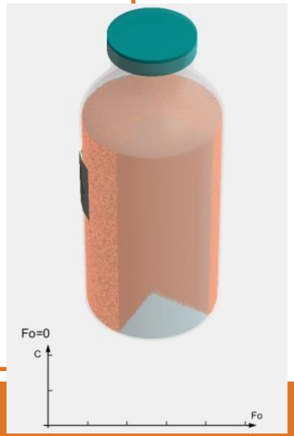
NON-FOOD

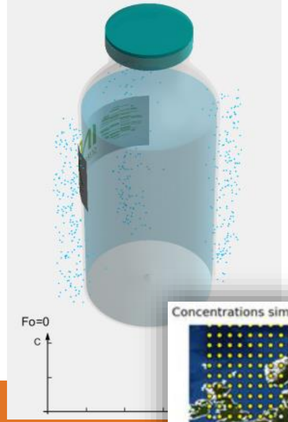


MINIMIZING
OIL UPTAKE
IN FRENCH-FRIES

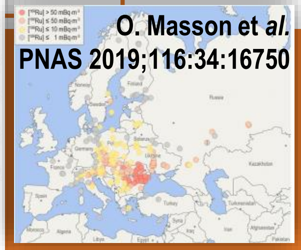
SAFETY OF
FOOD PACKAGING
(CHRONIC HAZARDS)

PACKAGING
DESIGN

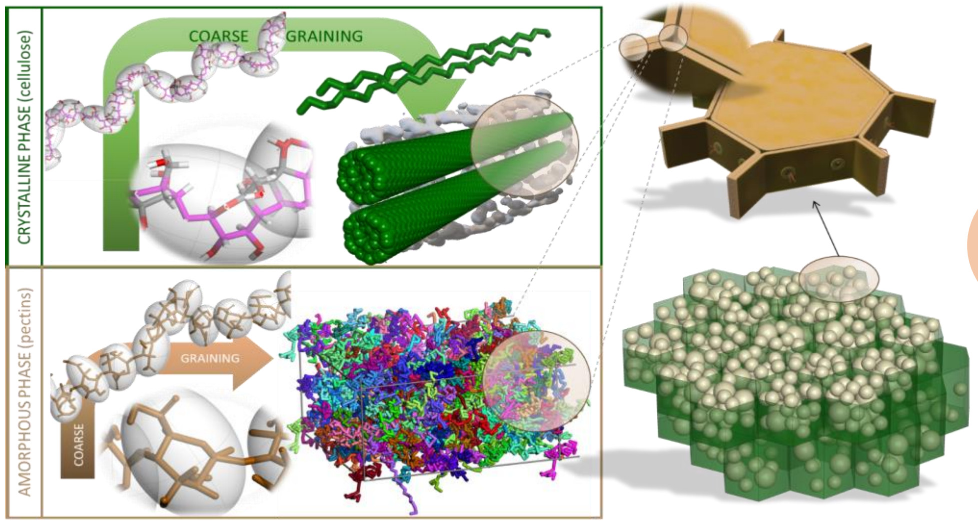




CONTAMINATION OF FOOD
STOCKS BY RADIONUCLIDES
(ACCIDENTAL HAZARDS)



SCIENCE & IMPACT



"Foresight" modeling in food

- *systemic, anticipation, prevention (future)*
- *Coarse-graining keeps trends, drops unessential details*
- ***analyze future developments***, attended or unattended (ingredient, food, packaging, supply chain, raw materials etc.)

AIM: ***minimizing risks and impacts***, societal innovation, future planning, may include optimization steps

OUTCOME: uncertain

TARGET: ***risk and impact assessment, weighting alternative scenarios***

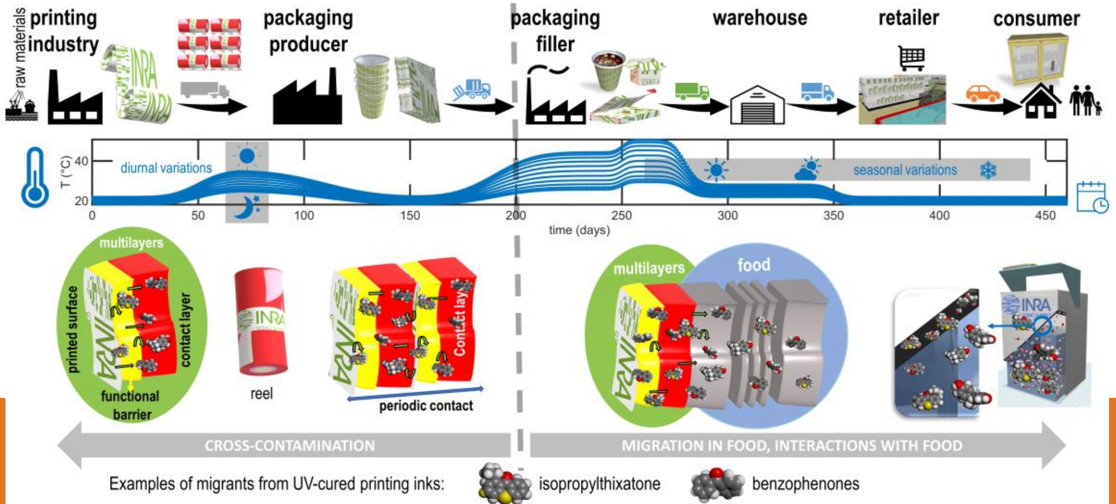
Conventional food modeling = present

- *punctual modeling and simulation*
- ***Coarse-graining preserves ALL important details (e.g., molecular, cellular structure, geometry, composition)***

AIM: ***improving food quality***, safety, efficiency, reducing cost

OUTCOME: likely

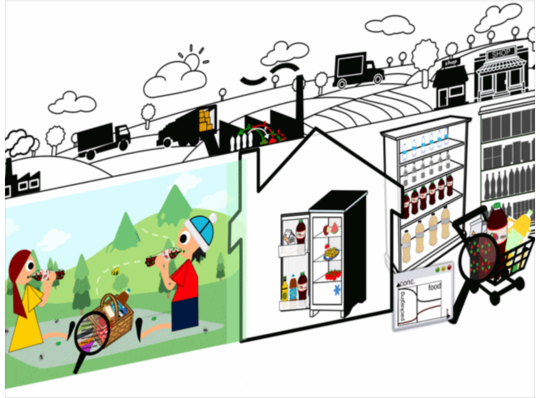
TARGET: ***efficient production, reverse engineering, local innovation***



Speed, flexible, agile, reusable, reliable

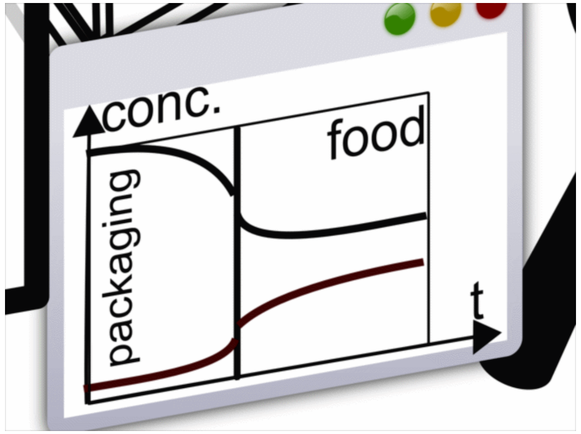
Property (transport, thermodynamics)

Statistical-Physics (equilibrium)



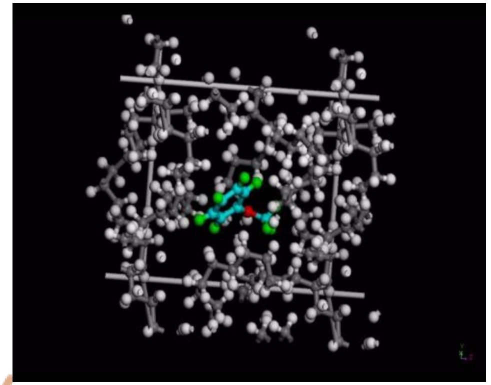
Fluxes, flows, kinetics

Deterministic, probablistic



Risk assessment

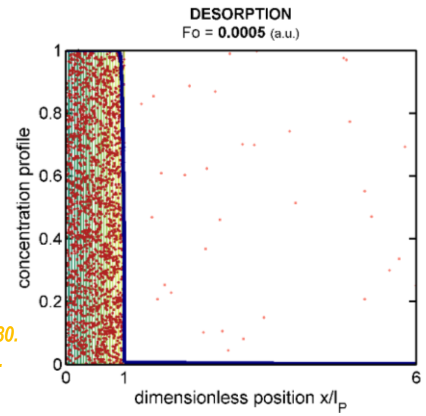
Probabilistic (no equilibrium)

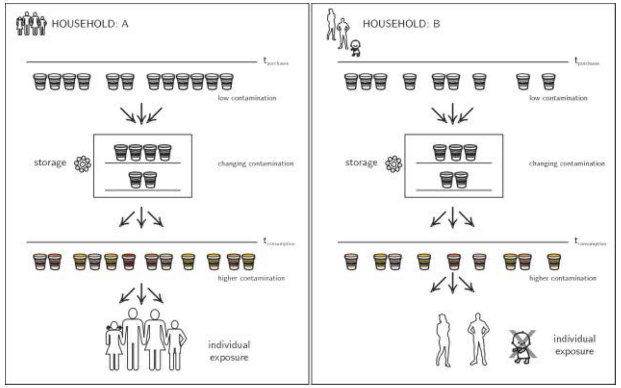


Free energy perturbation

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

Industrial & Engineering Chemistry Research **2010**, *49*, 7263-7280.
Industrial & Engineering Chemistry Research **2017**, *56*, 774–787.
Food Research International **2017**, *88*, *Part A*, 91-104.





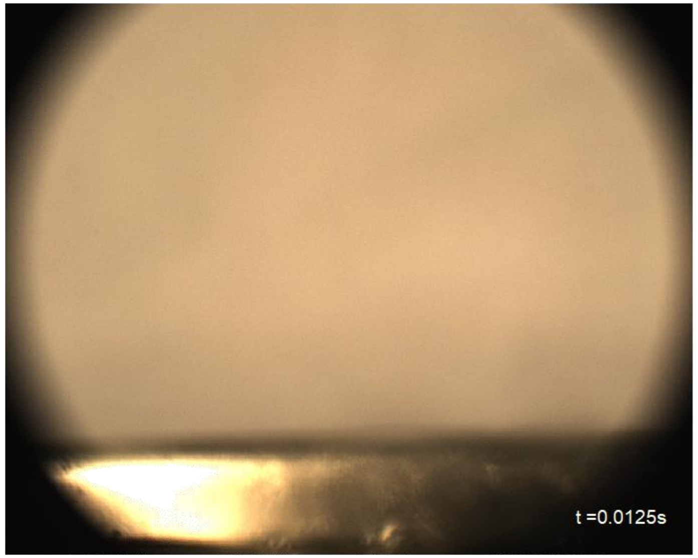
Equilibrium thermodynamics < Out-of equilibrium

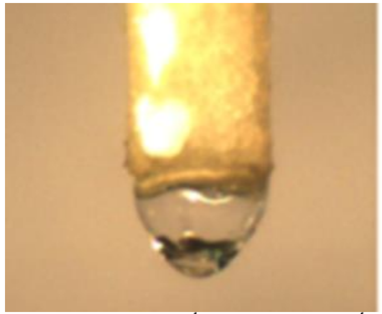
Scale hierarchy

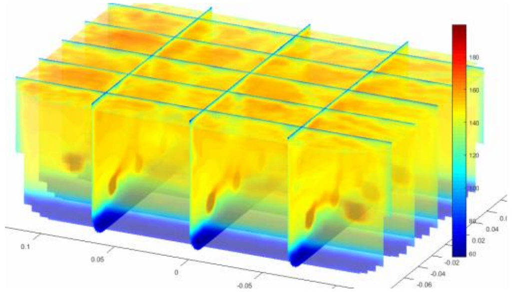
Key operations on models

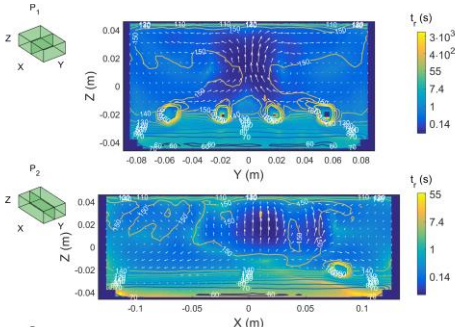
- Dimensionless (when possible)
- *Coupling (expensive)* vs *nesting (inexpensive)*

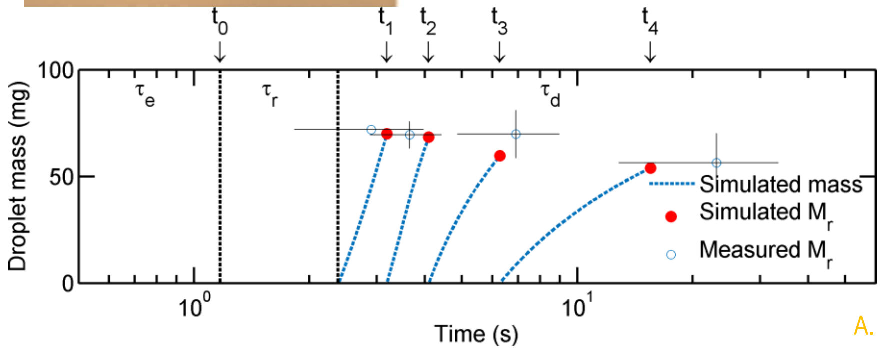
Oil dripping process (cooling)

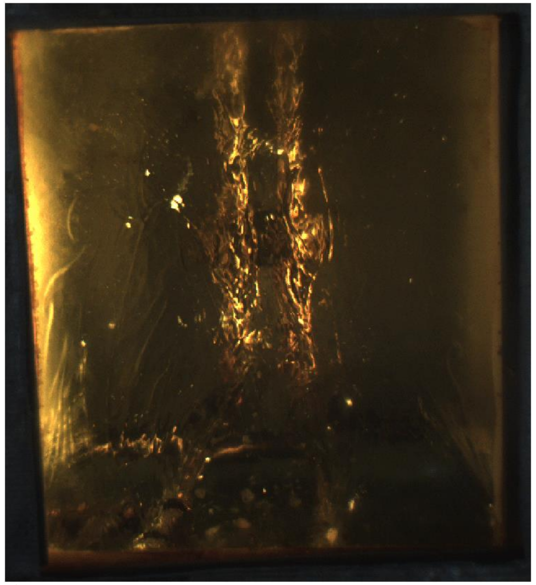




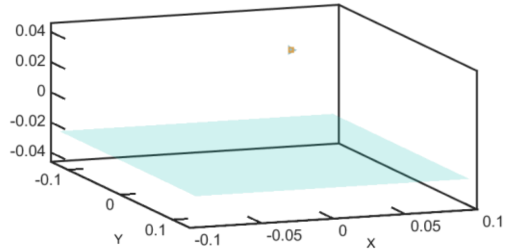








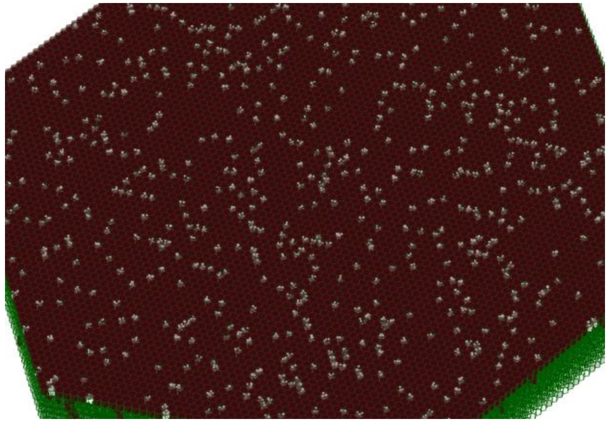
Oil oxidation during deep-frying



A. Patsioura, *et al*, *Food and Bioproducts Processing* ***2017, 101, 84-99.***
M. Touffet *et al.*, *Journal of Food Engineering* ***2018, 224, 1-16.***

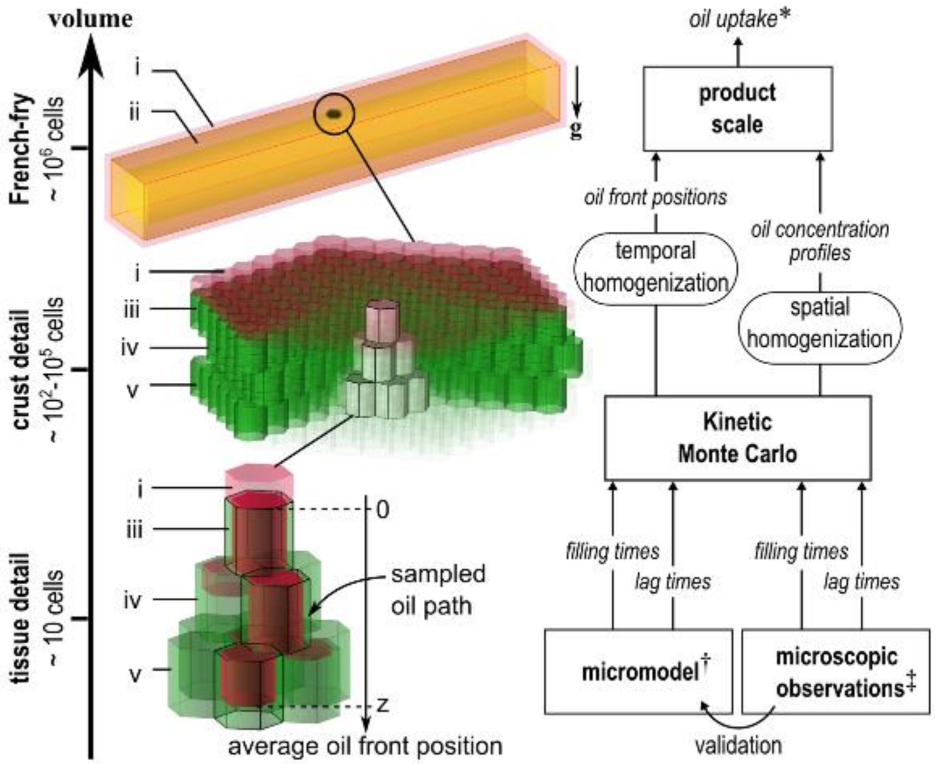
Key operations on models

- ▶ *Dimensionless* (when possible)
- ▶ *Coupling* vs *nesting* scales

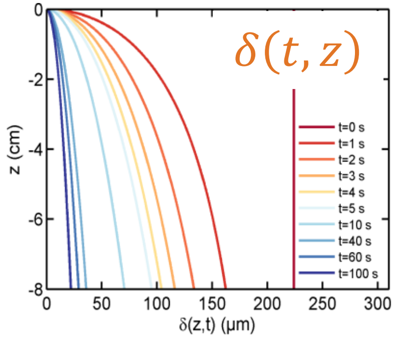


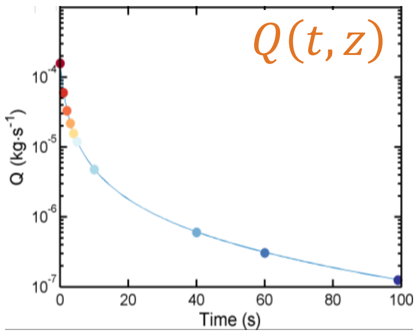
- ▶ *Chaining* ●→◆→●→■
- ▶ *Looping*
- ▶ *Ensemble averaging* (very important) $\bar{x}=\frac{\sum_{i=1}^{n}(x_i * w_i)}{\sum_{i=1}^{n} w_i}$
- ▶ *Serialization of scenarios*
- ▶ *Piping* (CFD, chemistry, mass transfer, thermodynamics models)

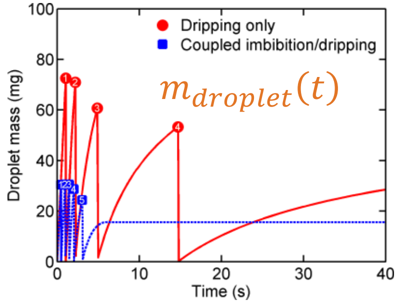
- ▶ ***Standards and good modeling practices***

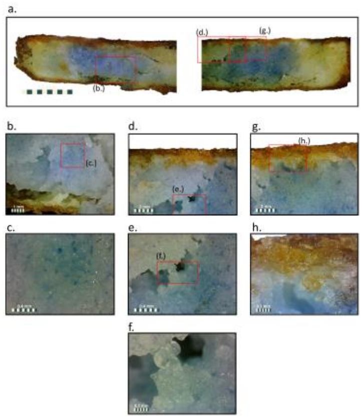


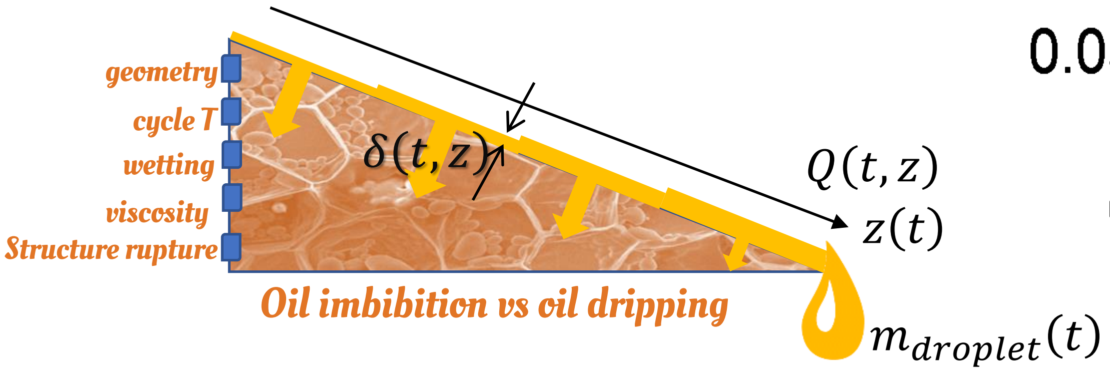
J.-M. Vauvre, A. Patsioura, R. Kesteloot and O. Vitrac, *AIChE Journal* **2015, 61, 2329–2353.**

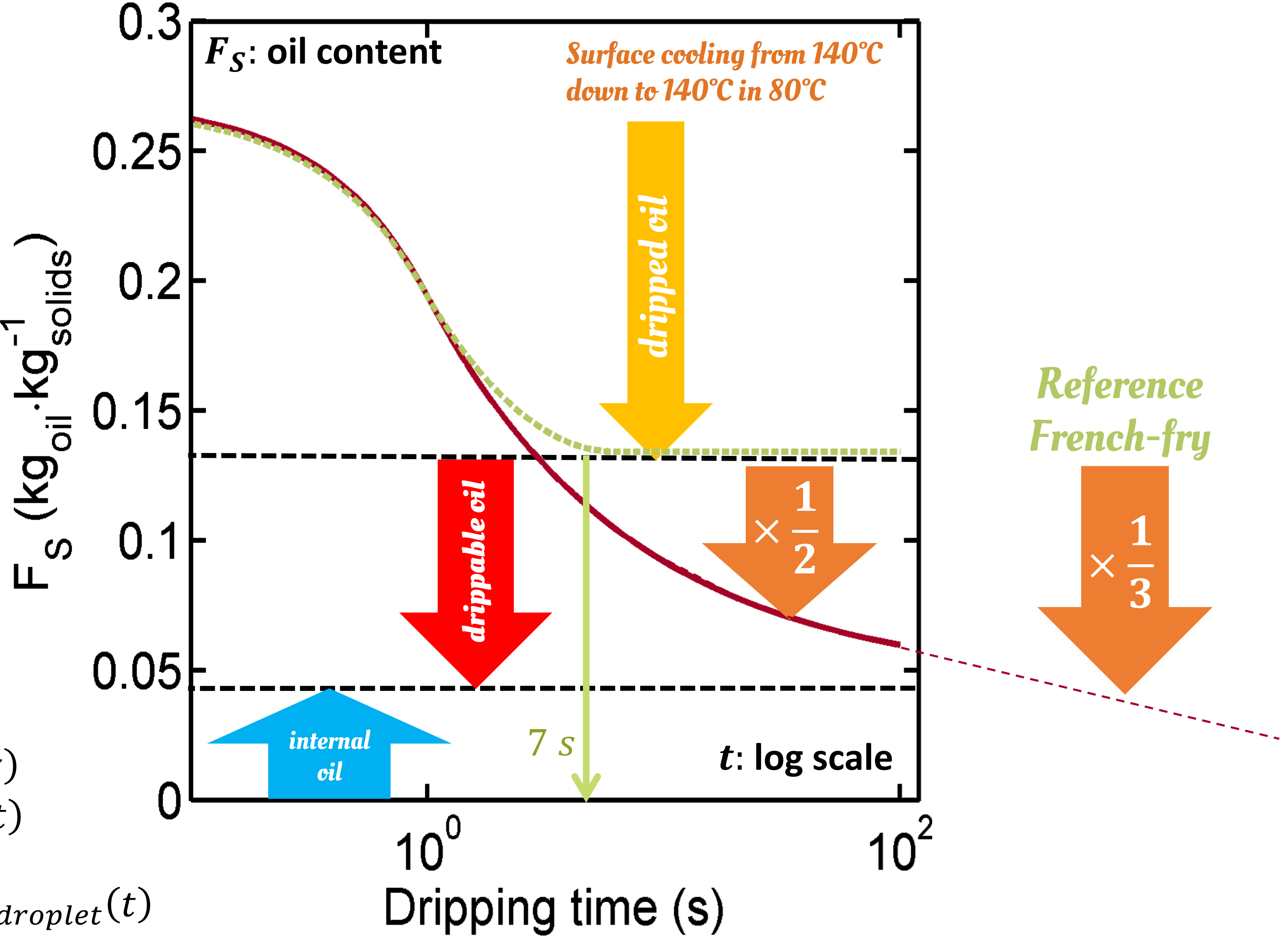










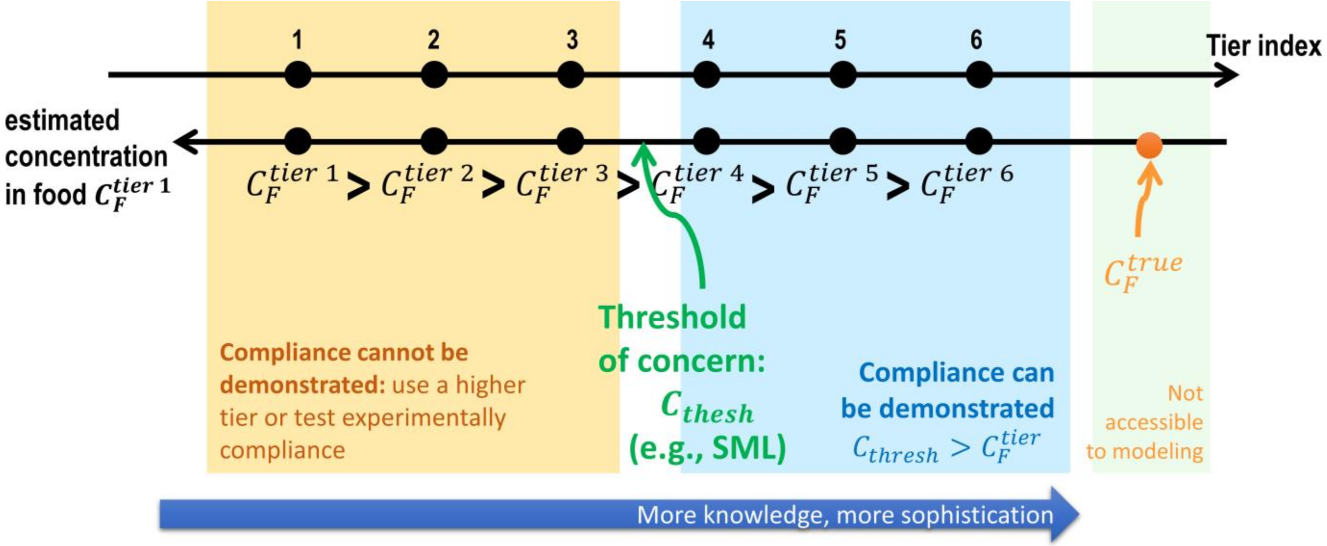


Multiscale model of oil dripping and oil pickup

INRA SCIENCE & IMPACT
université PARIS-SACLAY

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

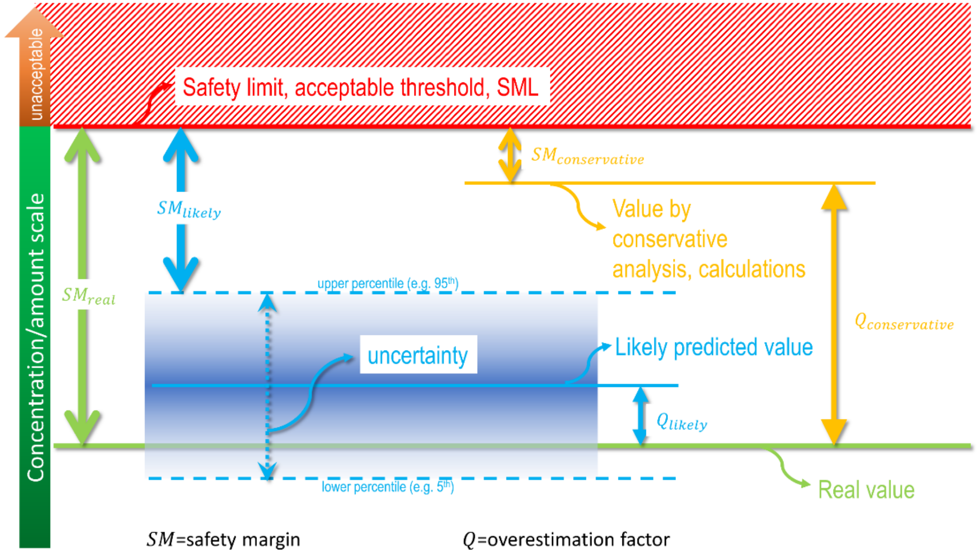


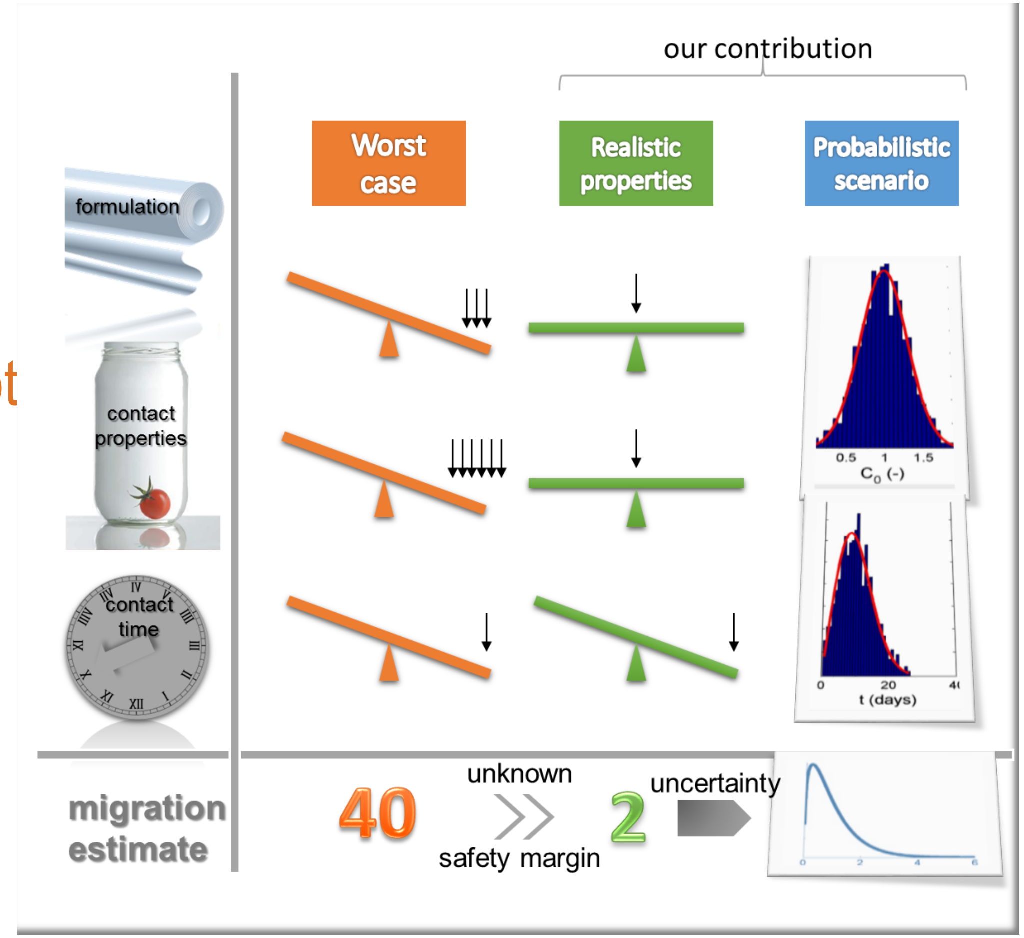
E. J. Hoekstra, R. Brandsch, C. Dequatre, P. Mercea, M.-R. Milana, A. Störmer, X. Trier, O. Vitrac, A. Schäfer and C. Simoneau, in: E. Hoekstra (Ed.): JRC Scientific and technical Reports EUR 27529 EN, European Commission, Ispra (Italy), **2015**.

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





INRA SCIENCE & IMPACT
université PARIS-SACLAY
How to manage uncertainty

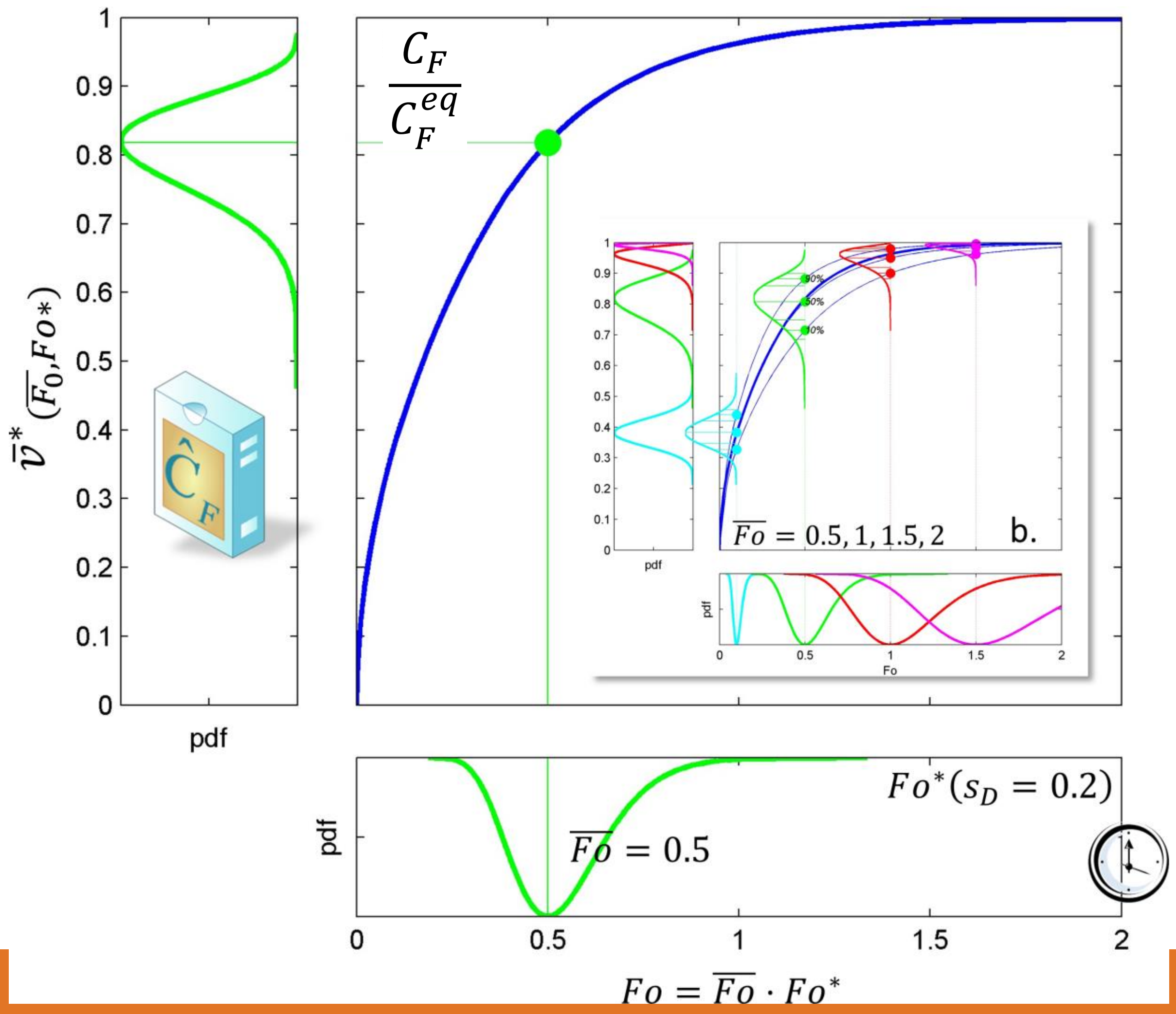
Y. Zhu, P.-M. Nguyen and O. Vitrac in: G. Robertson (Ed.): Elsevier Food Science Reference Module, Elsevier, Amsterdam, NL, 2019, pp. 64

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



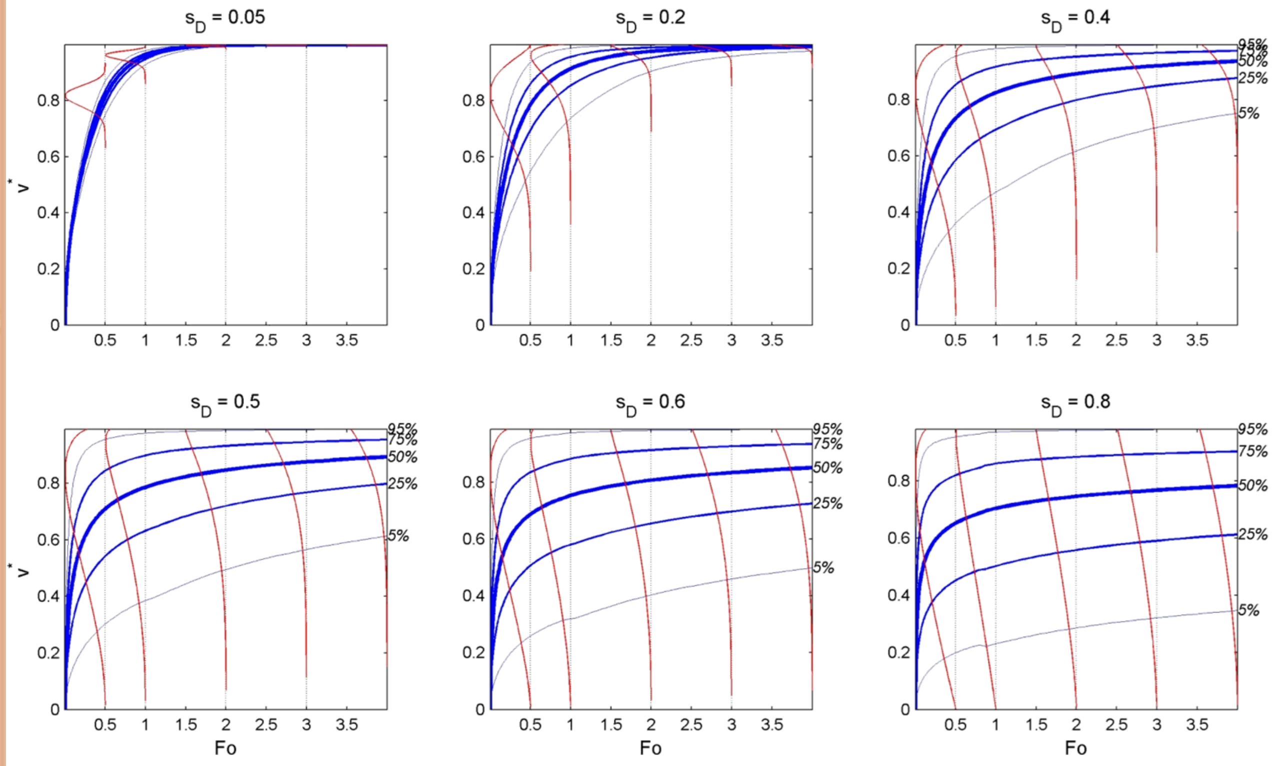
O. Vitrac and M. Hayert, *Aiche Journal* **2005, 51, 1080-1095.**
O. Vitrac, B. Challe, J.-C. Leblanc and A. Feigenbaum, *Food Additives and Contaminants t* **2007, 24, 75-94.**

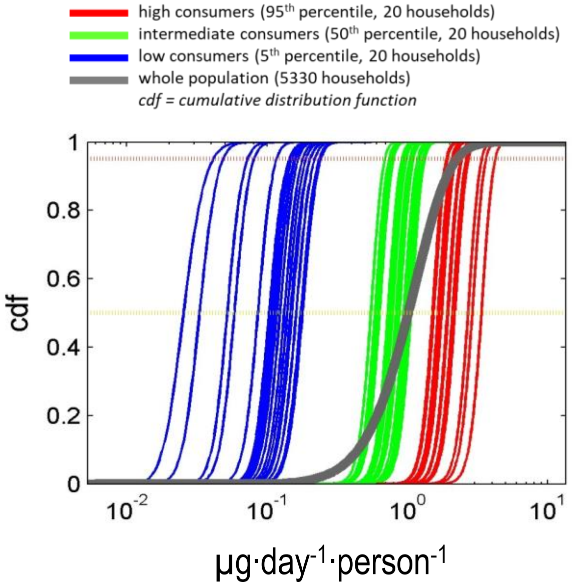
$$\underset{\text{product scale}}{p_r\left(C \le x\right)} = f\begin{pmatrix}\text{food, packaging, migrants} \\ \text{storage cond., uncertainty}\end{pmatrix}$$

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

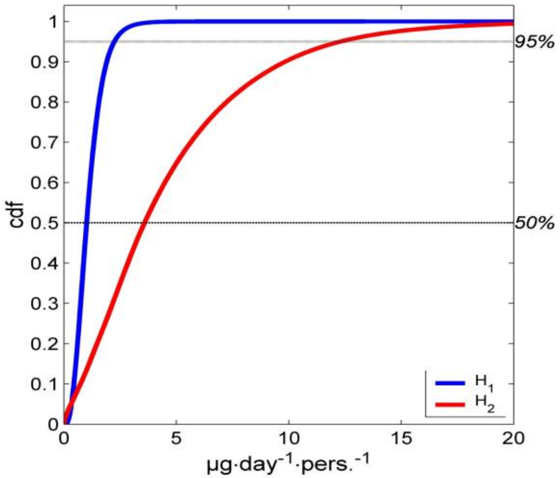
$$E_k = \frac{c_0 \cdot \overline{v}_\infty^*}{365 \cdot P_k} \cdot \sum_{i=1}^{N_k} \overline{v}_i^*\left(Fo_i, Bi, K, L\right)$$

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

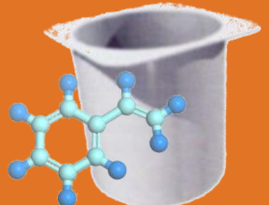




2 physico-chemical scenarios



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



Consumer exposure

styrene from yogurt pots in PS

INRA SCIENCE & IMPACT

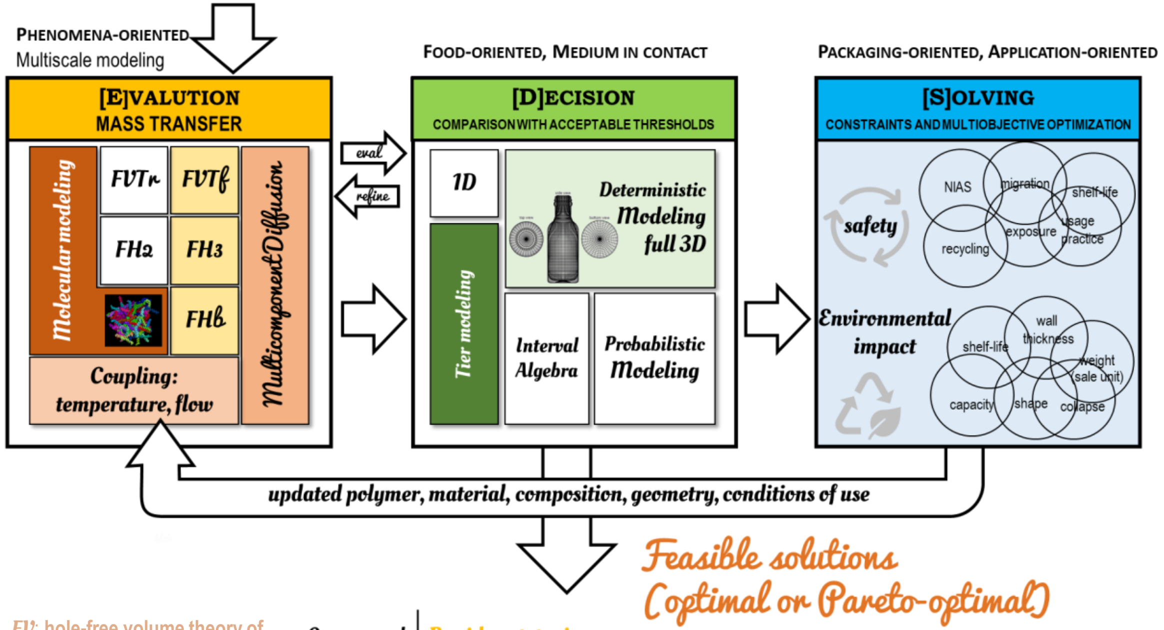
université PARIS-SACLAY

Y. Zhu, B. Guillemat and O. Vitrac, *Frontiers in Chemistry* **2019, 7.**

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**



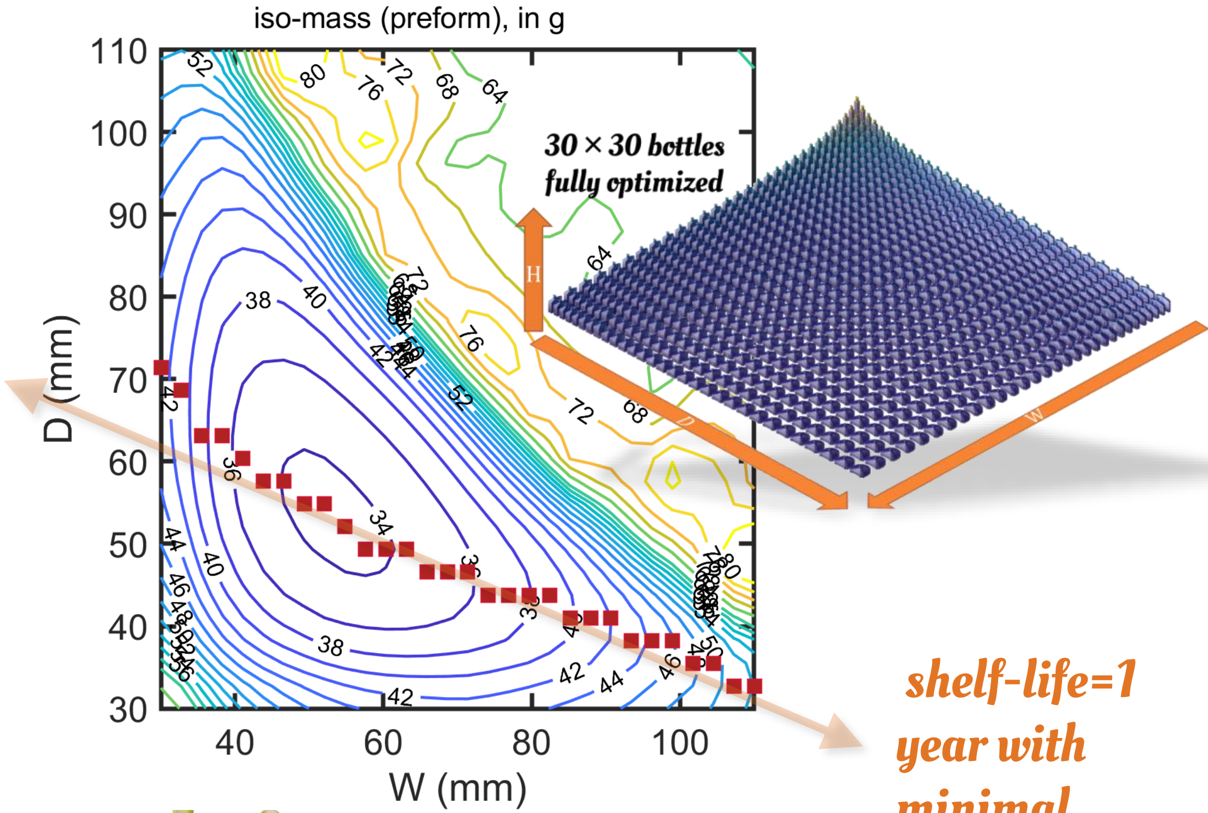
FV: hole-free volume theory of diffusion
(r=rigid and f=flexible solutes)

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

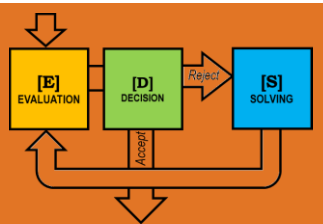
Our research **Rapid prototyping**

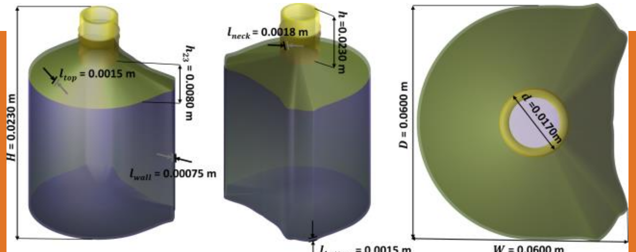
applications

- **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

INRA SCIENCE & IMPACT

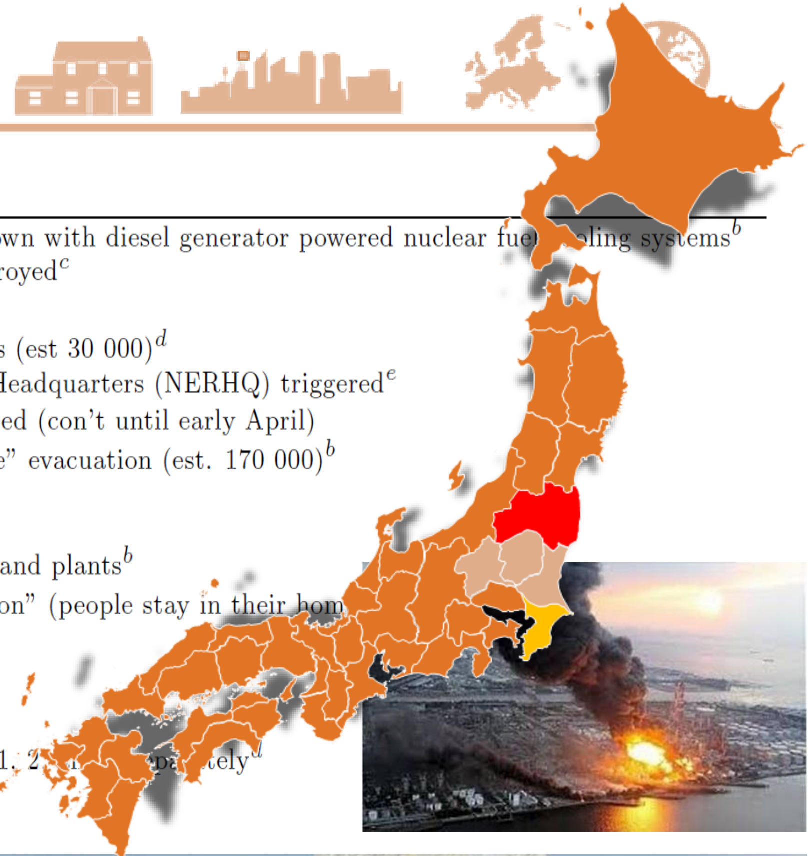
Day (2011)	Event	INES[a]	Results
March 11	Earthquake		All operating reactors at FNPP begin emergency shutdown with diesel generator powered nuclear fue… …ling systems[b]
	Tsunami		Four of the six reactors damaged, diesel generators destroyed[c]
			Evacuation of 3 km radius surrounding FNPP[d]
			Unevacuated 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]
		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 … …tely[d]
		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	

d+1: Airborne contamination

d+4: evacuation $\leq$ 20 km

d+10: contamination 200 km S

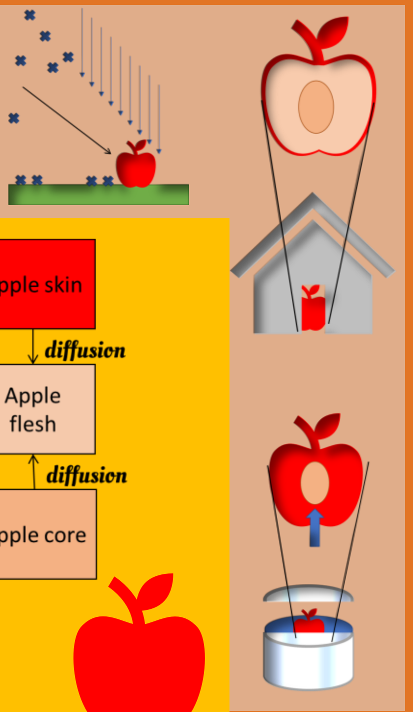
Nov 2017: end of export restrictions to EU



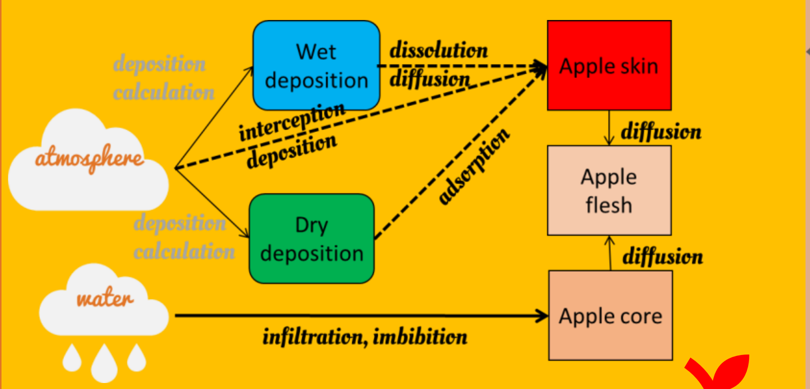
INRA SCIENCE & IMPACT

Contamination of food products after a nuclear disaster

Scenarios of food exposure accounting for storage and packaging conditions



Apple plugin



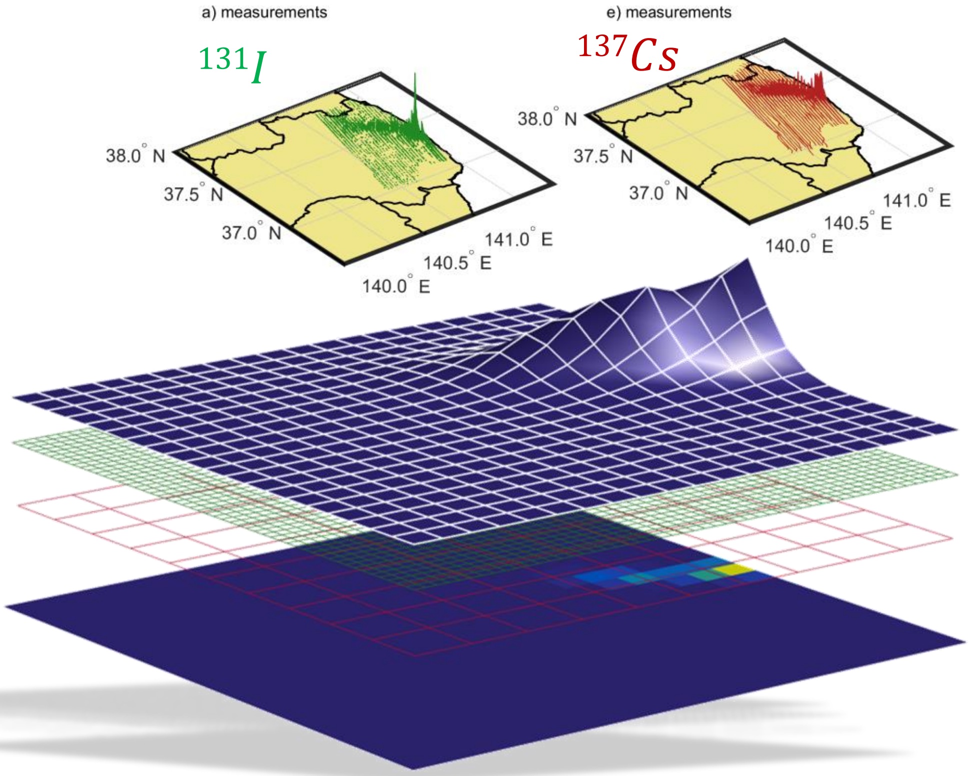
Collection of mechanisms with/without packaging

^{131}I

^{90}Sr

^{137}Cs

Relatively volatile radionuclide can contaminate large areas

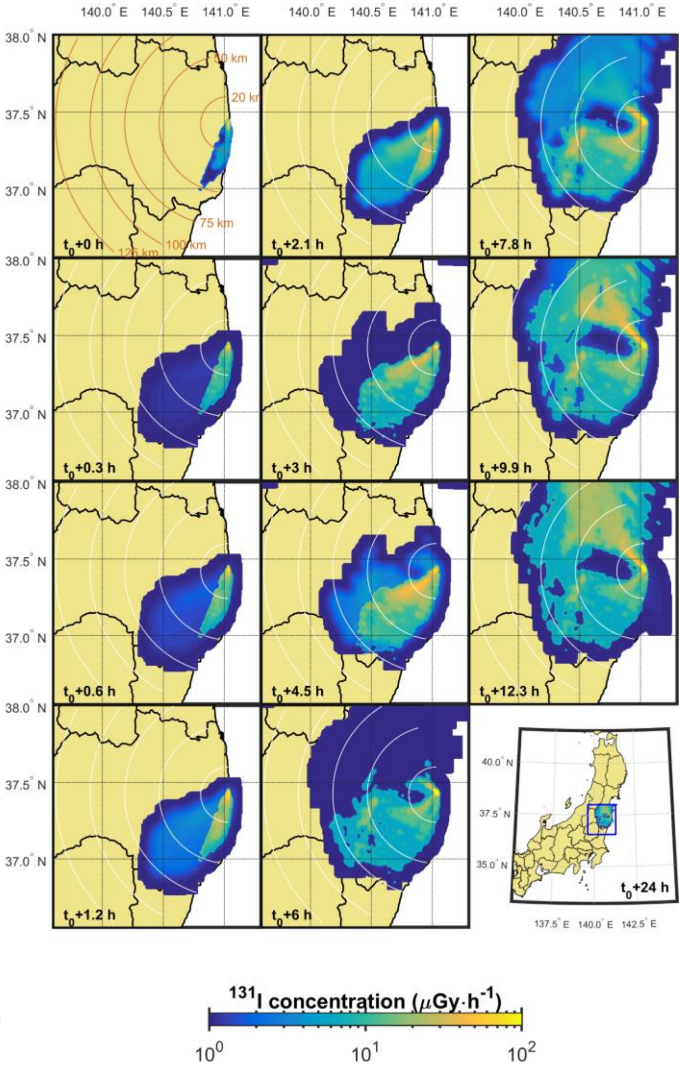


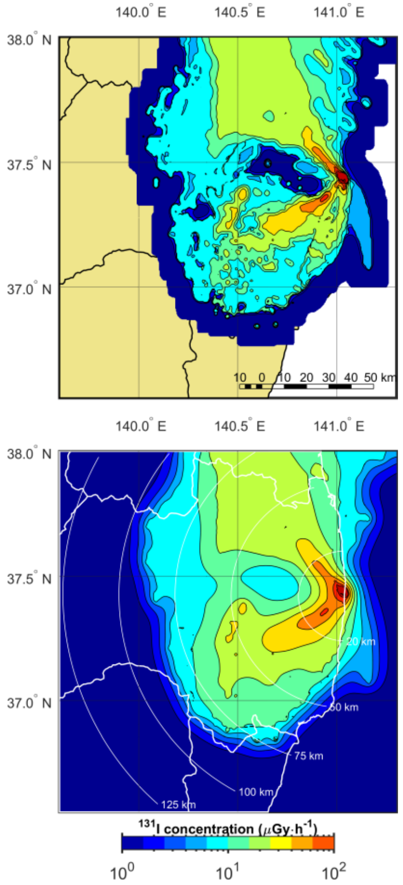
Combining multiple information with different resolutions and obtained on different periods

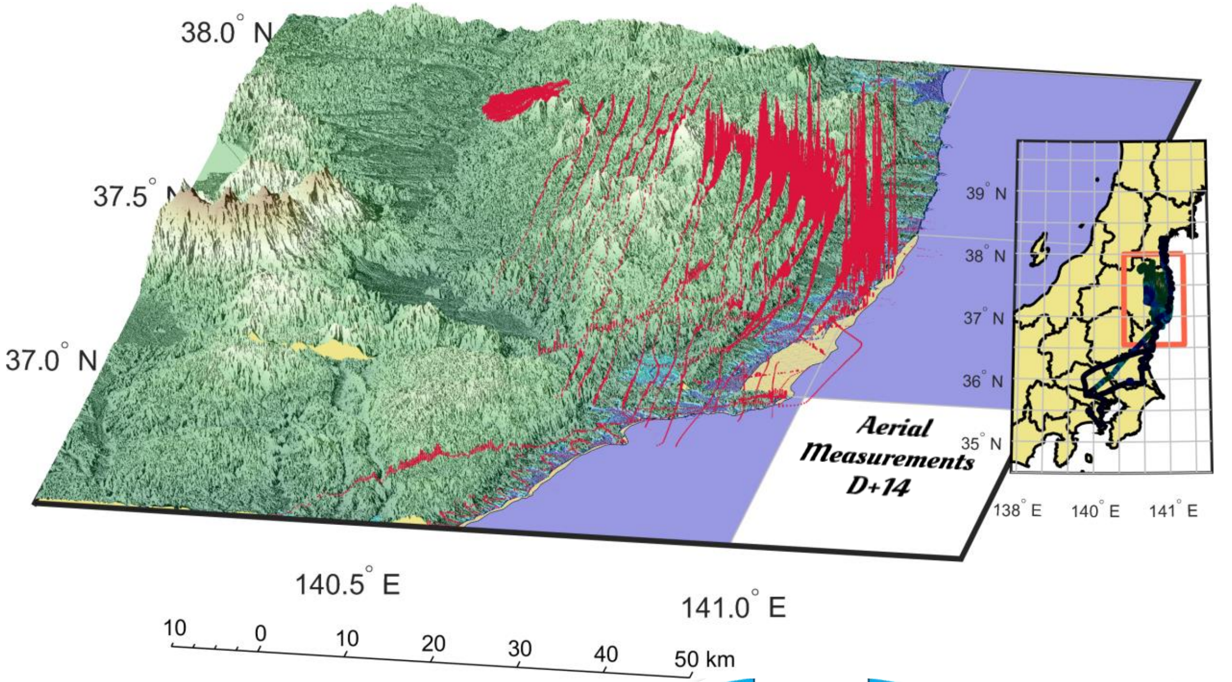
- *Meteorological data*
- *Dispersion data (measured, simulated)*

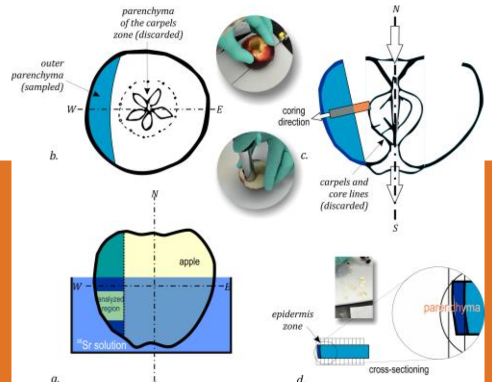
INRA SCIENCE & IMPACT

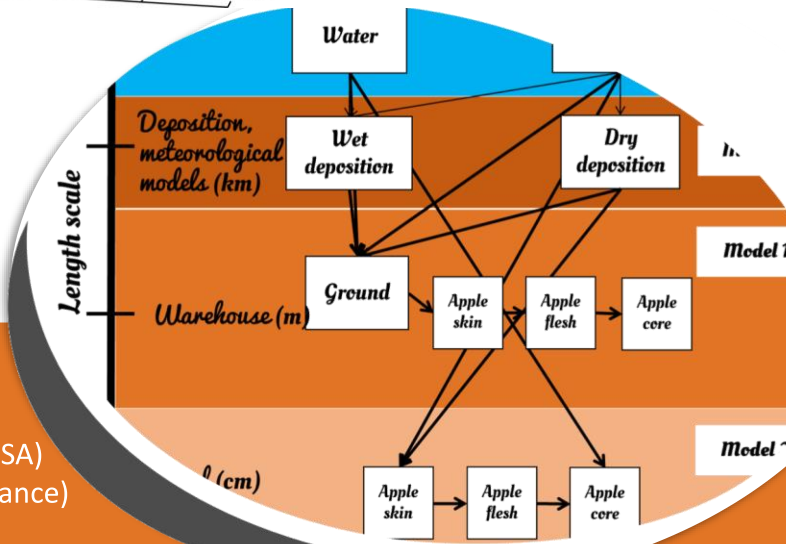
Collaborations
FDA (WEAC, Boston, MA,USA)
IRSN (Fontenay-les-Roses, France)







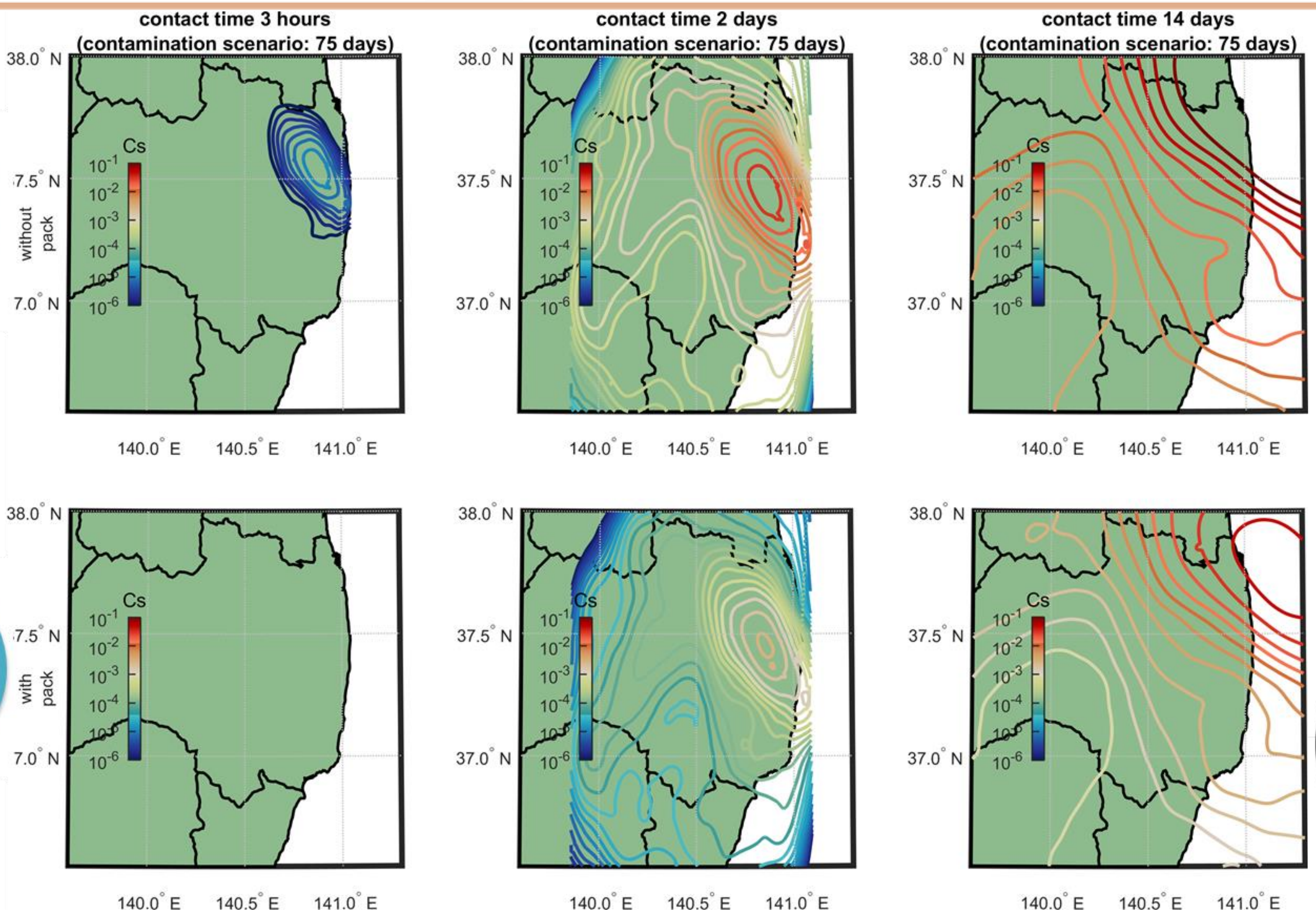




Collaborations

FDA (WEAC, Boston, MA,USA)

IRSN (Fontenay-les-Roses, France)



A tool for first responders

- *triage*
- *orienting future tests*

The Fukushima plant today

INRA SCIENCE & IMPACT

université PARIS-SACLAY

Work in progress wit IRSN

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

Large scale models are real serious games (cost-efficient, responsible, preventive or prospective)

Computer and the societal demand are the main drivers (meshless methods, more linked scales and phenomena)

Collaborative and participative groups across disciplines are encouraged

New approach for innovation in the industry (experiments are required only for validation)

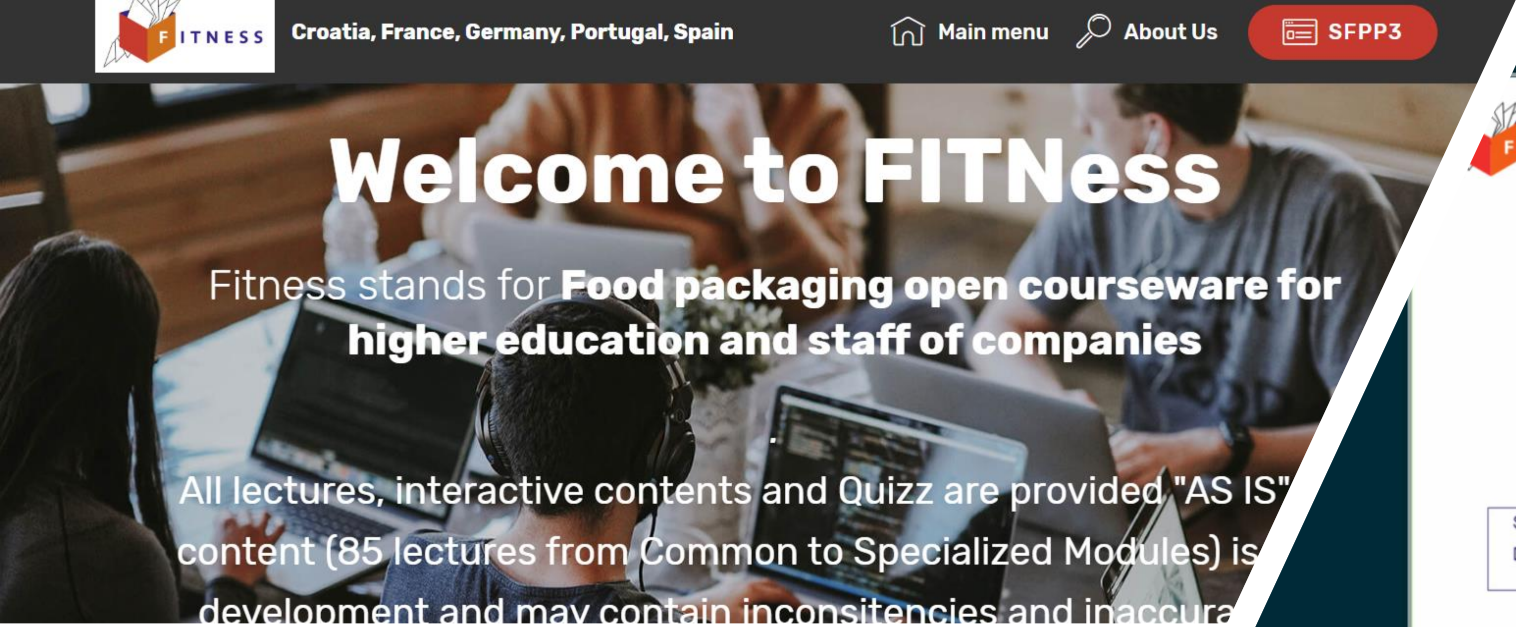
Trust is needed on model, simulation and decision (standards, frontiers in science/engineering)

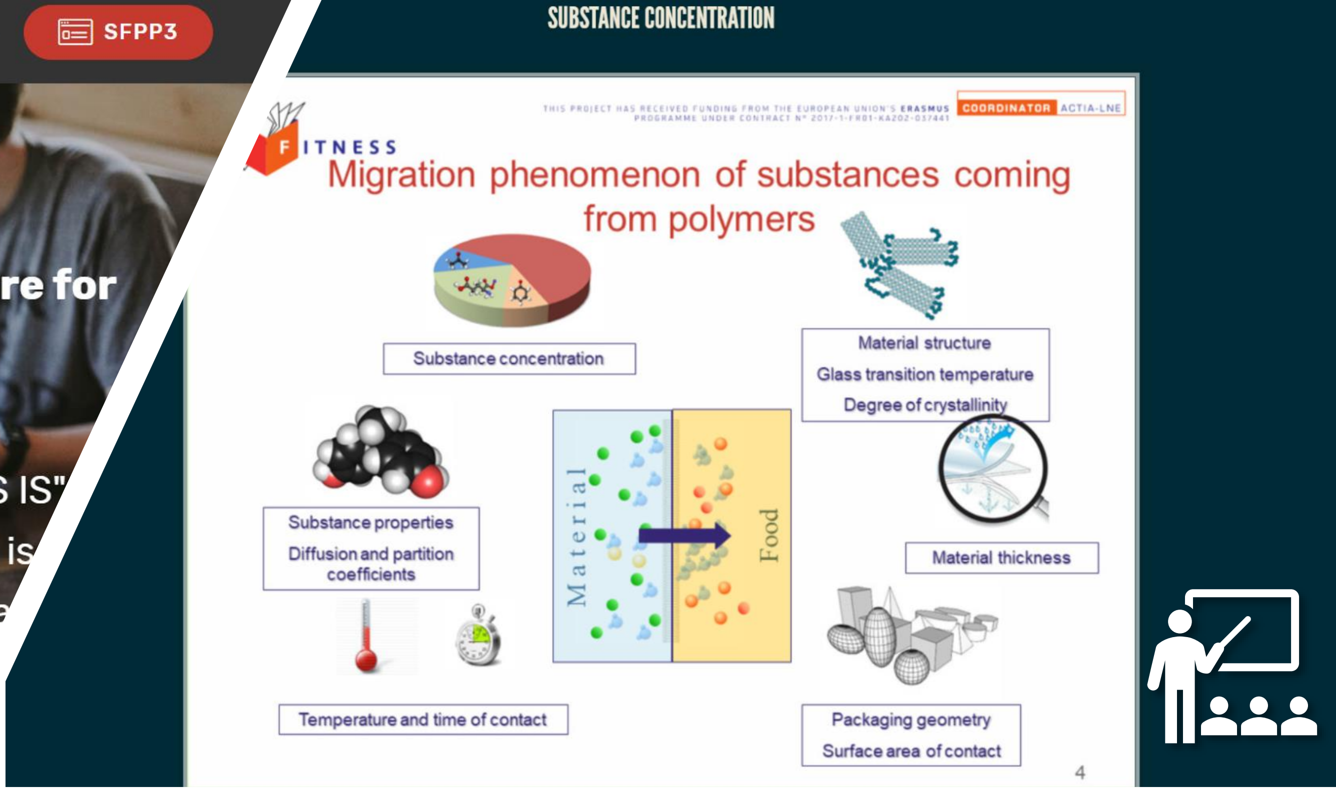
Teaching, training, real exercises, case-studies (e.g. European Initiative https://fitness.agroparistech.fr**)**

Think BIG with modeling

INRA SCIENCE & IMPACT

université PARIS-SACLAY





FITNESS

http://fitness.agroparistech.fr

Co-funded by the Erasmus+ Programme of the European Union

Online lectures

uthor: undef

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

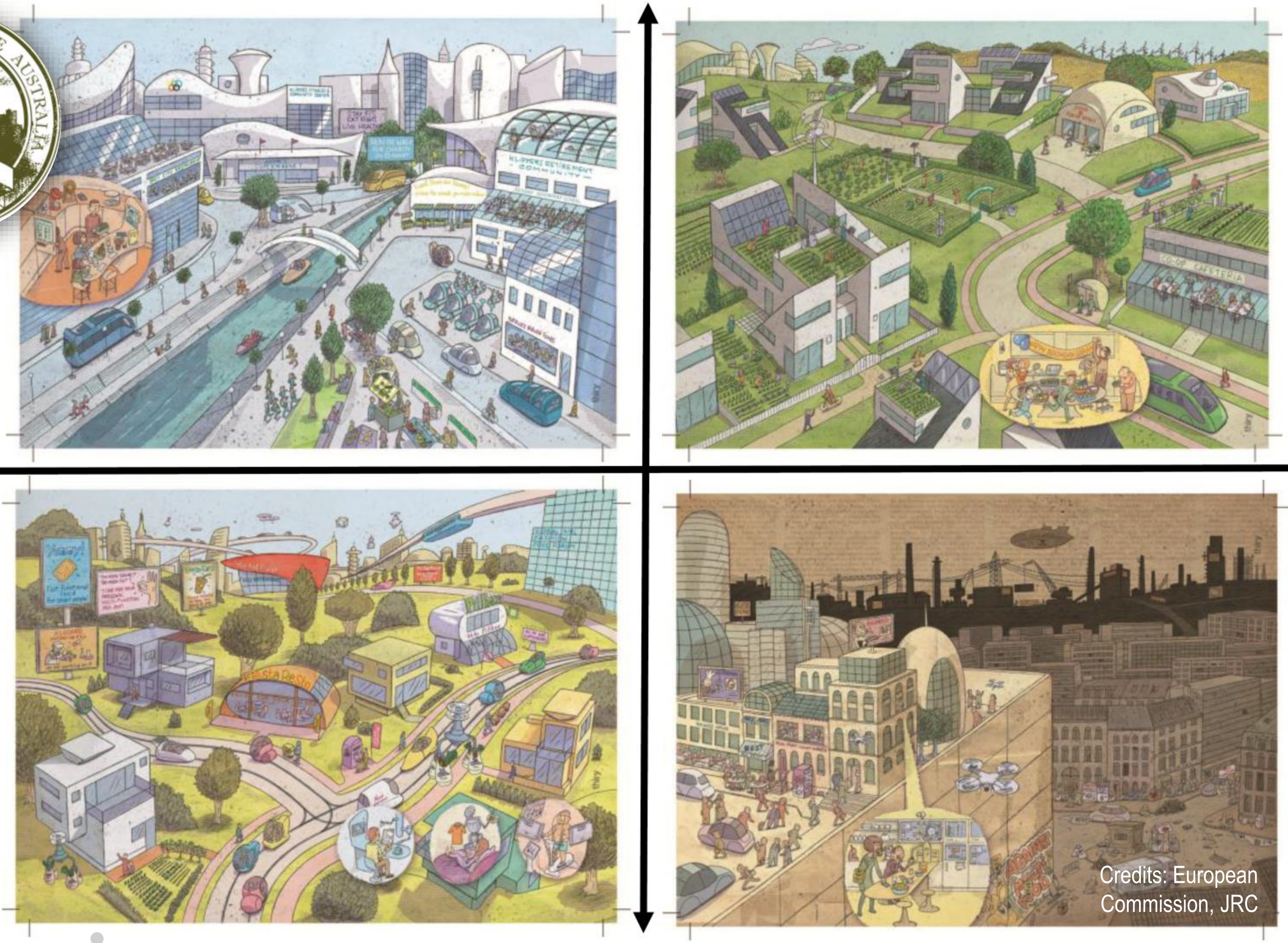
Migration modeling for multi-materials, multi-steps process, reusable materials - SPECIALIZED TRAININ MODULES

author: undef

part 1/1	references	extra	casestudies	howto	solutions

Strong community spirit (sustainable, safety and quality)

Low agriculture commodity and food price



High agriculture commodity and food price

Individualistic society (individual rights and initiatives valued)

Think BIG with modeling

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