



université
PARIS-SACLAY

INRAE Department Food, Bioproducts and Waste

AgroParisTech
Talents for a sustainable planet

LABORATOIRE
NATIONAL
DE MÉTROLOGIE
ET D'ESSAIS LNE



7th International
Symposium on Food
Packaging

Scientific Developments Supporting Safety and Innovation
3-6 May 2022 | Digital

Digital, Online – May 3-6, 2022

Computer-aided design of safe ➤ food packaging with maximized recycled content

UMR 0782 SayFood
Group Modeling and
Computational Engineering

UMT ACTIA 17.09

UMT
SAFEMAT
SAFETY
OF PACKAGING

Olivier Vitrac, INRAE, olivier.vitrac@agroparistech.fr

Julien Kermorvant, LNE-INRAE

Natacha Daoud, IPC-INRAE

Phuong-Mai Nguyen, LNE



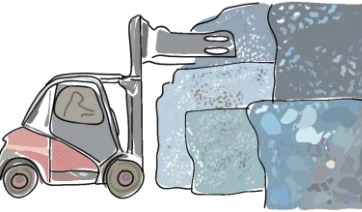
1964



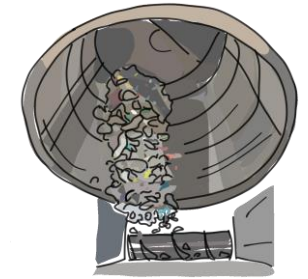
1974



Generalization of disposable bottles



Wastes became trade materials



Wastes are recycled



2008

for food contact



2022

Who can guarantee it?

Q1: HOW TO IDENTIFY THE SOURCING?
(food, non-food, decontaminated, intra EU)?

Q2: HOW TO USE THE RECYCLED CONTENT?
(direct contact, behind a functional barrier, low/high temperature)?

Q3: HOW TO DESIGN FOR WASTE REDUCTION AND FUTURE RECYCLABILITY?

➤ NEW RULES ARE COMING

With more risks and opportunities – good practices are imperative

French anti-waste law 2020-105

Draft order specifying the substances contained in mineral oils whose use is prohibited on packaging and in printing for the public

Public consultation: 49 comments

<http://www.consultations-publiques.developpement-durable.gouv.fr/projet-d-arrete-precisant-les-substances-contenues-a2559.html>



Food safety – recycled plastic in food packaging (updated 282/2008)

- transitional provisions,
- provisions for the appropriate evaluation of non-PET materials
- clear obligations for operators and competent authorities.

Public consultation: 96 comments

https://ec.europa.eu/info/law/better-regulation/have-your-say/initiatives/12013-Food-safety-recycled-plastic-in-food-packaging-updated-rules_en



In preparation

Draft act

Feedback period

06 December 2021 - 18

January 2022

FEEDBACK: CLOSED

UPCOMING

Commission adoption

Planned for

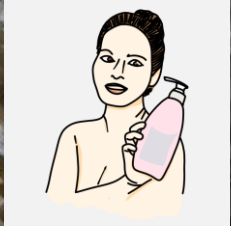
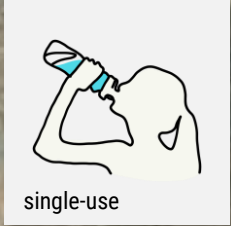
First quarter 2022



VIRGIN

virgin

DECONTAMINATED?



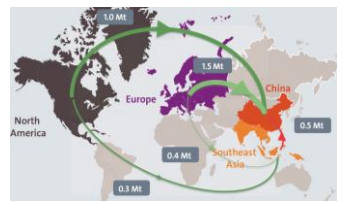
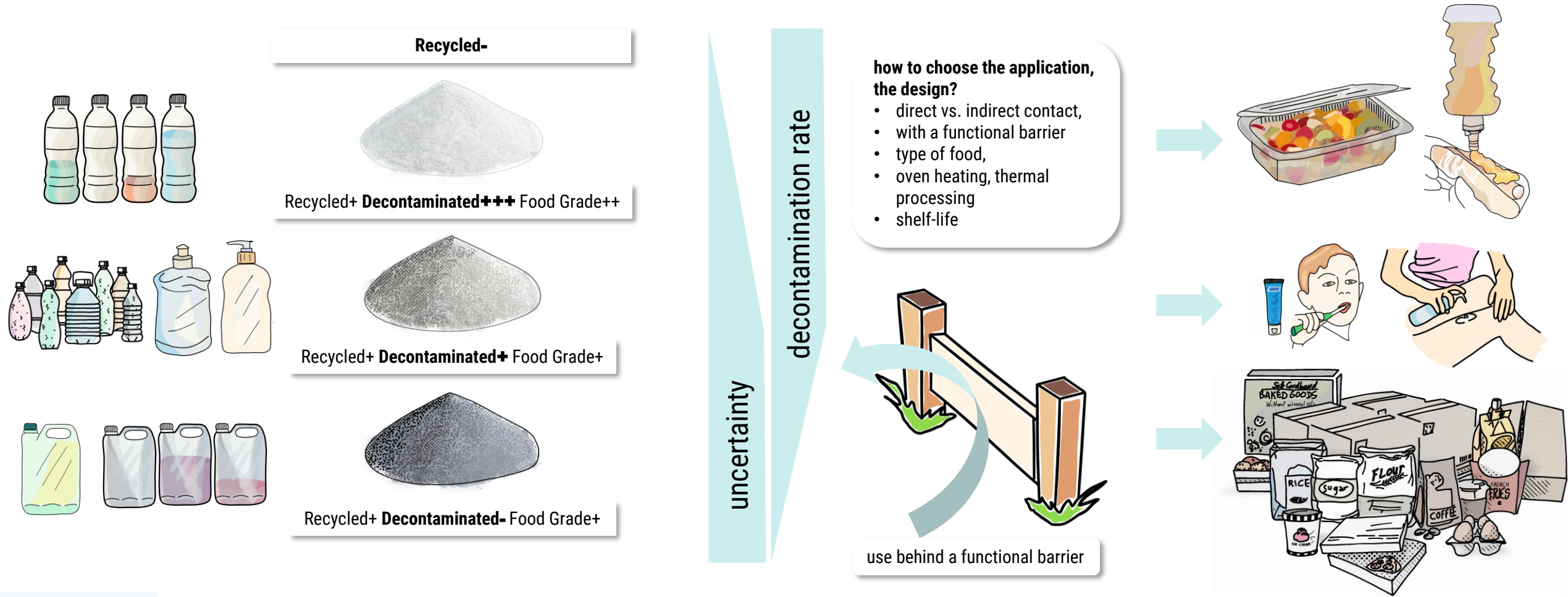
DECONTAMINATED?

HOT WASHED



➤ SOURCING, DESIGN AND RECYCLING ARE LINKED DECISIONS

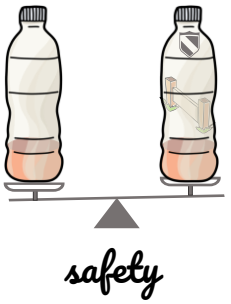
Beyond food contact



Which collecting, recycling route?

- Traceability?
- Purity?
- Integrity?

➤ ENABLING MORE RECYCLED STREAMS TO BE USED



decontaminated +++
FB-

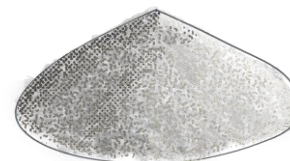
EQUIVALENT
SAFETY
=

decontaminated +
FB ++

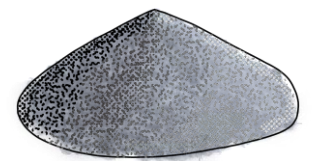
decontaminated +
FB ++



Recycled+ **Decontaminated+++** Food Grade++



Recycled+ **Decontaminated+** Food Grade+



Recycled+ **Decontaminated-** Food Grade+



➤ ENABLING MORE RECYCLED STREAMS TO BE USED

while offering the same safety



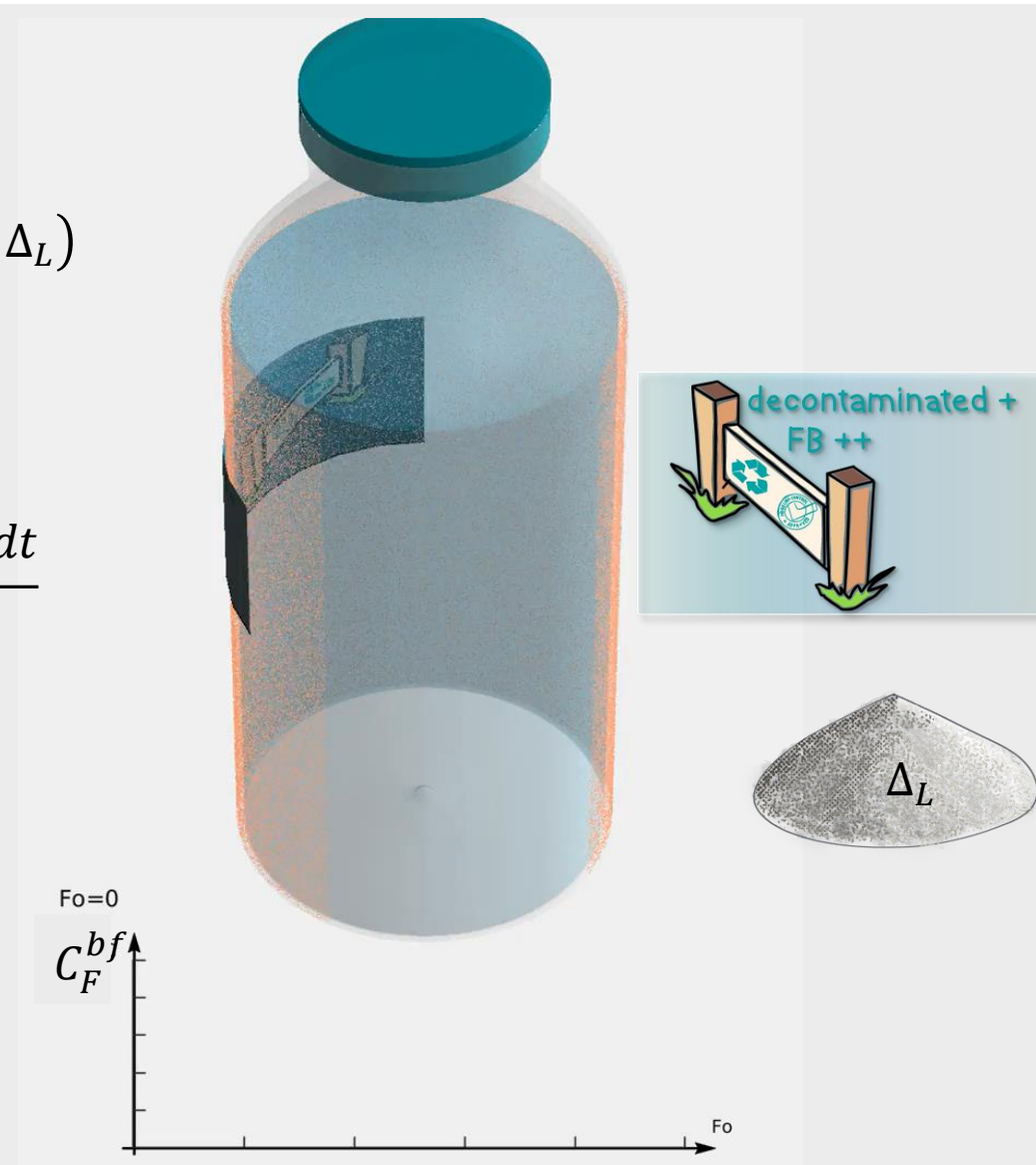
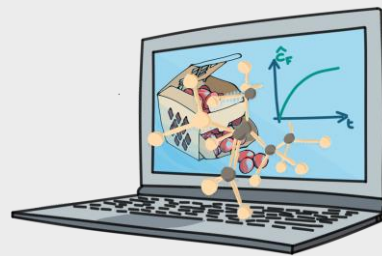
Mathematical problem:

$$C_F(Fo_{eq}, \Delta_H) = C_F^{bf}(Fo_{eq}, \Delta_L)$$

with

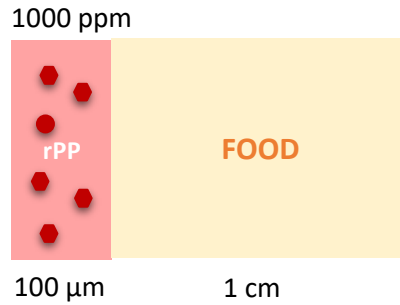
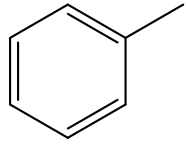
$$\Delta_H < \Delta_L$$

$$Fo = \int_0^t \frac{D[T(t)]_{layer}^{recycled} dt}{l^2}$$



> Model situation: rPP

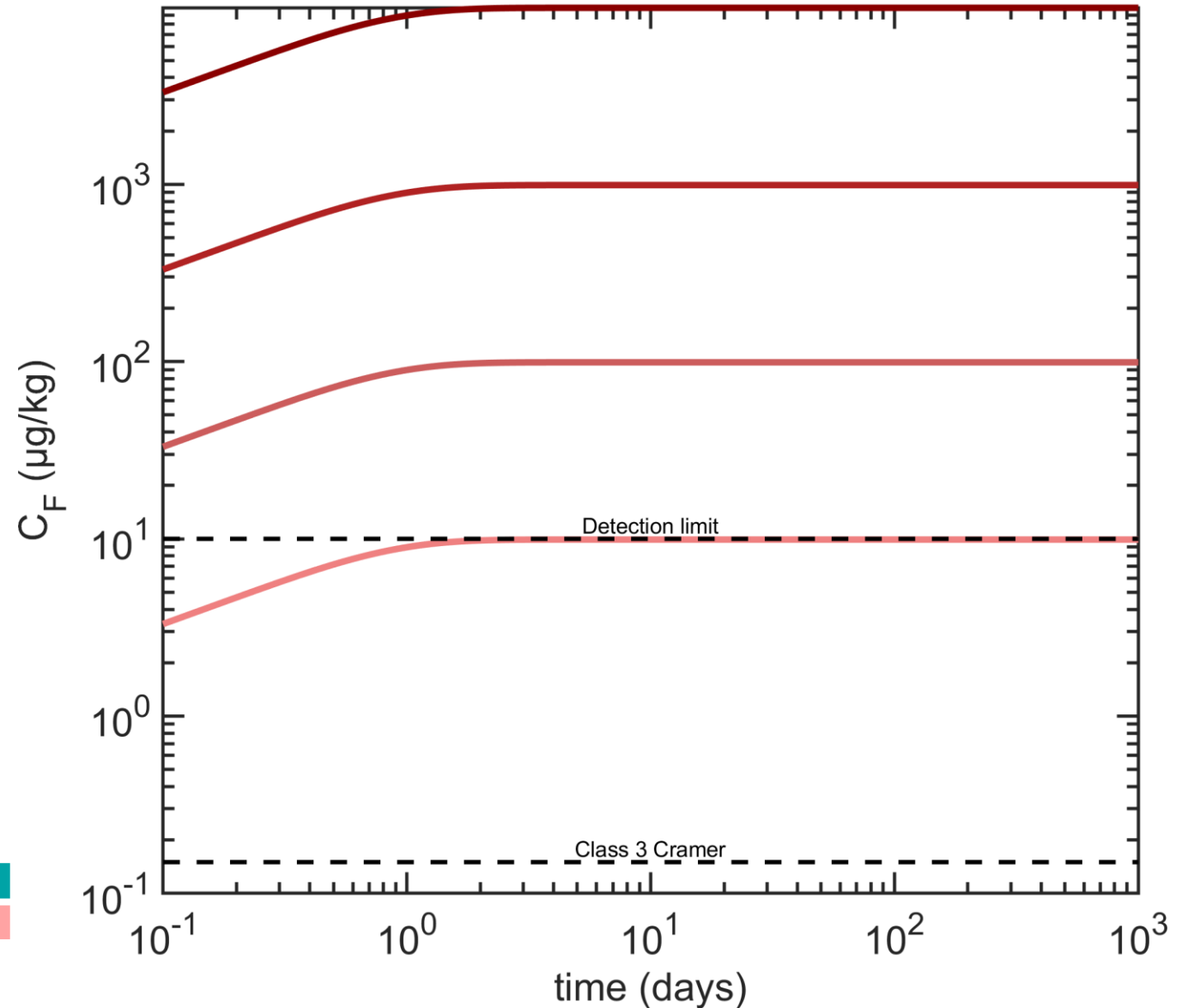
Toluene
@40°C



decontamination rate: Δ

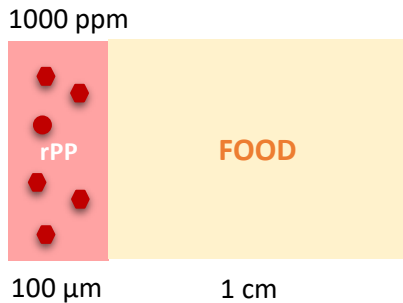
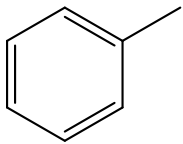
Polymer	D ($m^2 \cdot s^{-1}$)	Ref.
PP	10^{-13}	Fang <i>et al.</i> Macromolecules 2013, 46, 3, 874

- recycled - REF
- REF - $\Delta=90.0\%$
- REF - $\Delta=99.0\%$
- REF - $\Delta=99.9\%$

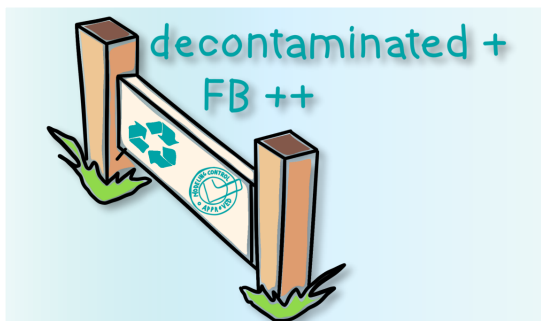
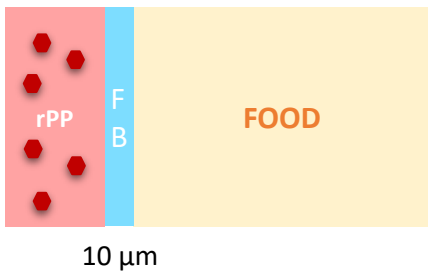


➤ Model situation: rPP+PET(10%)

Toluene
@40°C

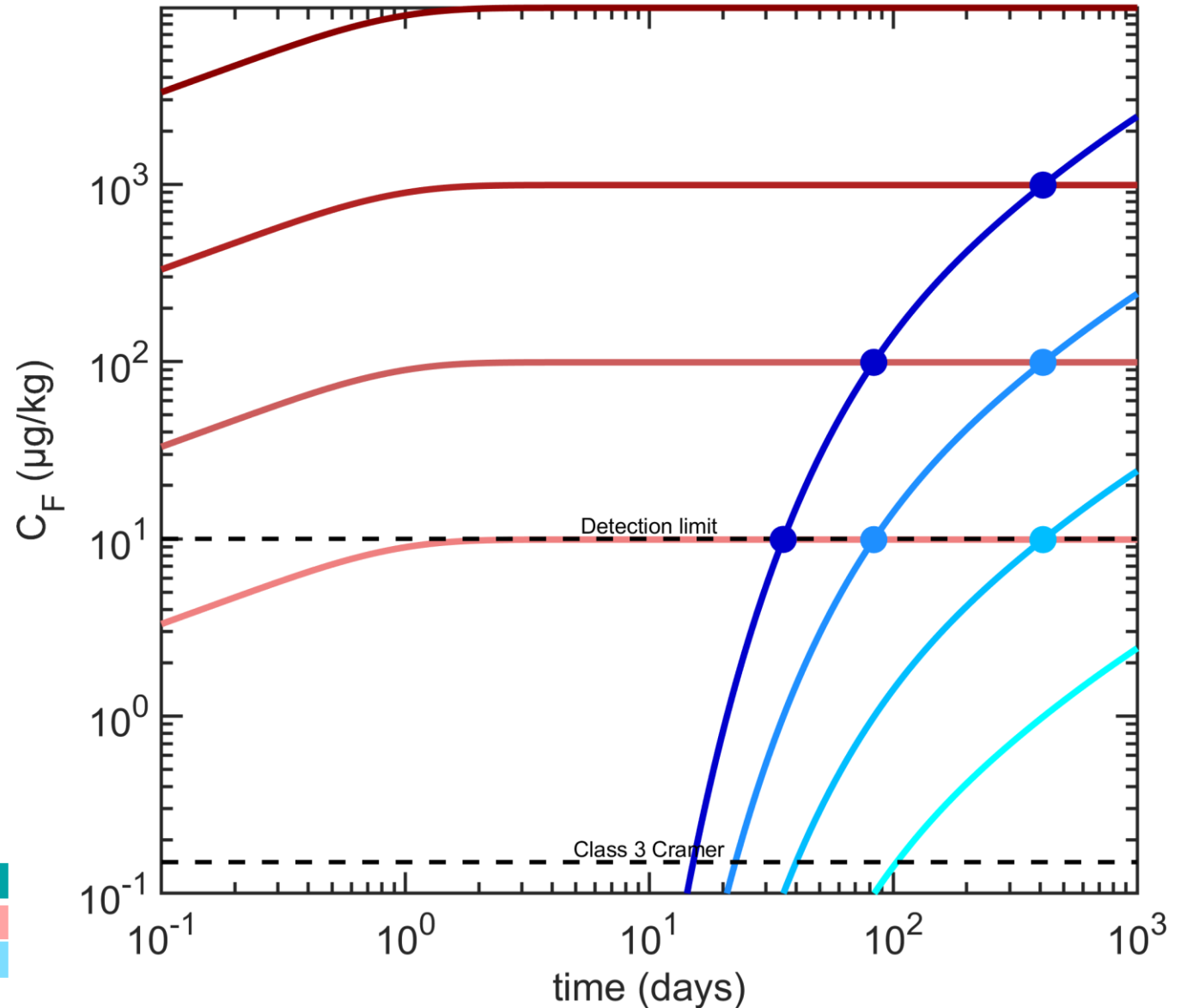


functional barrier
= dry PET
($T_g = 76^\circ\text{C}$)



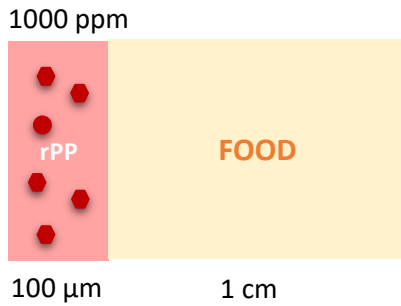
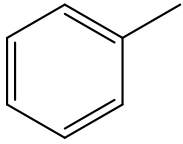
Polymer	$D \text{ (m}^2 \cdot \text{s}^{-1}\text{)}$	Ref.
PP	10^{-13}	Fang <i>et al.</i> <i>Macromolecules</i> 2013, 46, 3, 874
Dry PET	3.5×10^{-18}	Zhu <i>et al.</i> <i>Soft Matter</i> , 2019,15, 891

- recycled - REF
- REF - $\Delta=90.0\%$
- REF - $\Delta=99.0\%$
- REF - $\Delta=99.9\%$

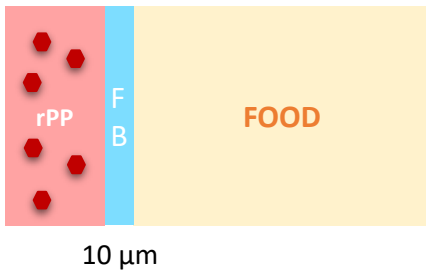


➤ Model situation: rPP+PET(10%)

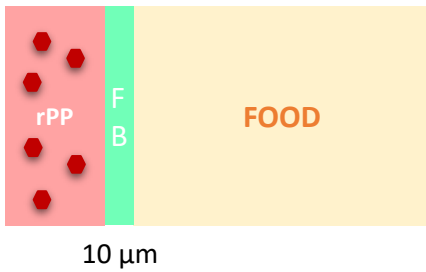
Toluene
@40°C



functional barrier
= dry PET
($T_g = 76^\circ\text{C}$)

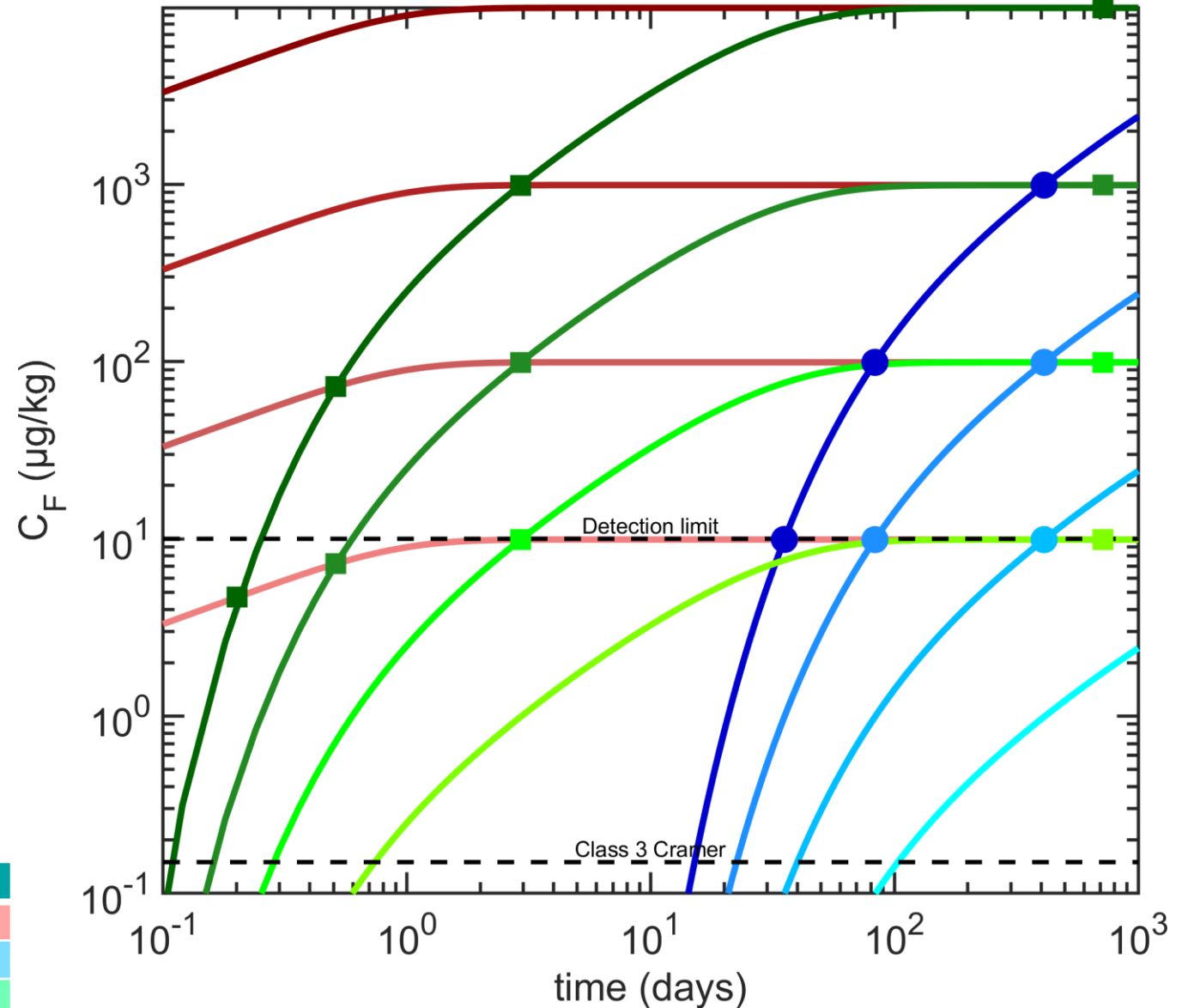


functional barrier
= plasticized PET
($T_g = 60^\circ\text{C}$)

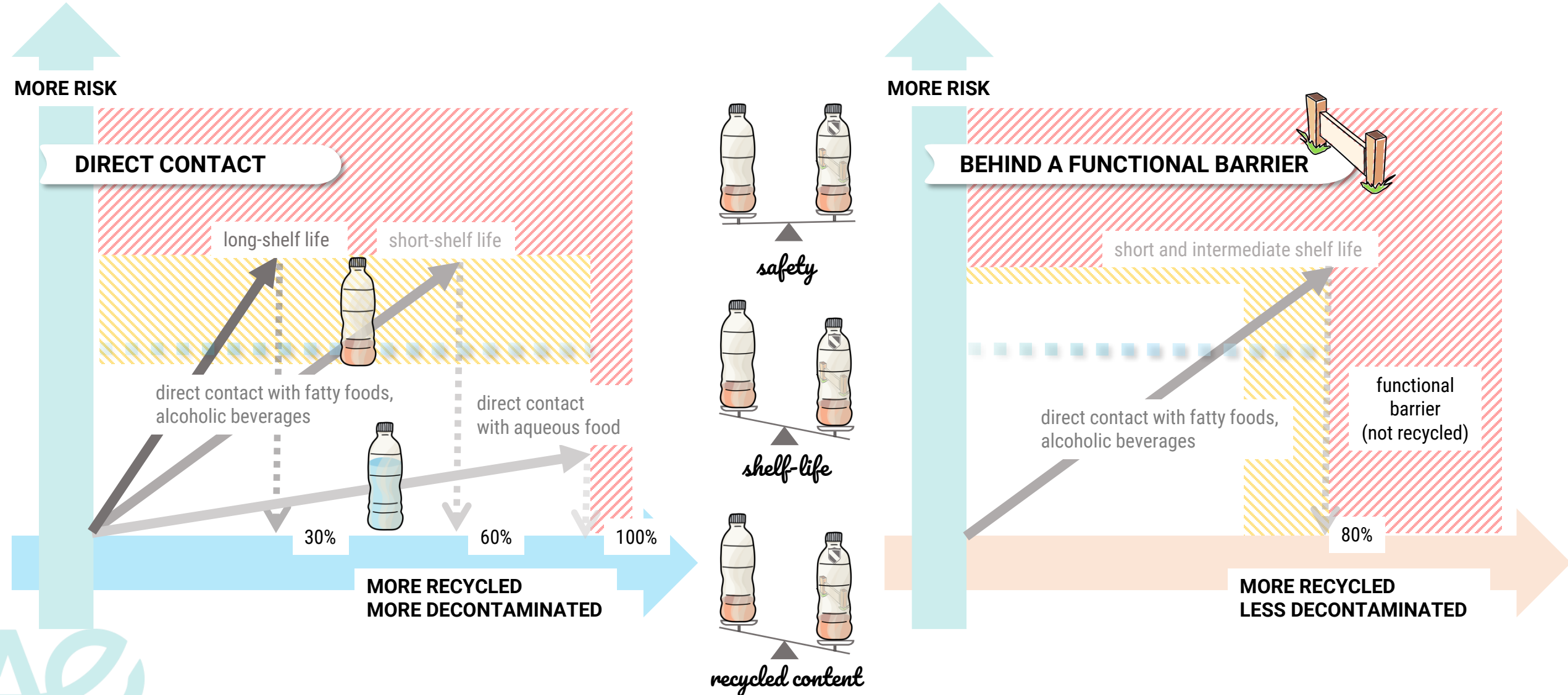


Polymer	D ($\text{m}^2 \cdot \text{s}^{-1}$)	Ref.
PP	10^{-13}	Fang <i>et al.</i> <i>Macromolecules</i> 2013, 46, 3, 874
Dry PET	3.5×10^{-18}	Zhu <i>et al.</i> <i>Soft Matter</i> , 2019,15, 891
plasticized PET	5×10^{-16}	Zhu <i>et al.</i> <i>Soft Matter</i> , 2019,15, 891

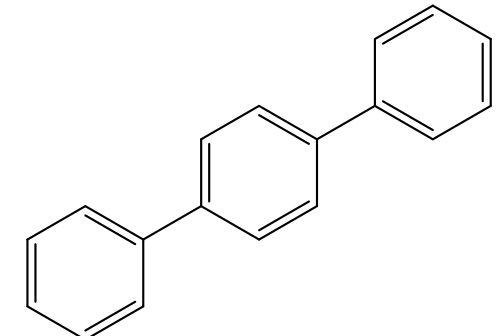
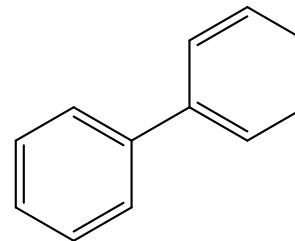
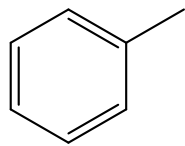
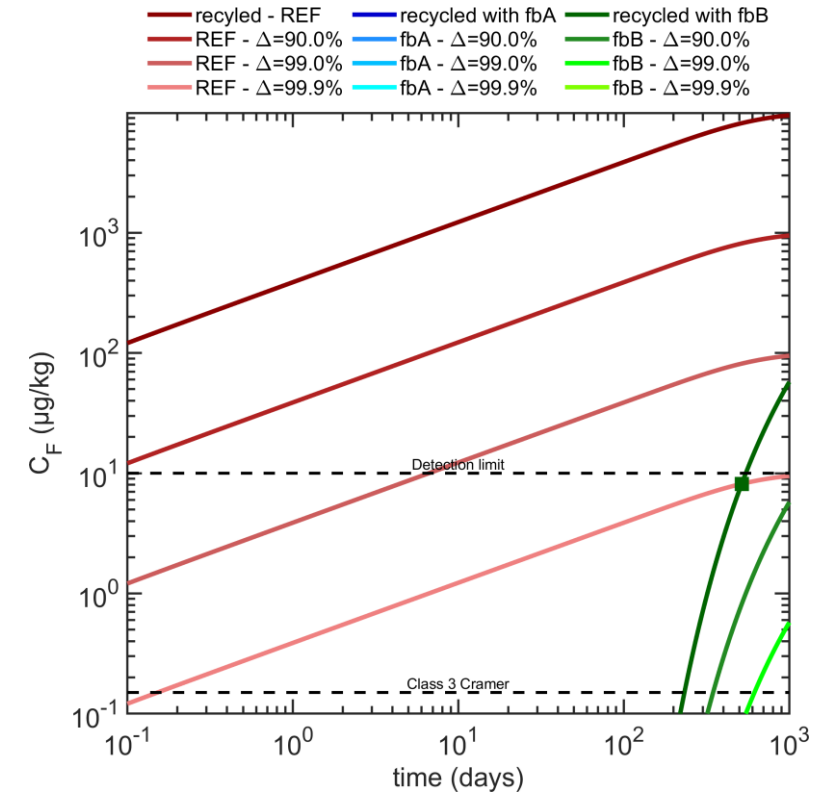
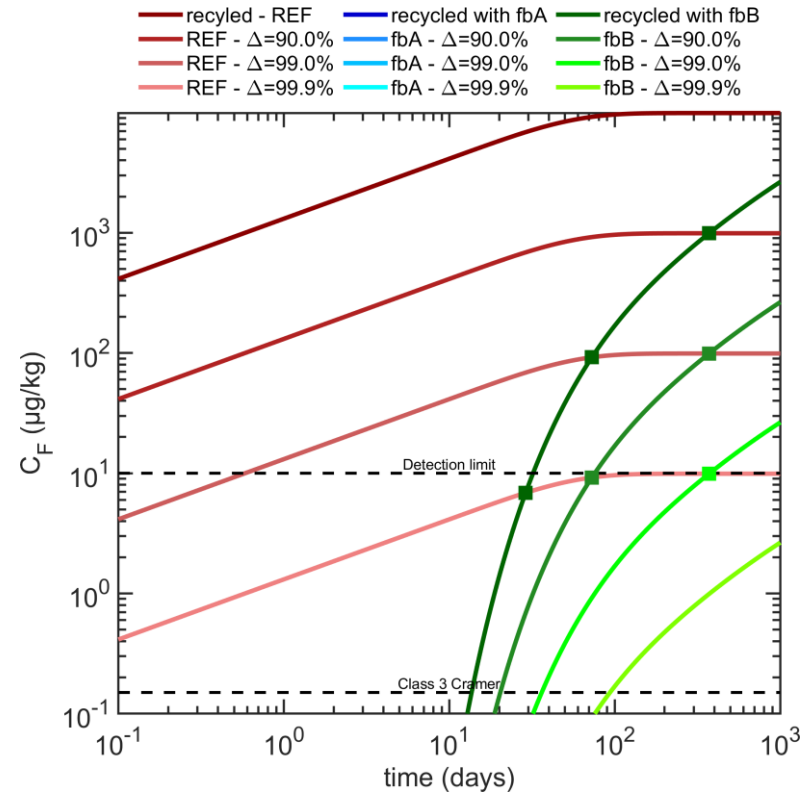
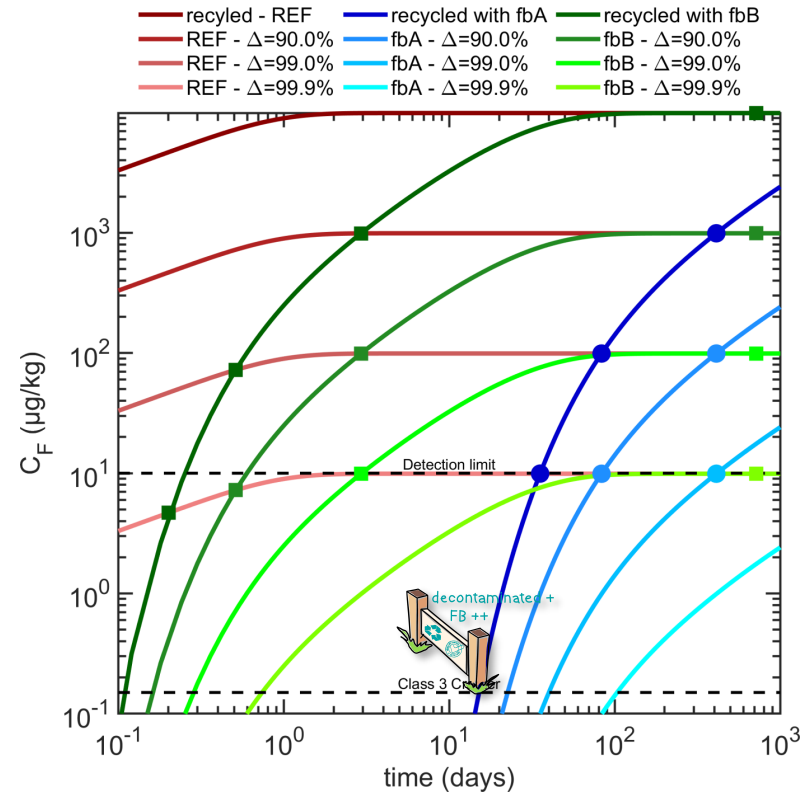
- recycled - REF
- REF - $\Delta=90.0\%$
- REF - $\Delta=99.0\%$
- REF - $\Delta=99.9\%$
- recycled with fbA
- fbA - $\Delta=90.0\%$
- fbA - $\Delta=99.0\%$
- fbA - $\Delta=99.9\%$
- recycled with fbB
- fbB - $\Delta=90.0\%$
- fbB - $\Delta=99.0\%$
- fbB - $\Delta=99.9\%$



➤ BENEFITS OF FUNCTIONAL BARRIERS (if well used)

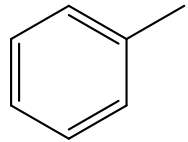















➤ Effect of the number of rings on the concept of equivalent safety

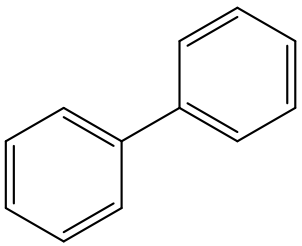













➤ Duration with equivalent safety for rPP

Functional barrier: "dry" PET (plasticized PET)



	0% 	90% 	99% 	99.9% 	 decontaminated +++ FB-
 0% 	>1000 days (716)	411 days (2.9)	83 days (0.5)	35 days (0.2)	  
 90%	>1000 days	>1000 days (716)	411 days (2.9)	83 days (0.5)	
99%	>1000 days	>1000 days	>1000 days (716)	411 days (2.9)	
 99.9%	>1000 days	>1000 days	>1000 days	>1000 days (716)	

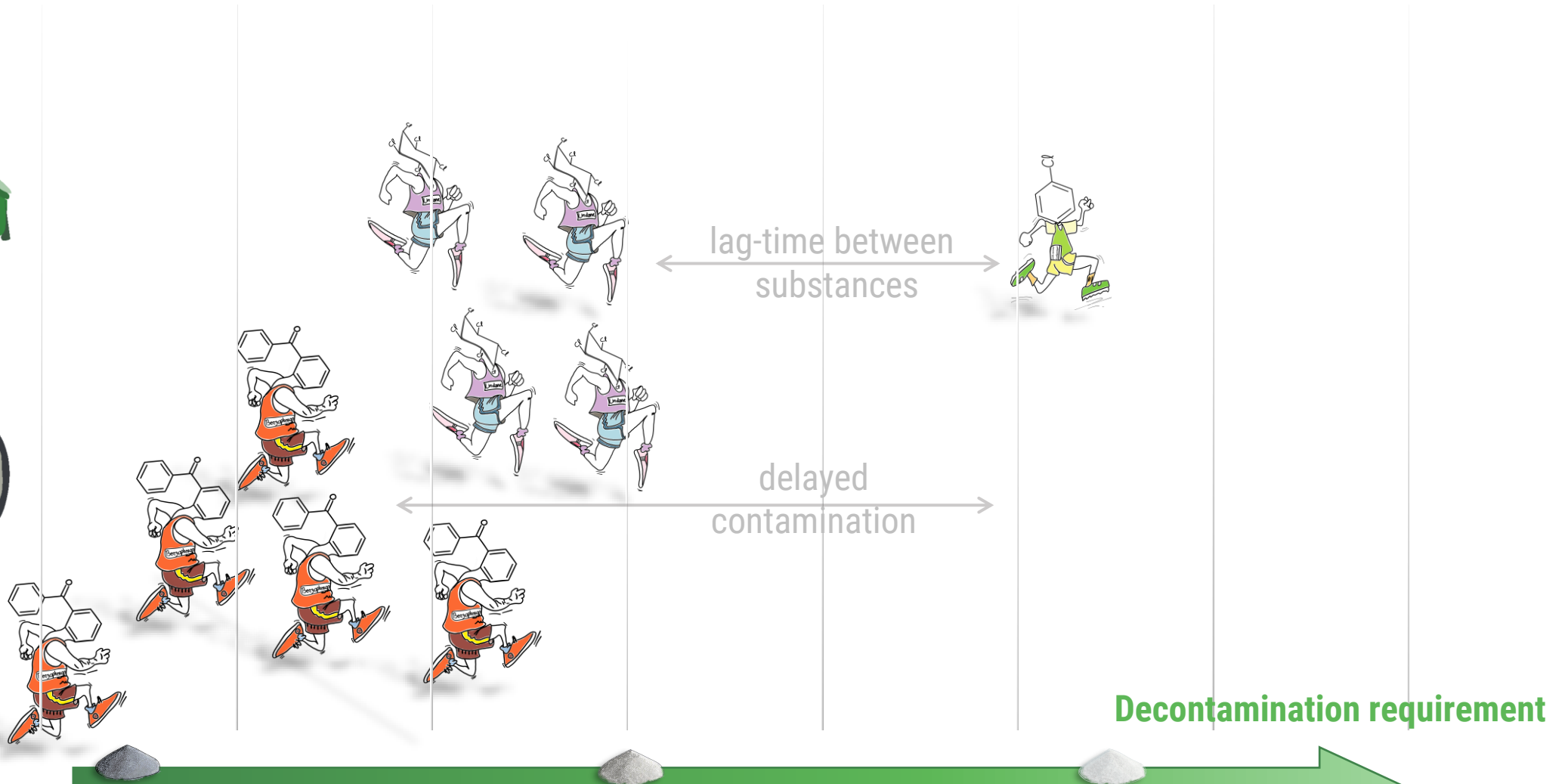
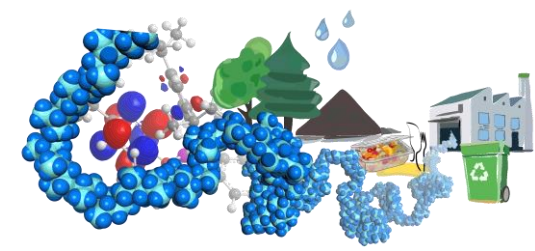


	0% 	90%	99%	99.9% 	 decontaminated +++ FB-
 0% 	>1000 days (1000)	>1000 days (371)	>1000 days (73)	>1000 days (29)	  
 90%	>1000 days (1000)	>1000 days (1000)	>1000 days (371)	>1000 days (73)	
 99%	>1000 days (1000)	>1000 days (1000)	>1000 days (1000)	>1000 days (371)	
 99.9%	>1000 days (1000)	>1000 days (1000)	>1000 days (1000)	>1000 days (1000)	



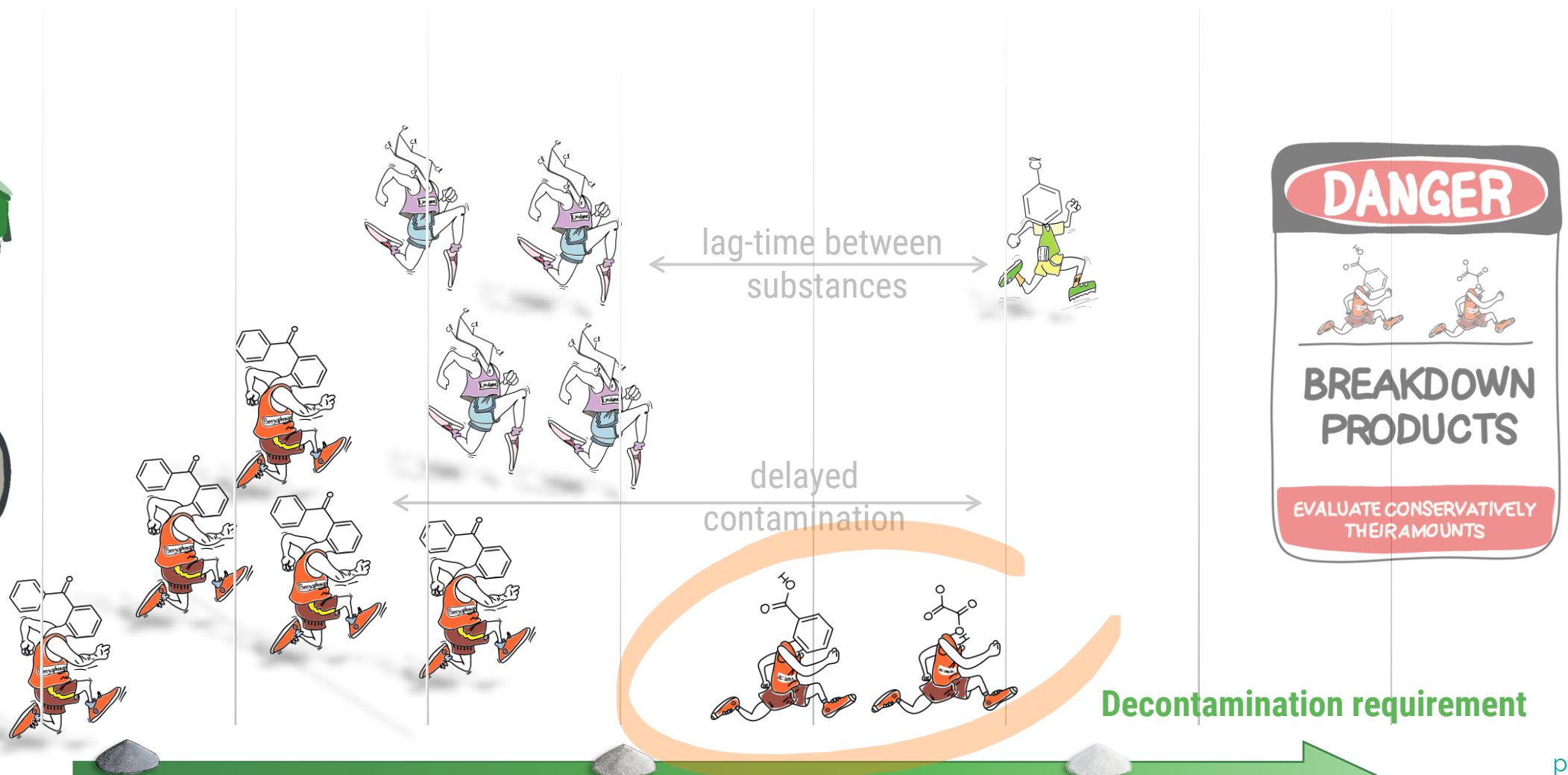
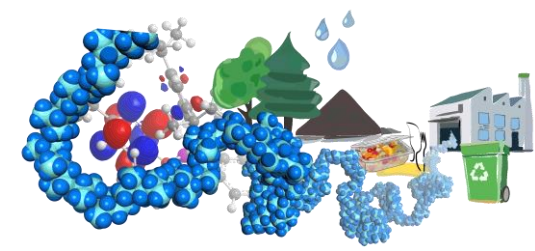
➤ TOWARDS A NEW CONCEPT OF FUNCTIONAL BARRIERS

FB are relative barriers, not absolute

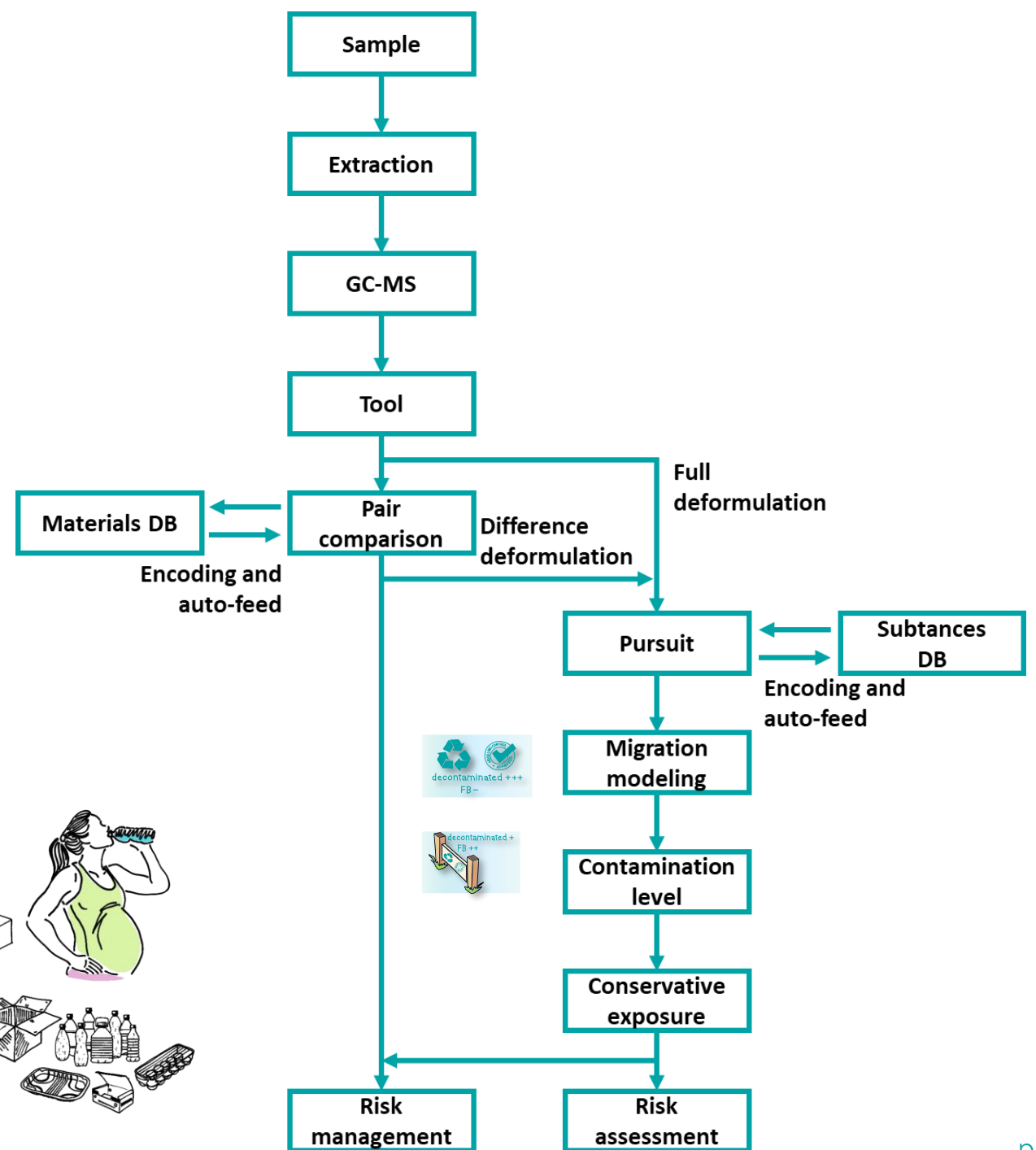
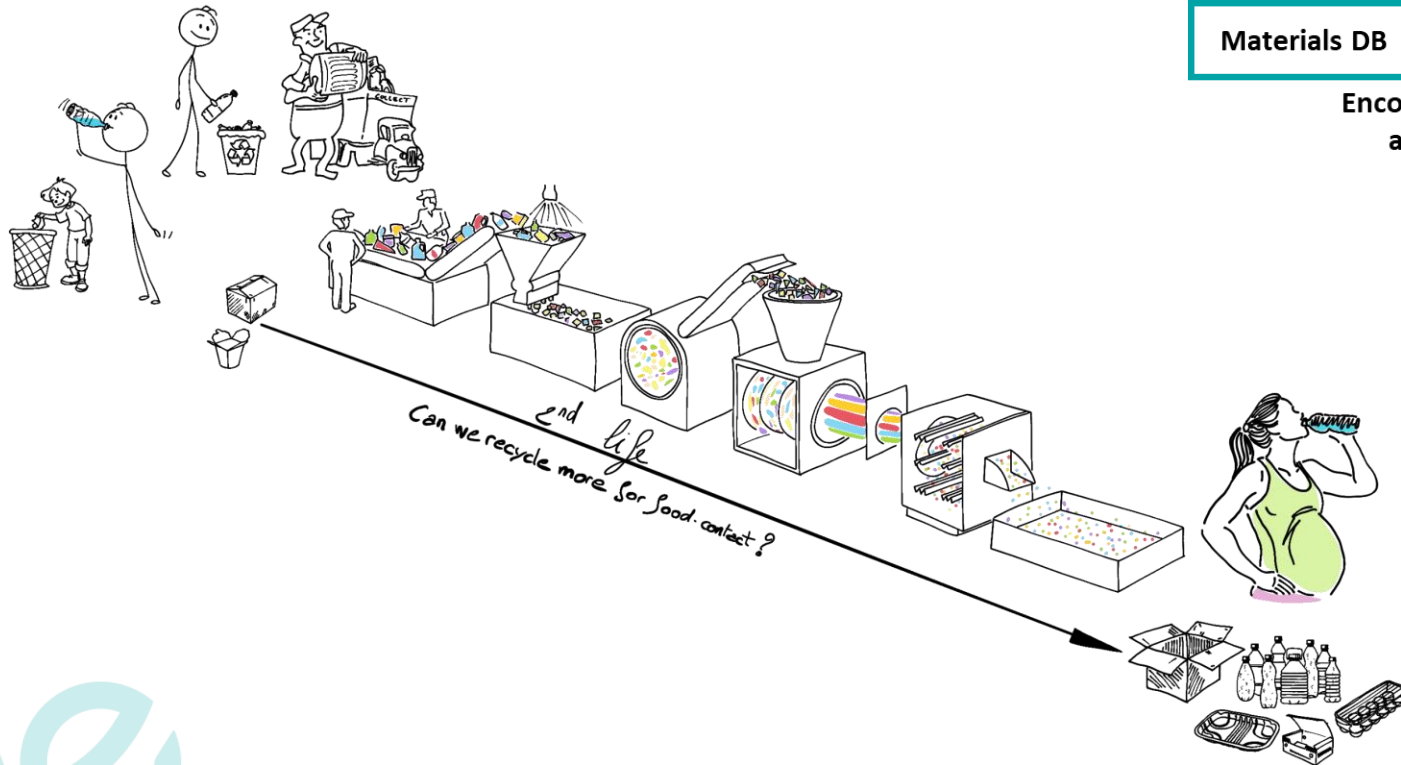


➤ TOWARDS A NEW CONCEPT OF FUNCTIONAL BARRIERS

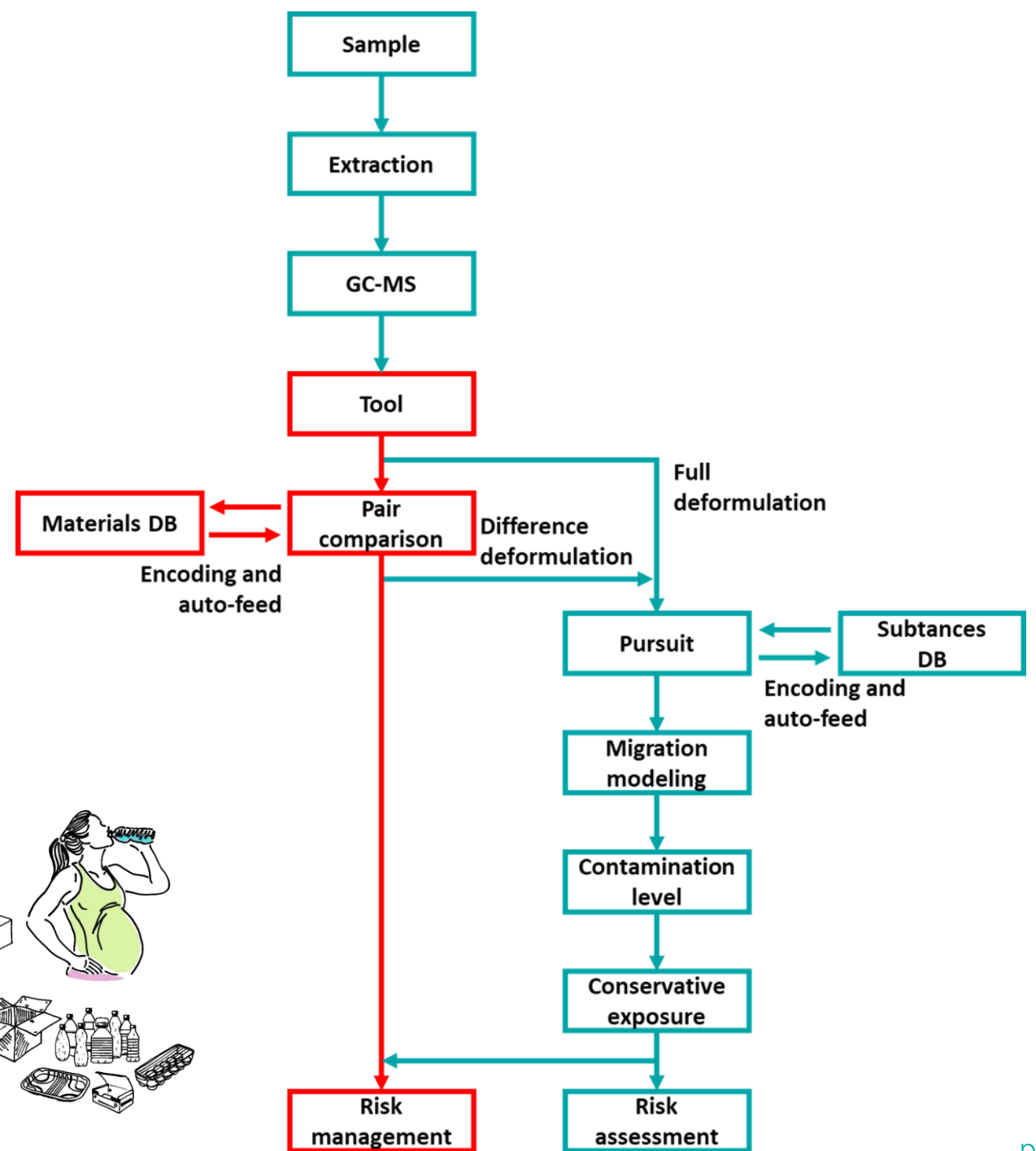
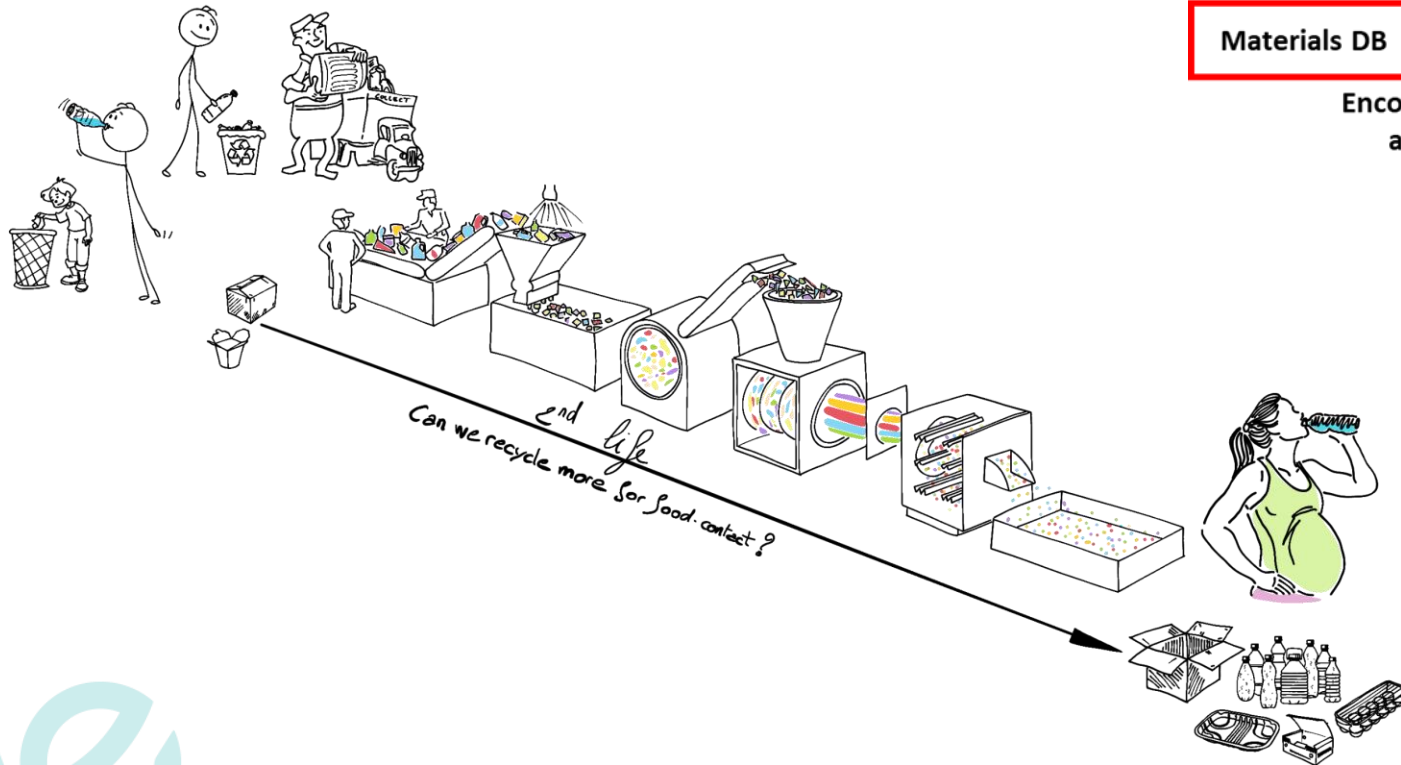
FB are relative barriers, not absolute



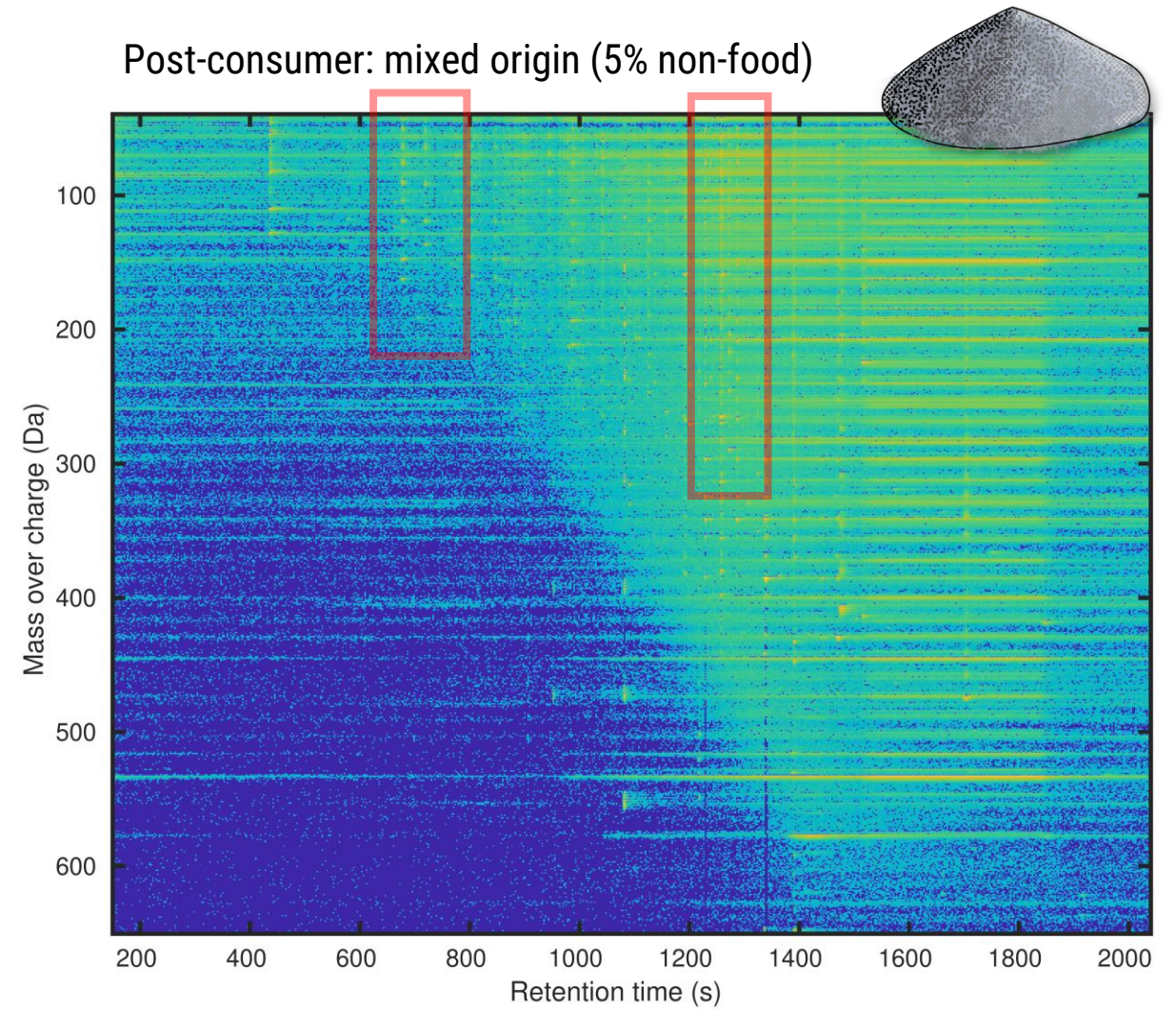
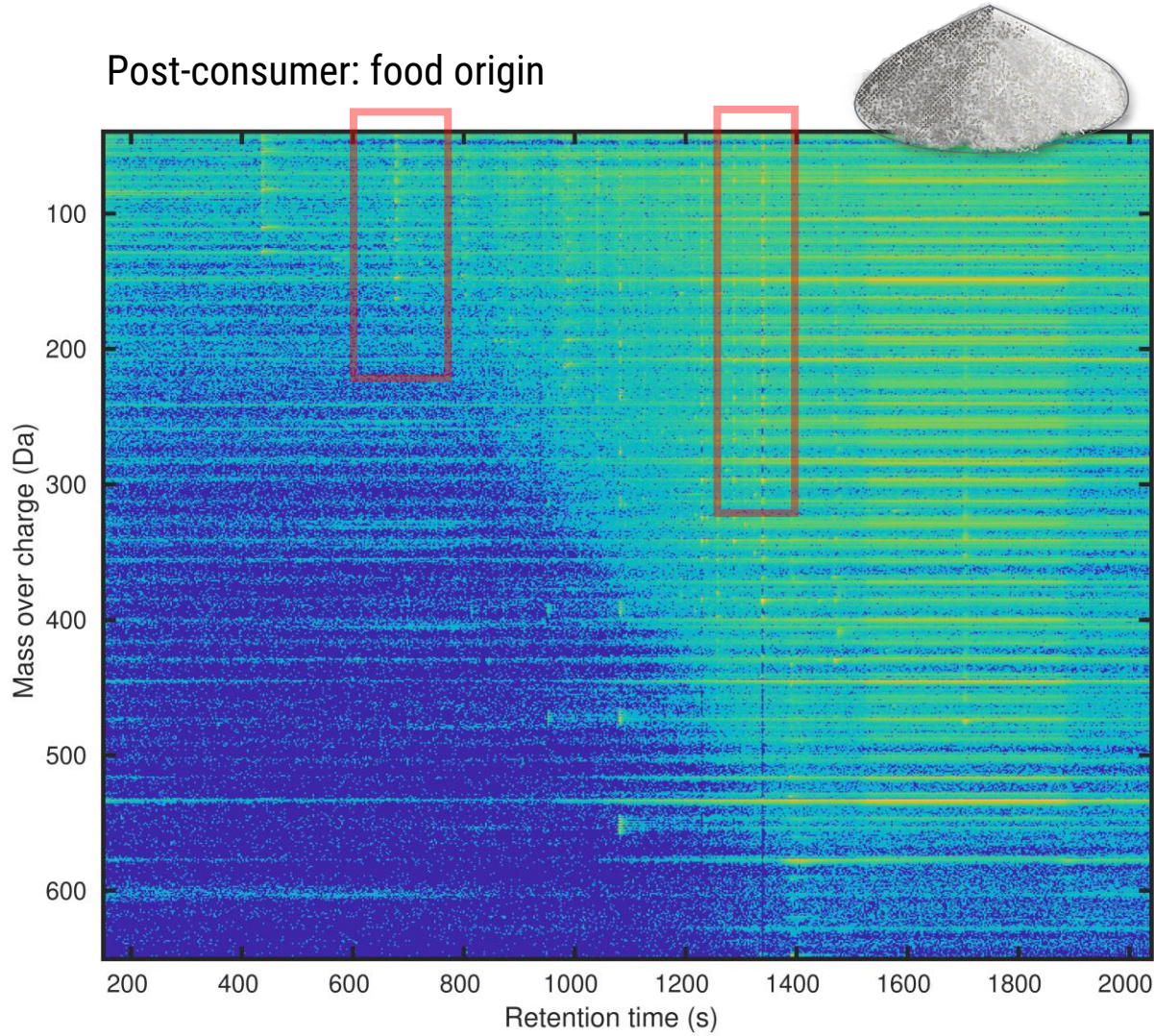
➤ STRATEGY FOR ROUTINE CONTROL OF RECYCLED STREAMS



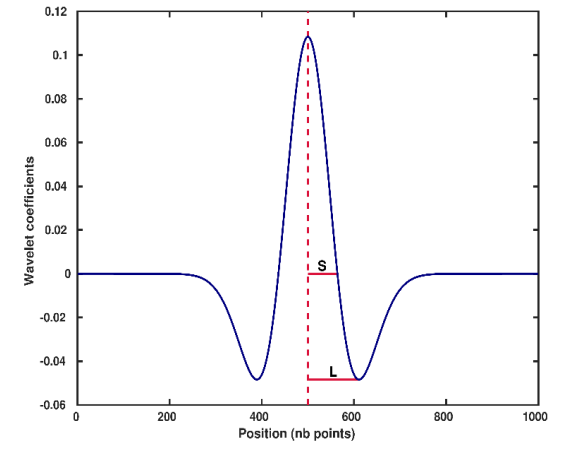
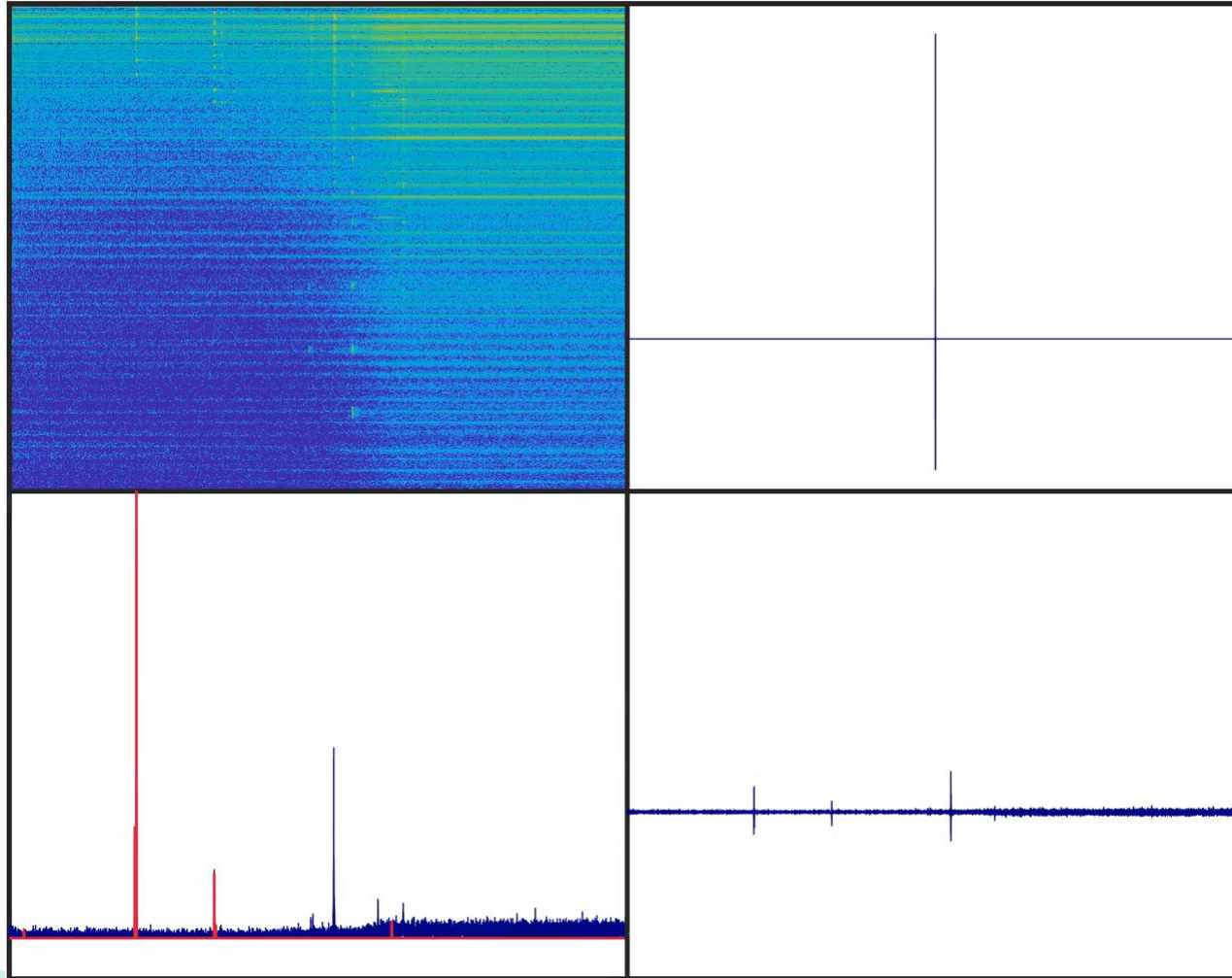
➤ STRATEGY FOR ROUTINE CONTROL OF RECYCLED STREAMS



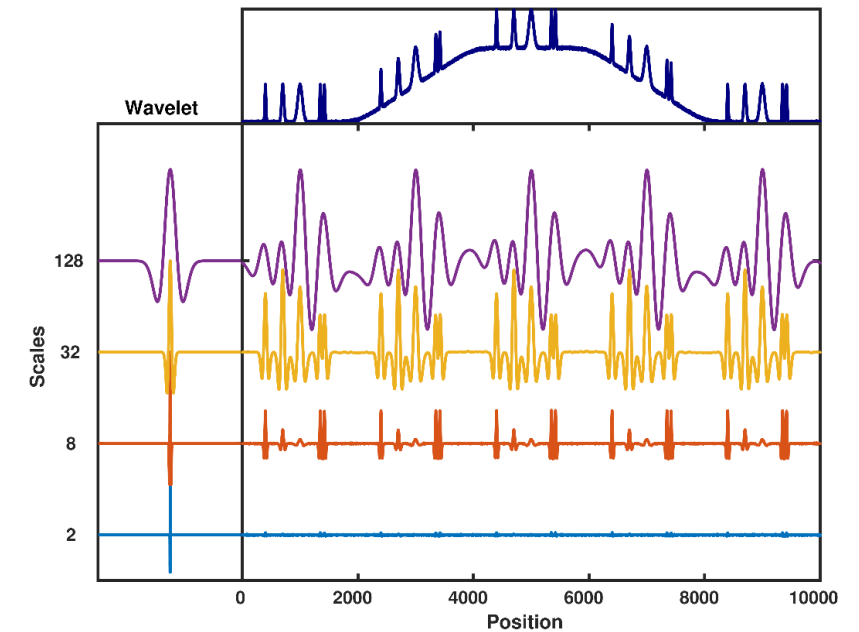
➤ TYPICAL EXAMPLE: post-consumer PET (not decontaminated)



➤ SIGNAL FILTERING, ENCODING AND RECONSTRUCTION

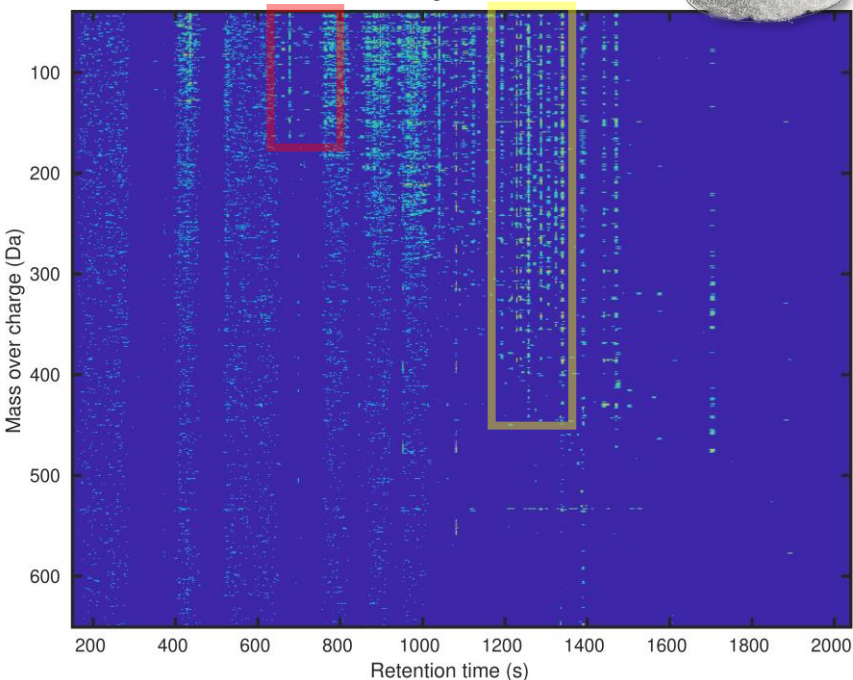


Symmetric wavelet transform
remove steady signal

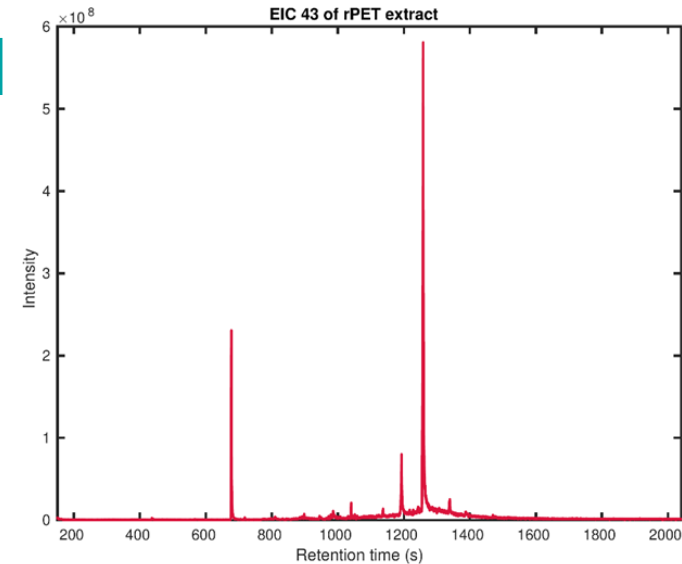
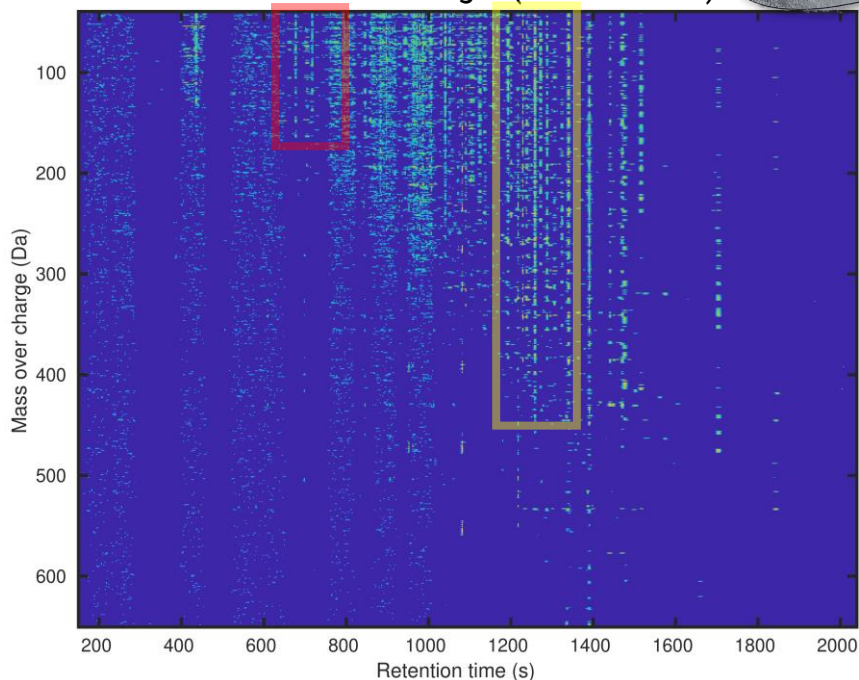


➤ SIGNAL TAGGING, COMPRESSION AND COMPARISON

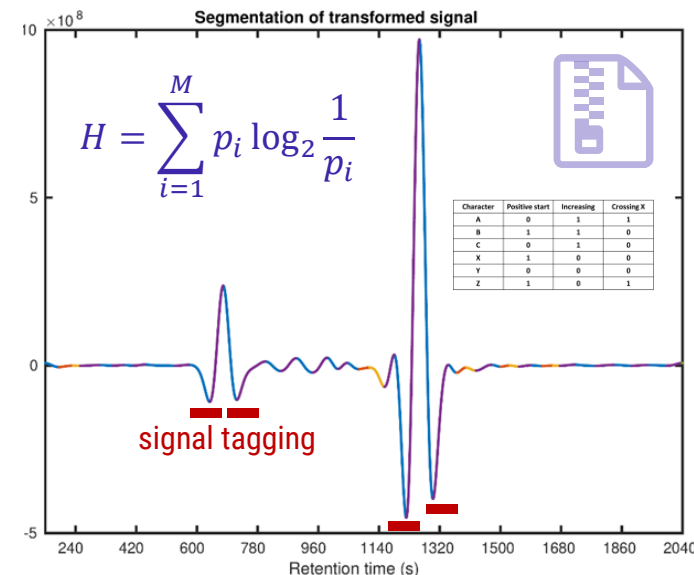
Post-consumer: food origin



Post-consumer: mixed origin (5% non-food)



One-to-one coding of monotonic segments



B Z C Y A Z A Z C Y A Z A Z A Z C Y A Z A Z A Z A Z A Z A Z C
Z C Y A Z A Z A Z A Z A Z A Z A Z A Z C Y A Z A Z A Z A Z A Z

Alignment

	A	B	C	Z	Y	X
A	1	0	0	0	0	0
B	0	1	0	0	0	0
C	0	0	1	0	0	0
Z	0	0	0	1	0	0
Y	0	0	0	0	1	0
X	0	0	0	0	0	1

Gap_{opening} = 0
Gap_{size} = 0

B Z C Y A Z A Z C Y A Z A Z A Z C Y A Z A Z A Z A Z A Z A Z C
Z C Y A Z A Z A Z A Z A Z A Z A Z A Z C Y A Z A Z A Z A Z A Z

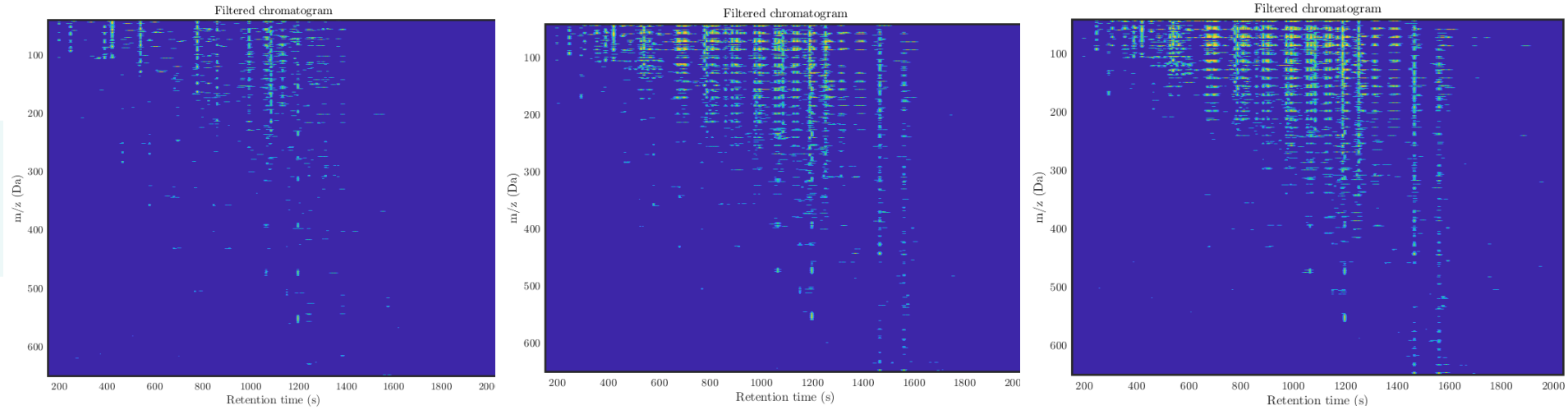
Mismatch Gap Match

$$Distance = \frac{Gap + Mismatch}{Match + Gap + Mismatch}$$

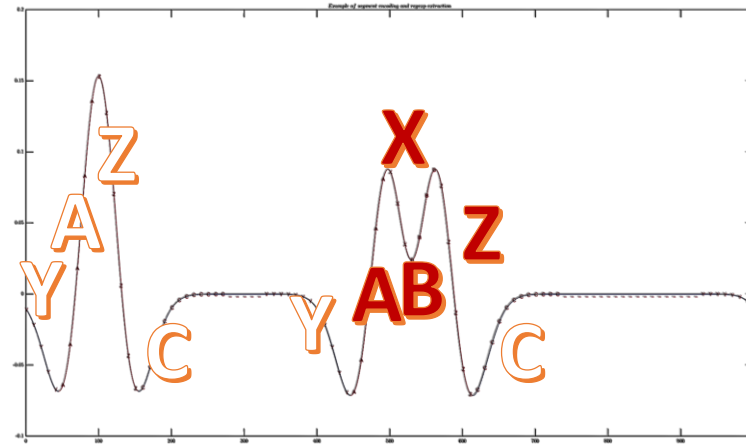
Levenshtein distance

Letter coding ZCYAZAZAZAZAZAZAZAZCYAZAZAZCYAZCYAZAZAZAX
(90 to 96% compression)


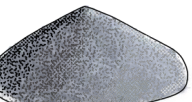


➤ INVARIANCE WITH CONCENTRATION (e.g. oligomers)

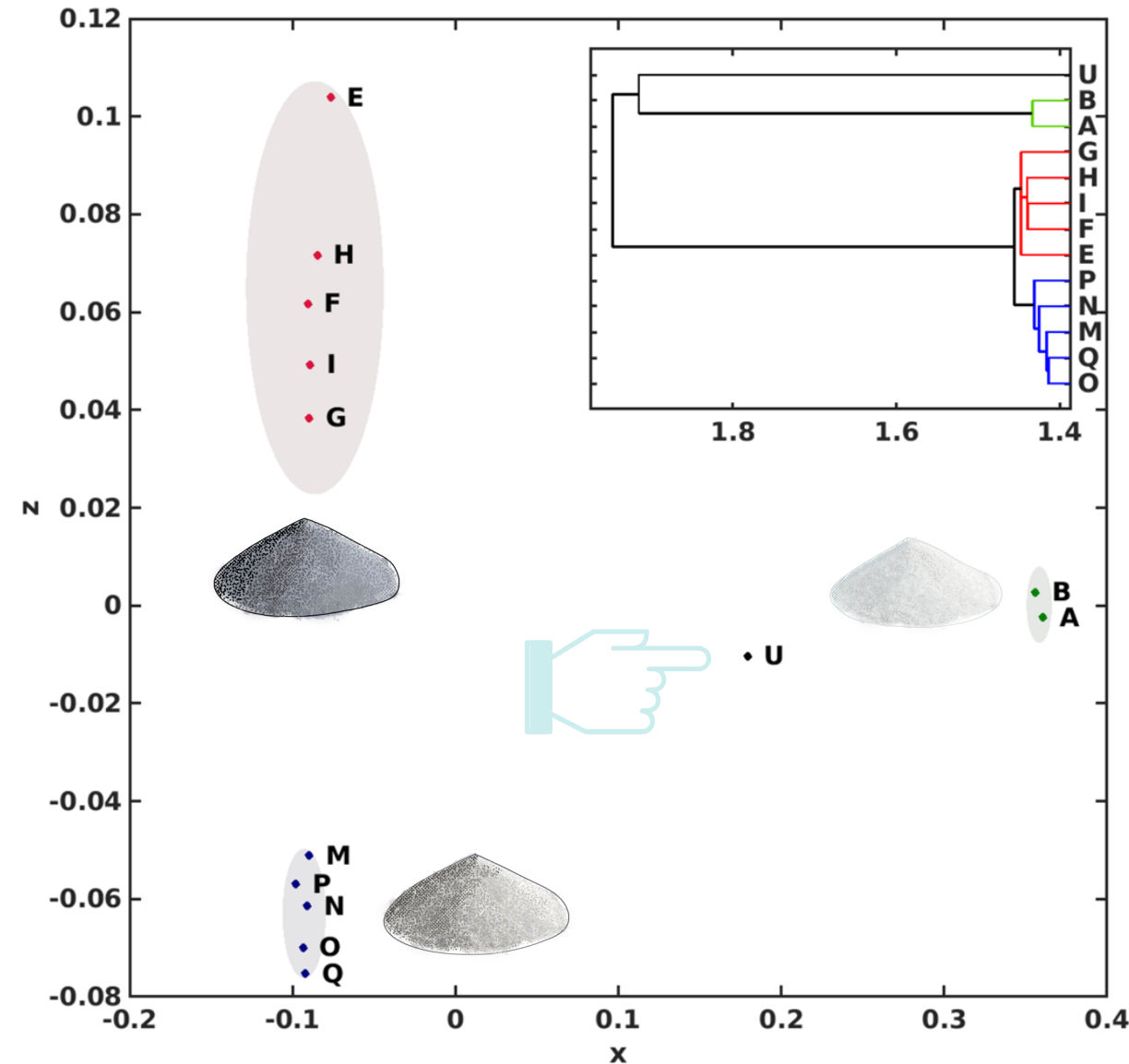


IDENTIFICATION OF A SIGNAL WITH REGULAR EXPRESSIONS: $[AX]+[BZ]+$



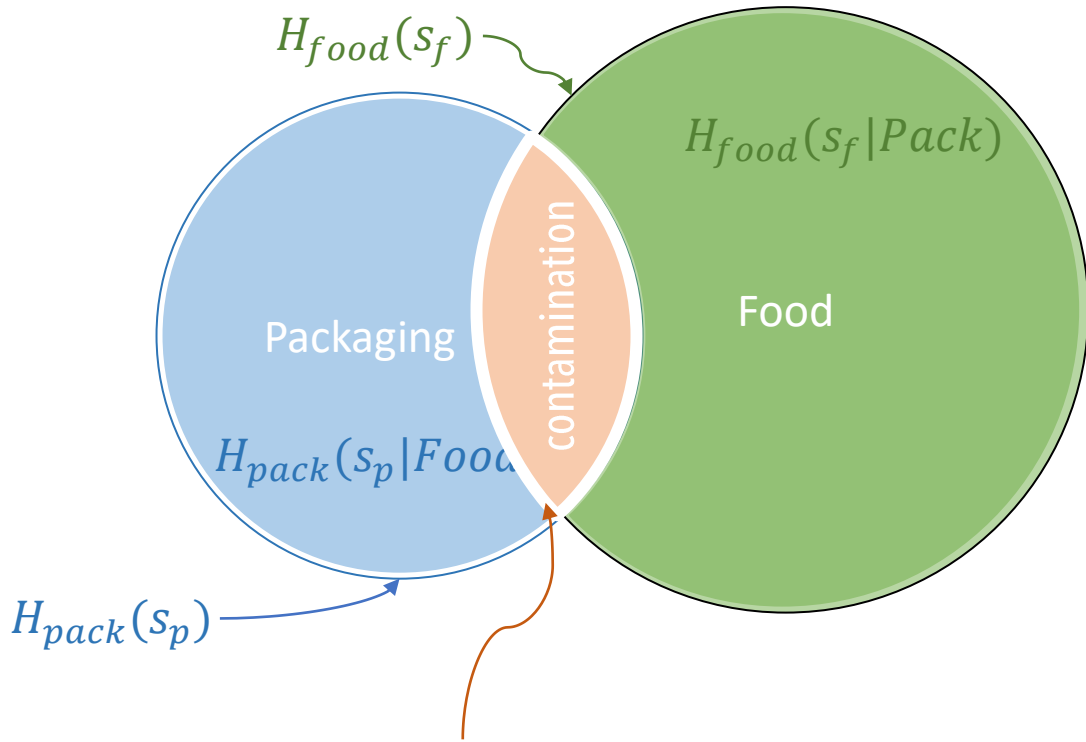
➤ RANKING AN UNKNOWN SAMPLE AMONG 12

-  Food grade and commercially available PET (A & B)
-  Post consumer mixed origin PET flakes (E, F, G, H & I)
-  Post consumer food origin PET flakes (M, N, O, P & Q)
-  Unknown PET sample (U)



IDENTIFICATION OF CONTAMINATION PATHWAYS

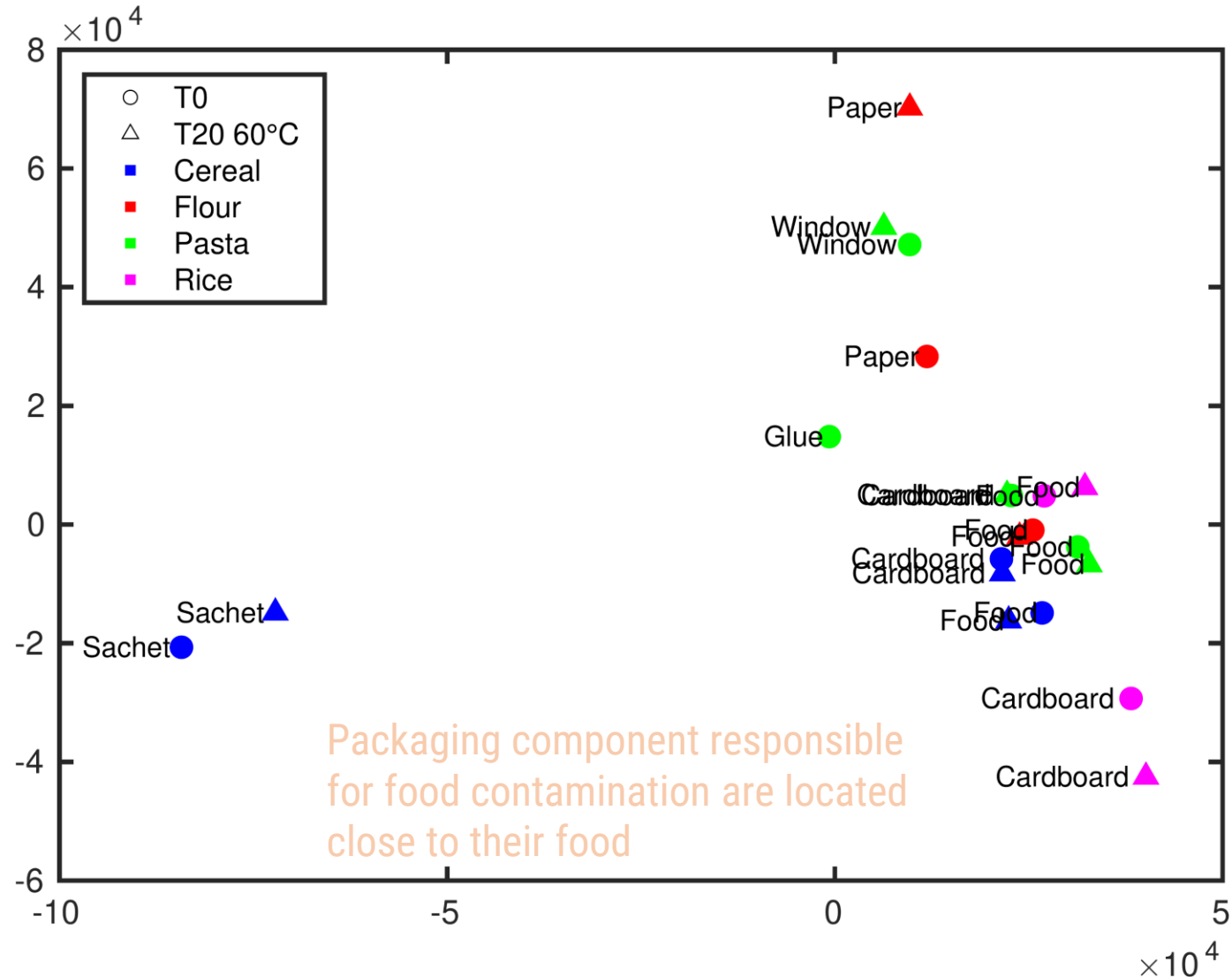
Distance built from the mutual information theorem and the full space of chemicals: $H(s_p, s_f)$



Mutual chemicals **may include** contaminants

$$H(s_p, s_f) = \sum_{s_p, s_f} pr(s_p, s_f) \log_2 \frac{pr(s_p, s_f)}{pr(s_p)pr(s_f)}$$

$$= H_{food}(s_f) + H_{pack}(s_p) - H(s_p, s_f)$$

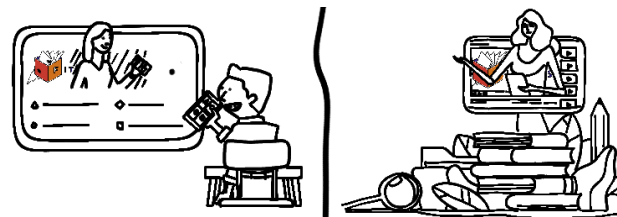




> SOME TAKEAWAYS

Why the computers are becoming essential to the circular economy

- The flow of materials and streams must be followed by a flow of compliance information
- The complexity is too high to be managed routinely (large variability)
- Lack of focus on the final article and food application
- Interactions with competing use of recycled plastics
- Providing incentives to develop safer and more sustainable solutions (free software)
- Starts with education



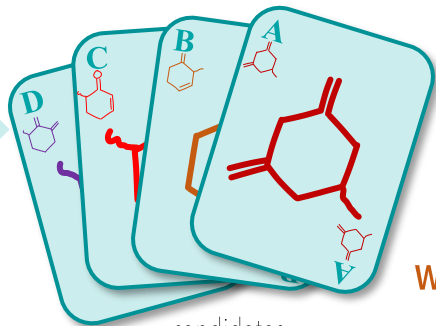


INTEGRATED SOFTWARE UNDER DEVELOPMENT

As part of the collaborative project PackSafe (ANR) - <https://anr.fr/Projet-ANR-21-CE21-0004>

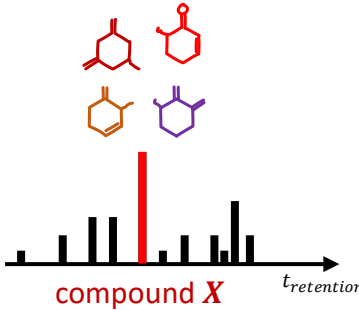


exposure assessment

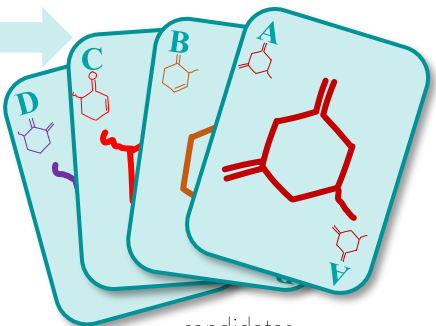


candidates

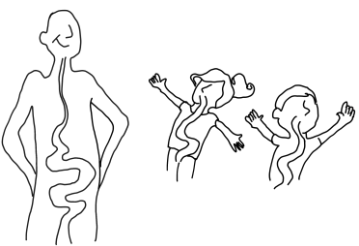
worst-case migration



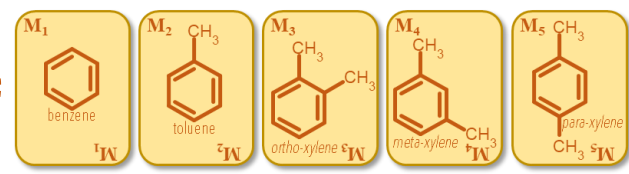
hazard analysis



candidates



acceptable threshold



C-hat_F

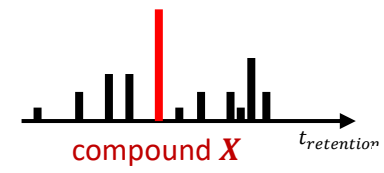


T ₁	T ₂	T ₃	T ₄	T ₅	T ₆	T ₆	T ₇
genotox 0.15 ppb	TOR 1 ppb	detection limit 10 ppb	organo- phosphate 18 ppb	Cramer III 90 ppb	Cramer II 540 ppb	Cramer I 1800 ppb	positive list SML
t _I	z _I	ε _I	t _I	s _I	° _I	° _I	t _I

T-hat

$$Severity(X) = 100 \times$$

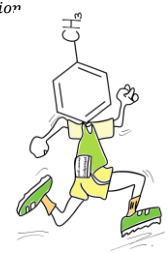
$$\max \left(\frac{\widehat{C}_F^A}{\widehat{T}_A}, \frac{\widehat{C}_F^B}{\widehat{T}_B}, \frac{\widehat{C}_F^C}{\widehat{T}_C}, \frac{\widehat{C}_F^D}{\widehat{T}_D} \right)$$



compound X

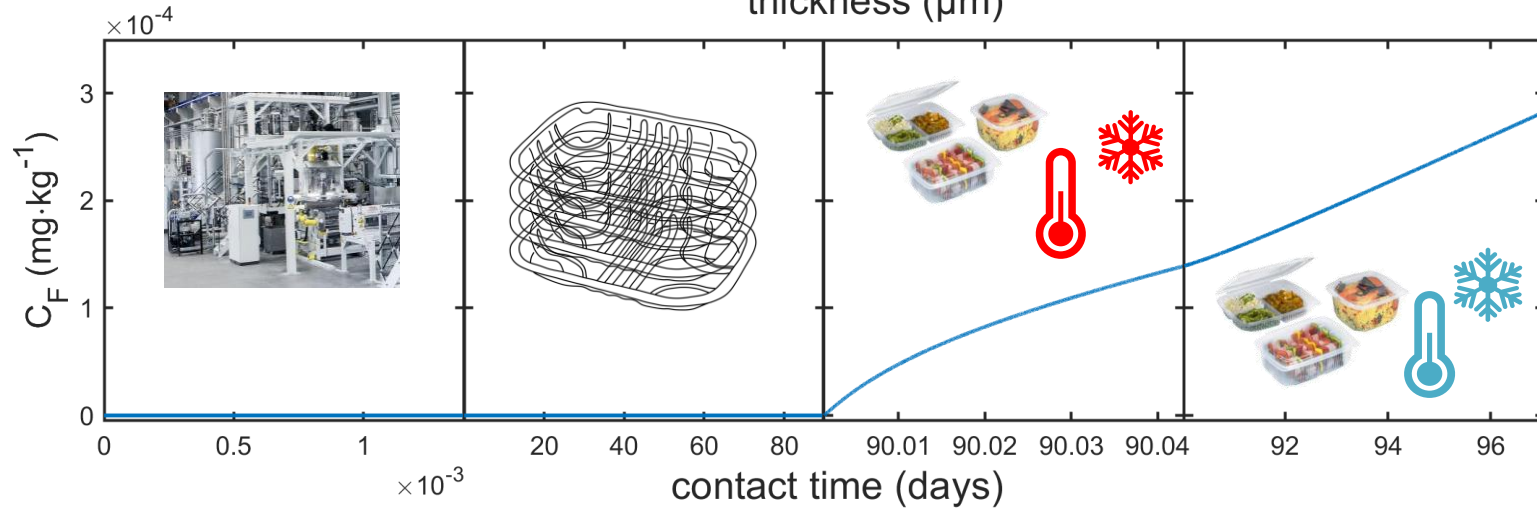
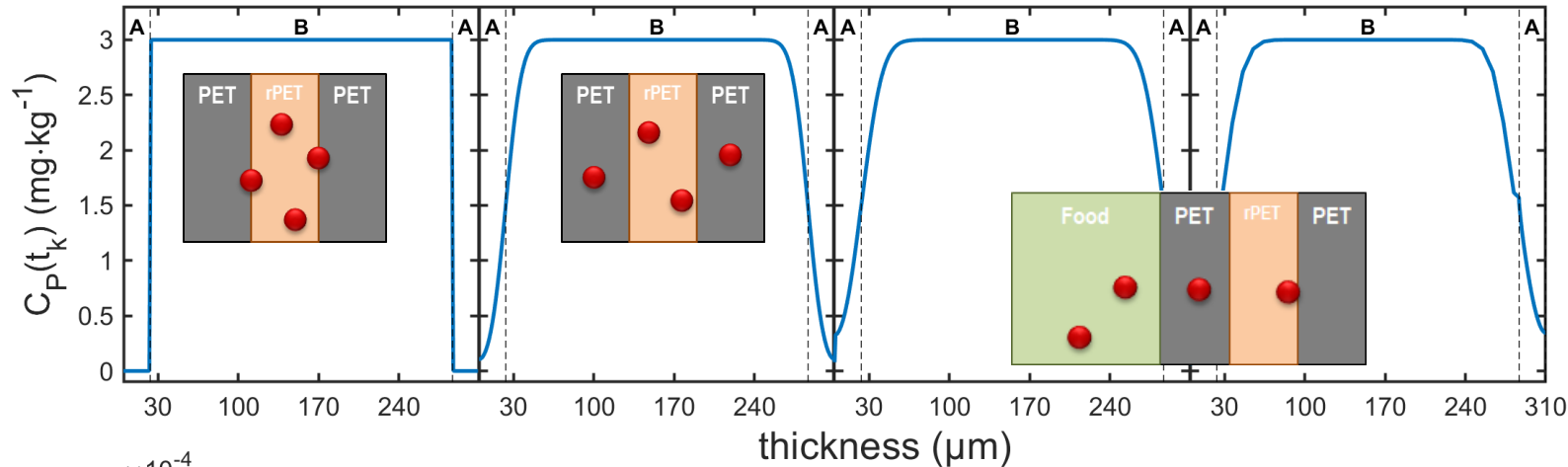
t-retention

all compounds

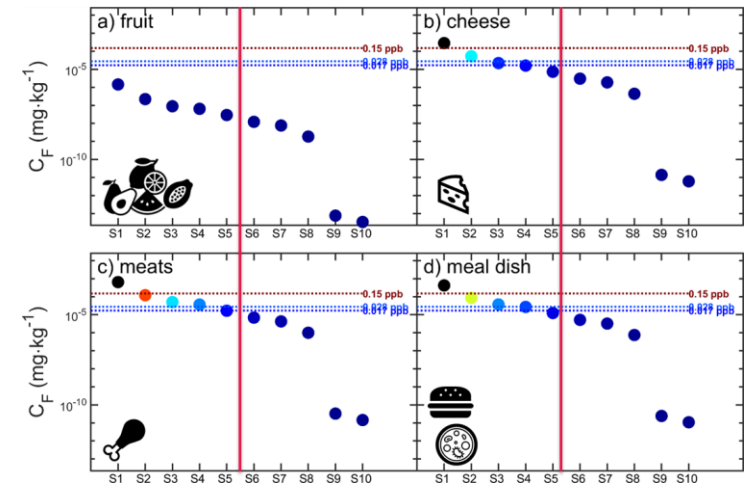


➤ Example of application for PET trays

Case of toluene



catastrophic
critical
moderate
minor
negligible



thermoforming

Hot filling

Storage (stacks)

Storage



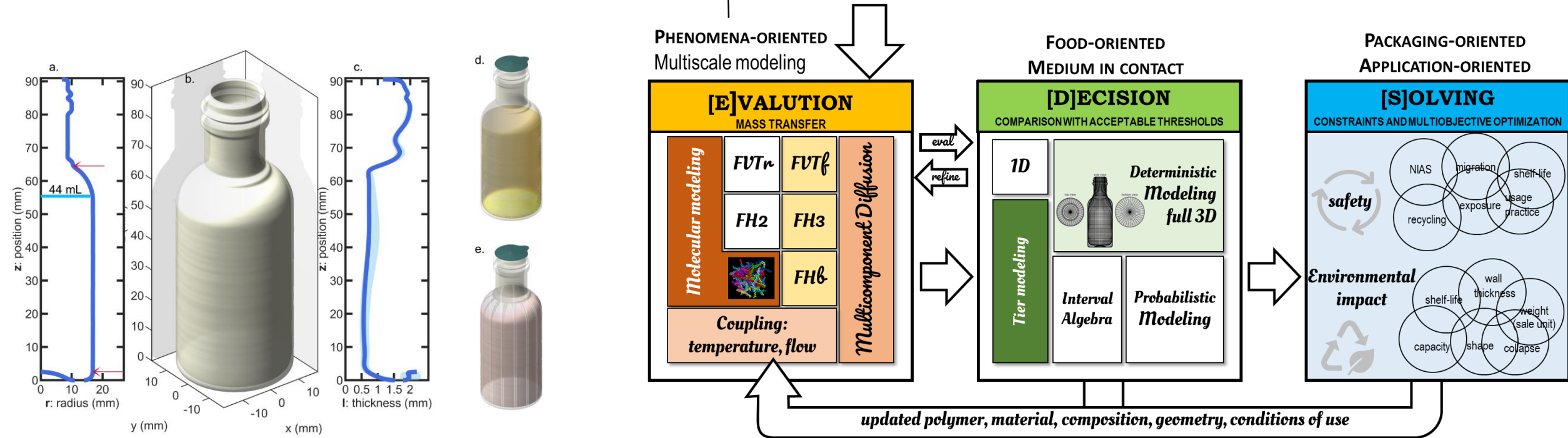
UPGRADED FMECAengine

for the optimization of shapes and functional barrier thicknesses

Ongoing SafeFoodPackaging Portal (pure Python): <https://github.com/ovitrac/SFPPy>



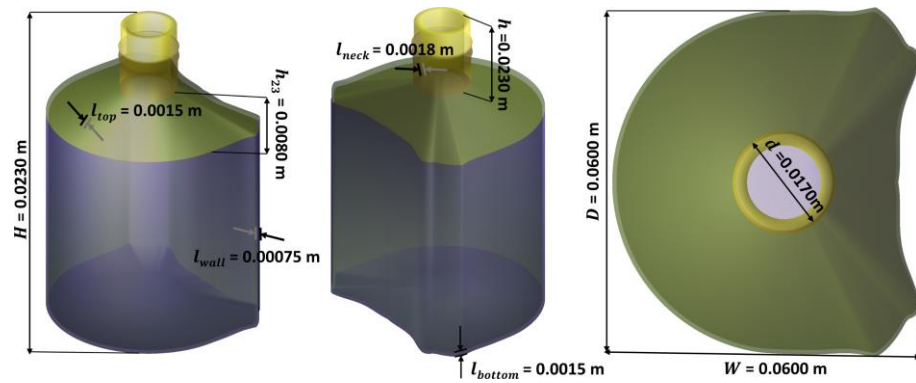
Computer-aided drafting



Feasible solutions
Optimal or Pareto-optimal

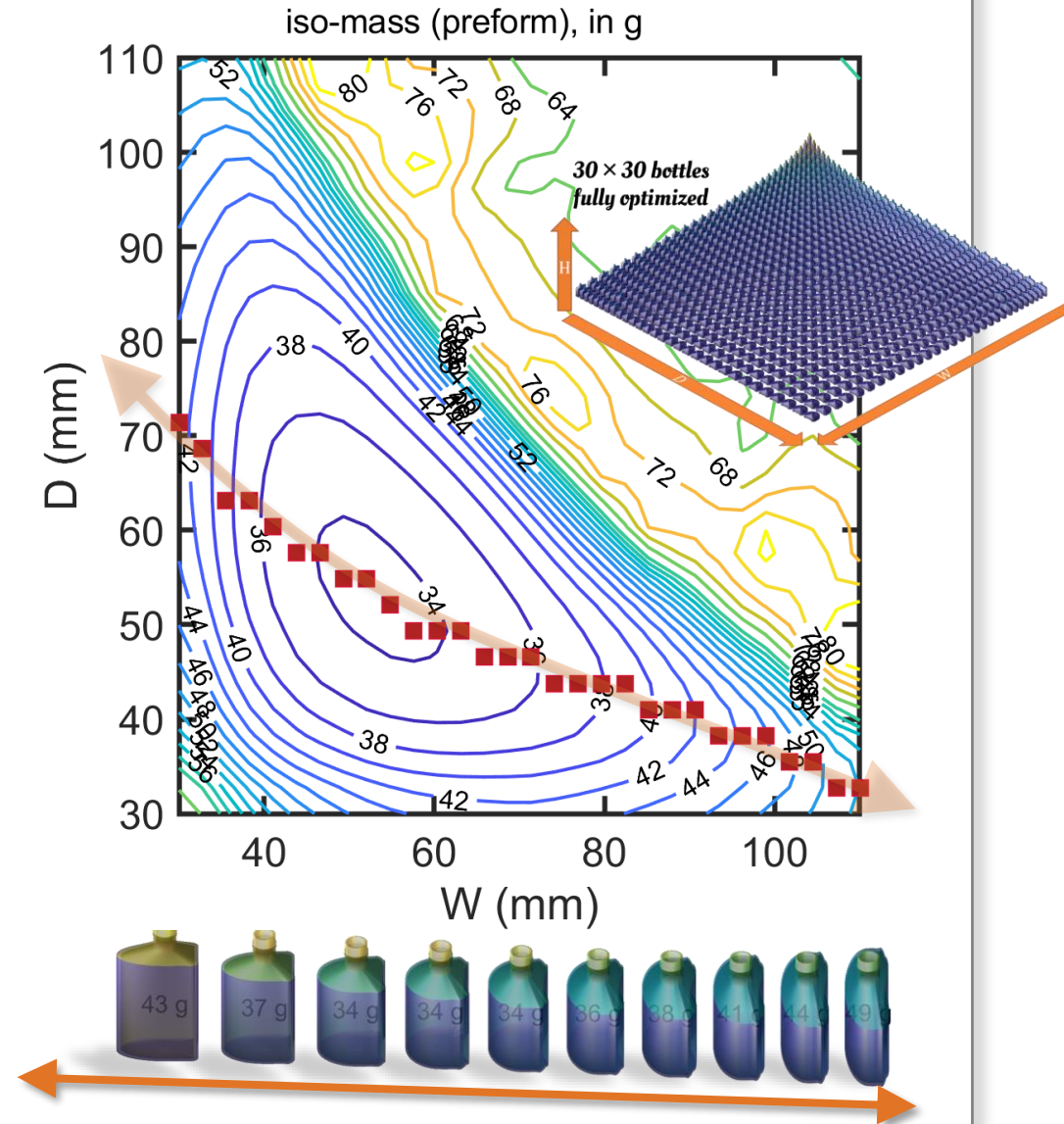
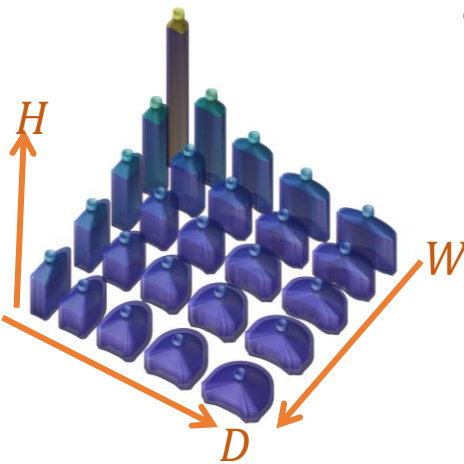
- AIChE Journal. 2013;59:1183-212 10.1002/aic.14056.
- Frontiers in Chemistry. 2019;7 10.3389/fchem.2019.00349.
- Risk assessment of migration from packaging materials into food. Elsevier Food Science Reference Module. Amsterdam, NL: Elsevier; 2019.

➤ VIRTUAL OPTIMIZATION of miniature PET bottles for alcoholic beverages served in planes



For each design (300 × 300), the detailed 3D geometry is optimized to match

- The overall shape
- The prescribed capacity
- A **weight loss** lower than 1% after one year
- A variation of **alcoholic strength** lower than 0.3% after one year
- The amount of **recycled PET**
- **Mechanical resistance**
- Risk of fire



➤ Train yourself to become green

Three months online curriculum on packaging design

<https://fitness.agroparistech.fr/>



roatia, France, Germany, Portugal, Spain

Main menu About Us job offers

Welcome to FITNESS

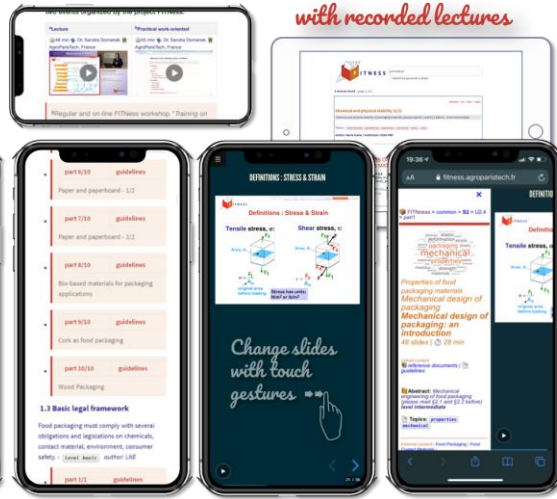
Fitness stands for **Food packaging open courseware for higher education and staff of companies**

All lectures, interactive contents and Quiz are provided "AS IS". The content (85 lectures from Common to Specialized Modules) is under development and may contain inconsistencies and inaccuracies. It will be updated regularly.

trainee/ student view



with recorded lectures



ecodesign

Search by keywords in slides

7 lectures found | page 1 of 1

# num. lectures	book	recorded	guidelines	extra	case-studies	how-to	solution
5	0	0	0	0	0	0	0

specialized > S5 > U5.3 > part1

Computer-aided FMECA applied to mass transfer

Computer-aided approaches facilitate the deployment of FMECA approaches. The lecture illustrates various situations calculated with the open-source software FMECAEngine identification of critical steps, components, substances - level advanced

Topics: design prevention safe-by-design migration risk safety modeling

Author: Olivier Vitrac | Institution: INRAE

Read Lecture

2 slides found

THIS PROJECT HAS RECEIVED FUNDING FROM THE EUROPEAN UNION'S ERASMUS PROGRAMME UNDER CONTRACT N° 2017-1-FR01-KA202-037441

COORDINATOR ACTIA-LNE

COMPUTER-EVOLUTIONARY ECO-DESIGN & SAFE-BY-DESIGN

Case of plastic bottles for alcoholic beverages

Beverage Consumption rate Storage Supply chain

Life cycle

ACCELERATING THE INNOVATION PROCESS FULL DIGITAL PROTOTYPING

max min min

➤ THINK HARD ABOUT TOLERANCES AND LINKED DECISIONS

CIRCULAR ECONOMY MAY INTRODUCE SYSTEMIC RISKS

