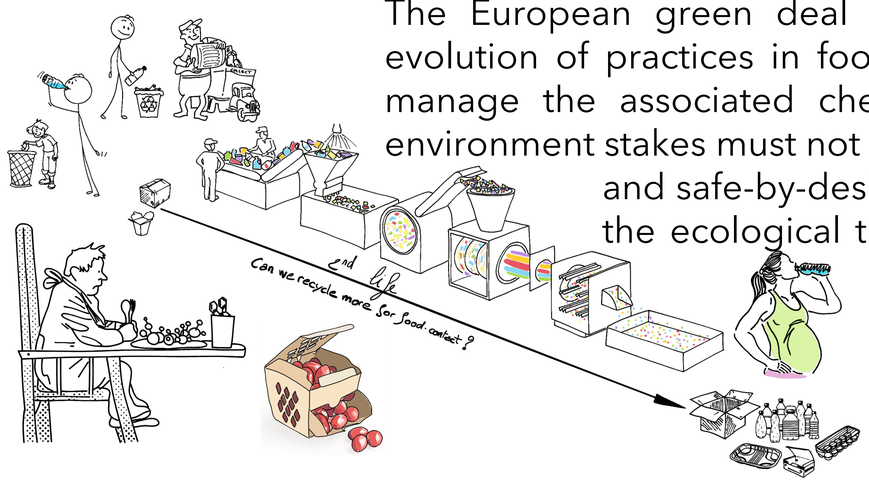
New strategies to evaluate and manage recycled materials for food contact

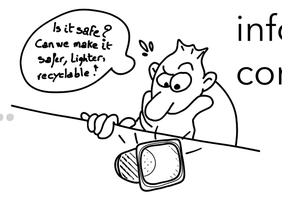
Summary

The European green deal is at the origin of the rapid evolution of practices in food packaging and the need to manage the associated chemical risks. Food safety and environment stakes must not be opposed. Rapid assessment and safe-by-design approaches are essential to the ecological transition: food-grade recycling loops, reusable food packaging.

The recent research works within UMT ACTIA 22.07 "***SafeMat***" aim at developing the engineering science to support safe and eco packaging design: analytical methods combined with numerical procedures, direct imaging of chemical contaminants in materials, assessment of functional barrier performance, etc. The principle of a public repository of the chemical information and observatory of recycled materials is considered.



recycle, reduce, reuse... in a safe way



General goal: developing the engineering science behind responsible packaging design

UNKNOWN STREAMS

Recycled- OR Recycled+ and decontaminated+++

Recycled+ and decontaminated+

Recycled+ and decontaminated+

ANALYTICAL TECHNIQUES

- **Routine low-resolution GC-MS techniques**
- Coupling with spectro/ imaging techniques (future)

WEB - AI

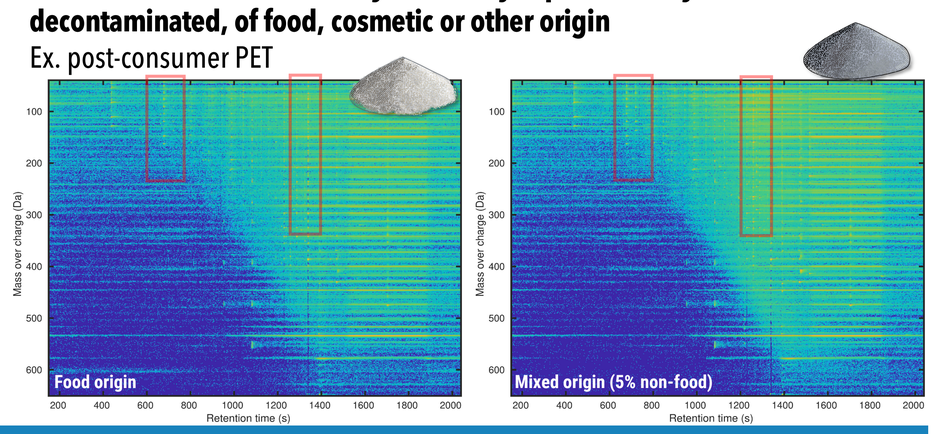
- **New chemometrics techniques based in information theory**
- Sample bank

MIGRATION MODELING

- **Plastics and non-plastics**
- Cross-contamination
- Decontamination process
- **Functional barriers**

TYPICAL CHALLENGE: difficulty to identify experimentally if a material is decontaminated, of food, cosmetic or other origin

Ex. post-consumer PET



Results (1/2): cross mass transfer beyond plastics - contamination of commercial foods by many substances from paper and boards (survey 2022, French market)

Searched and found substances in commercial food packaging

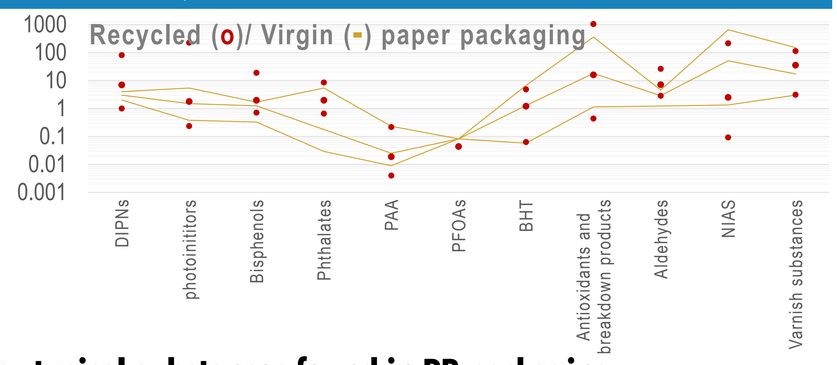
Mineral oil	Phthalates	PAH	PAA	Antioxidants and breakdown products	NIAS and others
MOSH	Diisobutyl phthalate	Naphtalene	aniline	Butylated Hydroxytoluene	Benzophenone
MOAH	Dipropyl phthalate	2-Methyl-naphthalene	o-toluidine	Irganox 1076	4-methyl benzophenone
DIPNs	Diisobutyl phthalate	1-Methyl-naphthalene	o-anisidine	Irgafos 168	Isopropyl-9H-thioxanthen-9-one (ITX)
	Dibutyl phthalate	Acenaphthylene	4-chloroaniline	Tris-(2,4-di-tert-butylphenyl)phoshate	diethylene glycol dibenzoate
	Benzyl butyl phthalate	Acenaphtene	p-cresidine	4-hydroxybenzophénone	Di(propylene glycol) dibenzoate
	Bis(2-ethylhexyl) phthalate	Fluorene	2,4,5-trimethylaniline	2,4-Di-tert-butylphenol	anthraquinone
	Di-n-octyl phthalate	Phenanthrene	4-chloro-2-methylaniline		2-ethyl-anthraquinone
	Dinonyl phthalate	Anthracene	2,4-diaminotoluene		Bisphenol A
	Dimethyl phthalate	Fluoranthene	2,4-diaminoanisole		Bisphenol F
	Diethyl phthalate	Pyrene	2-naphthylamine		Bisphenol S
	Diallyl phthalate	Benz(a) anthracene	5-nitro-o-toluidine		PFOA
	Dimethylglycol phthalate	Chrysene	4-aminobiphenyl		PFOS
	Dihexyl phthalate	Benz(b) fluoranthene	4-aminoazo-benzene		DEAB
	Dicyclohexyl phthalate	Benzo(k) fluoranthene	4,4'-oxydianiline benzidine		Michler's keton
	Diethylhexyl adipate	Benzo(a)pyrene	4,4'-methylenedianiline		Octanal
	Dibutyl sebacate	Indeno(1,2,3-c,d) pyren	2-aminoazotoluene		Nonanal
	Diisononyl phthalate	Dibenz(a,h) anthracene	4,4'-methylenedi-o-toluidine		Decanal
	Diisodecyl phthalate	Benzo(g,h,i) perylene	3,3'-dimethyl-benzidine		Aldehyde caproique
			4,4'-thiodianiline		Bis(2-ethylhexyl) fumarate
			3,3'-dichlorobenzidine		bis(2-ethylhexyl) maleate
			4,4'-methylene bis[2-chloroaniline]		2-Ethylhexyl acrylate
			3,3'-dimethoxy-benzidine		

FoodSafeBioPack

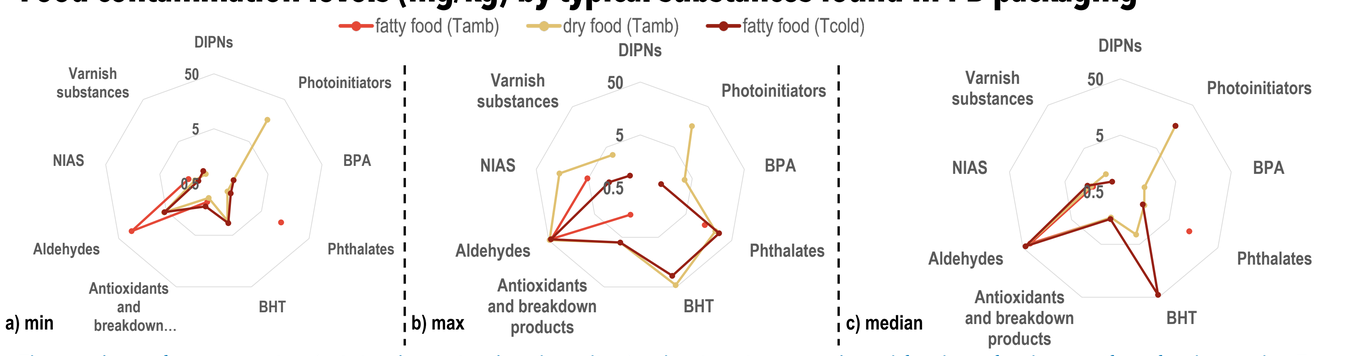
Project ANR-20-CE21-0009

Concentration ranges (mg/kg) of main substance classes in PB packaging

Three values of concentration (maximal, minimal and median) are presented for virgin fibers and recycled PB packaging. It was noticed that recycled PB contain larger amounts of contaminants (*e.g.* DIPNs – tracers of recycled PB, photo-initiators, bisphenols, phthalates).



Food contamination levels (mg/kg) by typical substances found in PB packaging



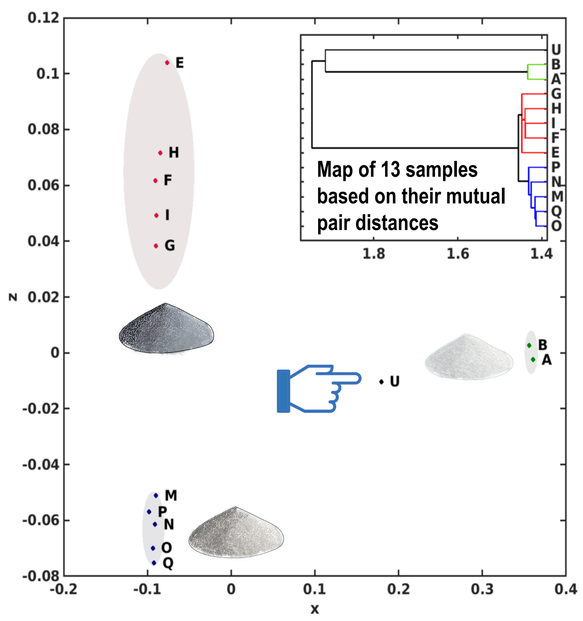
Three values of concentration (minimal, maximal and median) at buying time are plotted for three food types (fatty food stored at T_{amb}, fatty food stored at T_{cold} and dry food stored at T_{amb}). It is worth to notice that food contamination levels are already high, with migration rates $(m_{i,F}/(m_{i,F}+m_{i,P}))$ up to 50% of the total amounts in most cases.

Results (2/2): chemometrics techniques based in information theory

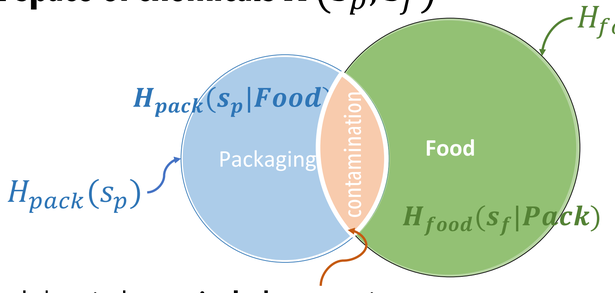
Blind comparison of samples with Principal Coordinate Analysis

- 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)

GC-MS low resolution and numerical procedures to robustly extract the fingerprint of arbitrary contamination patterns → ranking of samples according to their origins → enabling orientation of unknown streams.

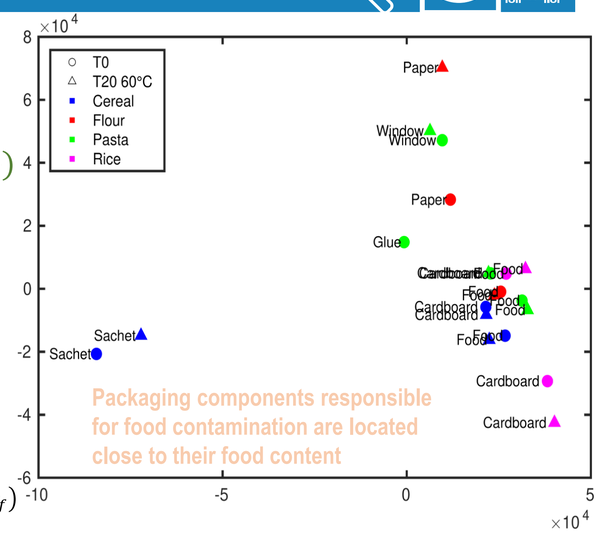


Identification of contamination pathways: Distance built from the mutual information theorem and the full space of chemicals $H(s_p, s_f)$



Mutual chemicals **may include** contaminants

$$H(s_p,s_f)=\sum_{s_p,s_f} pr(s_p,s_f)\log_2\frac{pr(s_p,s_f)}{pr(s_p)pr(s_f)}=H_{food}(s_f)+H_{pack}(s_p)-H(s_p,s_f)$$



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18e congrès de la Société Française de Génie des Procédés
Toulouse 2022

UMT SAFEMAT SAFETY OF PACKAGING

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