Fingerprints from GC-MS data

to manage recycled streams for food contact

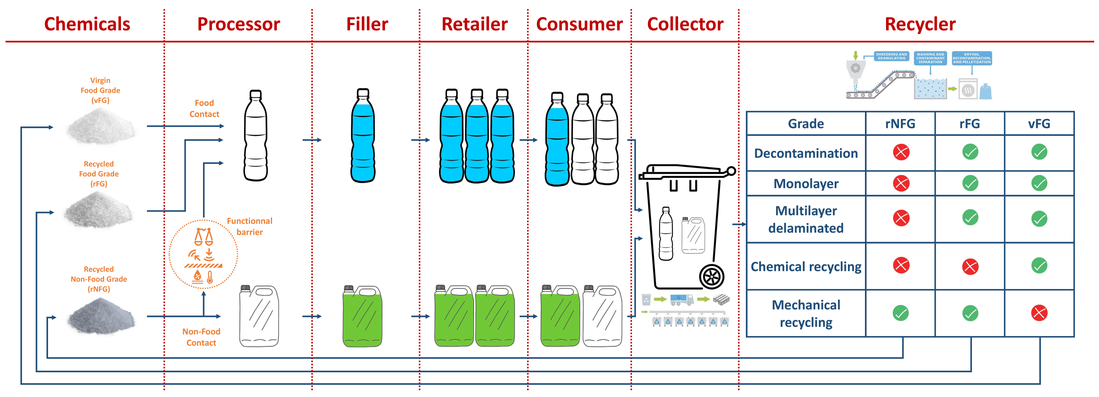
INDUSTRIAL PhD (CIFRE) with LNE

Development of analytical methods for the identification and quantification of non-intentionally added substances in food packaging

Summary

Recycled materials are highly variable (rNFG, rFG, vFG) and not all streams are acceptable for direct food contact or a use behind a functional barrier. The PhD explores the possibility to orient streams according to their fingerprints.

Fingerprints are generated and numerically compressed from a wavelet decomposition of common analytical signals (GC-MS, ^{1}H NMR, FTIR). The approach remains pluggable with existing tools and approaches.

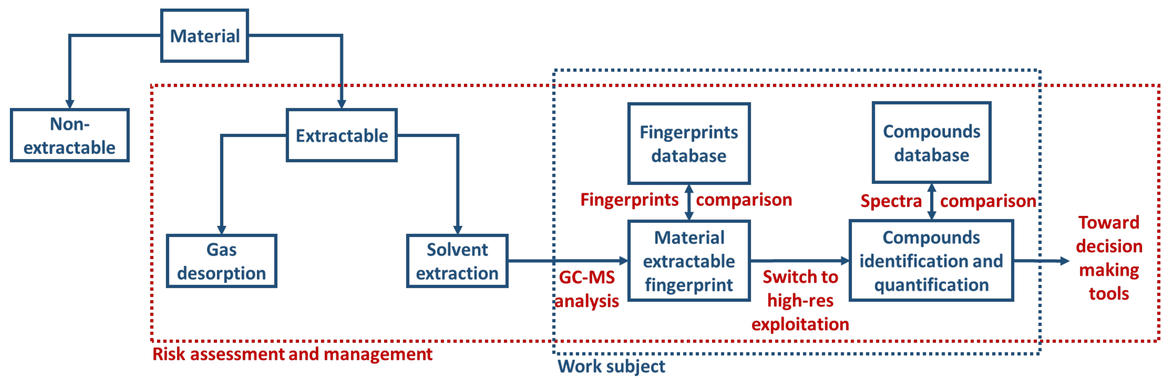


Grade	rNFG	rFG	vFG
Decontamination	✗	✓	✓
Monolayer	✗	✓	✓
Multilayer delaminated	✗	✓	✓
Chemical recycling	✗	✗	✓
Mechanical recycling	✓	✓	✗

Case-study materials

Data is acquired by GC-MS analysis of solvent extracts from either polypropylene food packaging, food grade or mixed grade recycled PET.

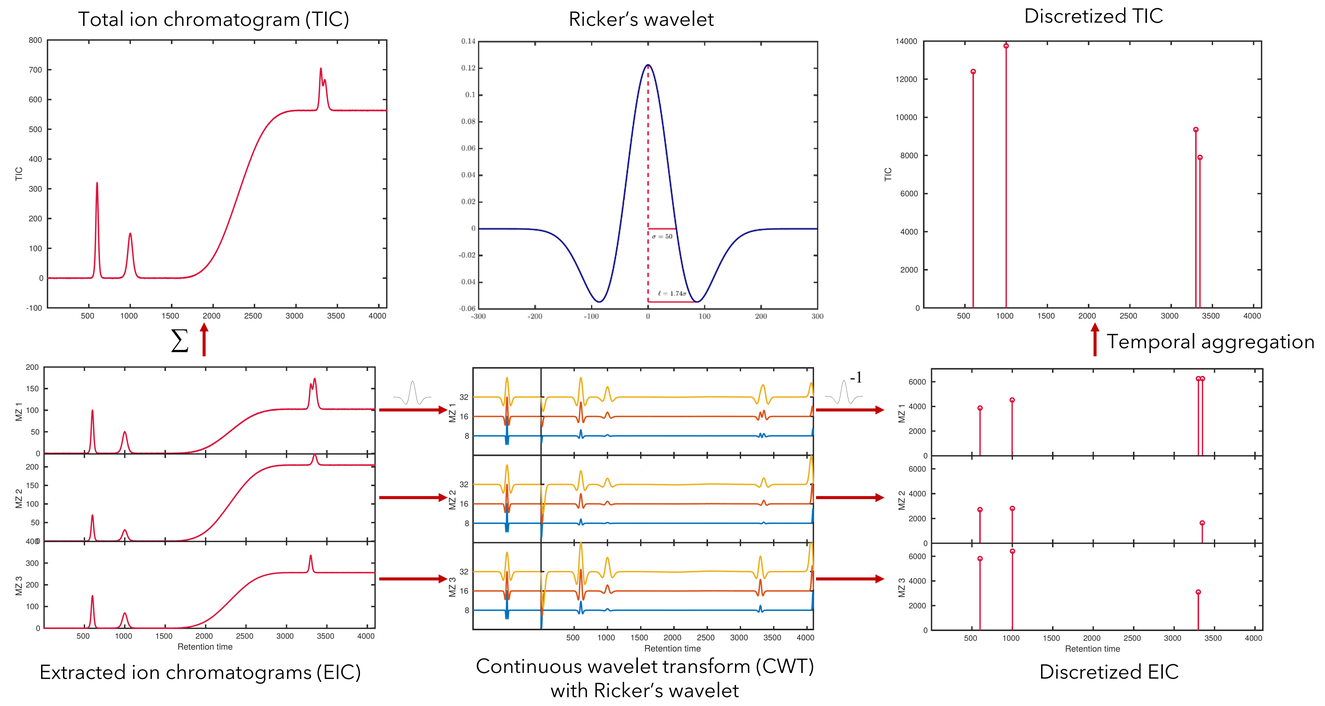
Each data file is a chromatogram containing temporal signals of ions with a mass over charge comprised between 40Da and 650Da composed by unwanted noise and baseline from column bleeding and sought peaks from injected samples.



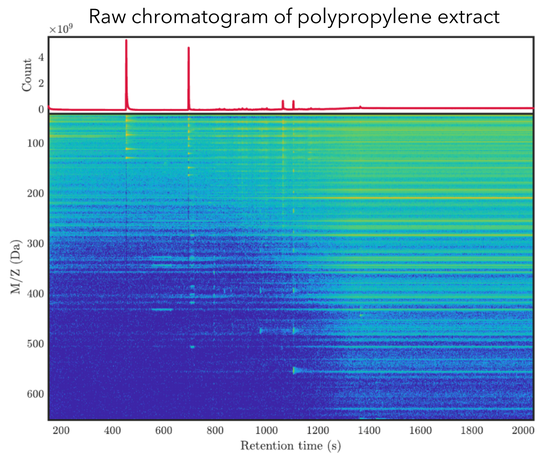
Numerical methods

Ion chromatograms are transformed along elution time. Negative lobes enable an easy tagging of patterns of individual and coeluted compounds. Steady baselines and high frequency noise are removed automatically by the transformation at a given scale. Specific mathematical properties enable to reconstruct quantitatively the theoretical elution profile from the representation of the signal at different scales. The final result is compatible with GC-MS software.

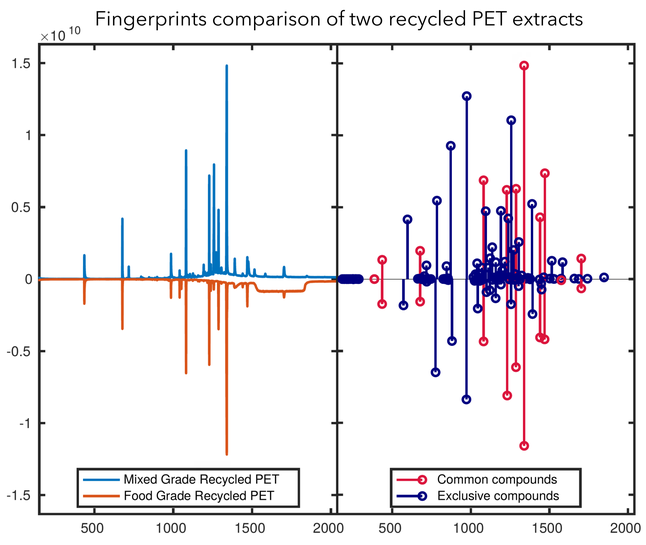
The depicted numerical example shows the transformed signal at 3 scales based on three ions signals.



Results and discussion



Current multiscale implementations (23 scales) clean and encode efficiently signals in 2-6 mins.
For unknown streams, 80-85% of coumpounds are automatically identified and associated to a fingerprint.



Conclusions and perspectives

Using a multiresolution description of signals with the Ricker's wavelet, the proposed methodology enables direct a deconvolution of compounds and fingerprints. Extracted signals facilitate pair comparison, tracking of compounds and the identification of unknown chemicals.

Future evolutions will couple identification of likely compounds with migration modeling for risk assessment. Feeding large fingerprint databases will help the non-supervised identification of streams via deep-learning,

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