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La technique SBSE dédiée à l'analyse de composés odorants par GC-MS-Sniffing

Annabelle Cingöz, A.Borcy, C. Henneuse

January, 26-27, 2015

SBSE Technical Meeting

Organisé par VEOLIA

Environment

Introduction – Packaging and « Off-Flavour »

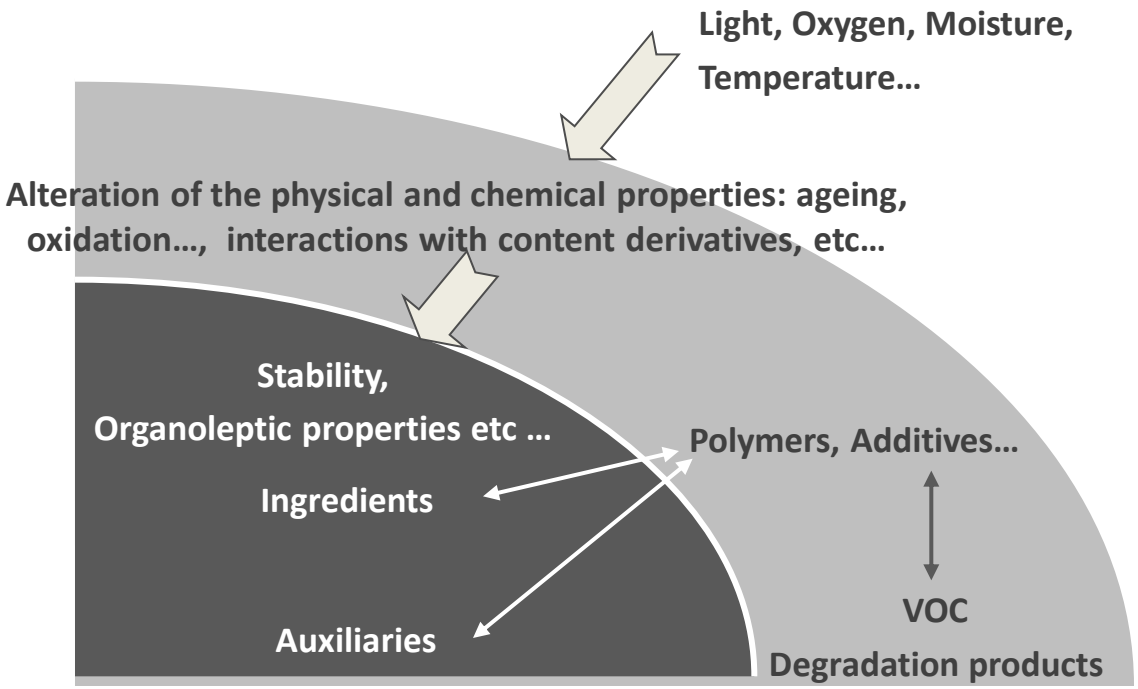
Packaging requirement: -ensure the integrity of the content

-ensure the safety of the consumers

➔**European regulation**
N° 1935/2004
N° 10/2011 (plastic)

Off-Flavour: - Are caused by the packaging, ageing, food/packaging material interactions

- Occur by volatile transfer, diffusion into the food or chemical reactions



Odorous compounds emitted by different polyolefin formulations for caps and closure applications after accelerated ageing (solar simulation)

- Analysis of a formulation without anti-UV additive (worst case)
- Influence of slip agents and anti-UV additives
- Comparison with a commercial reference

Experimental protocol

- Conditioning

Polymer material in contact with water

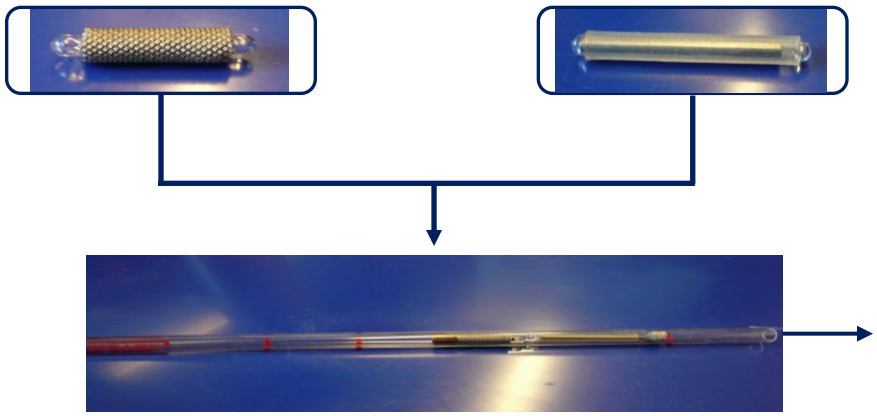
Accelerated ageing in Q-SUN Xenon Test chamber (solar radiation simulator chamber)

Controlled temperature 40°C

- Extraction of volatiles: sequential EG-PDMS procedure

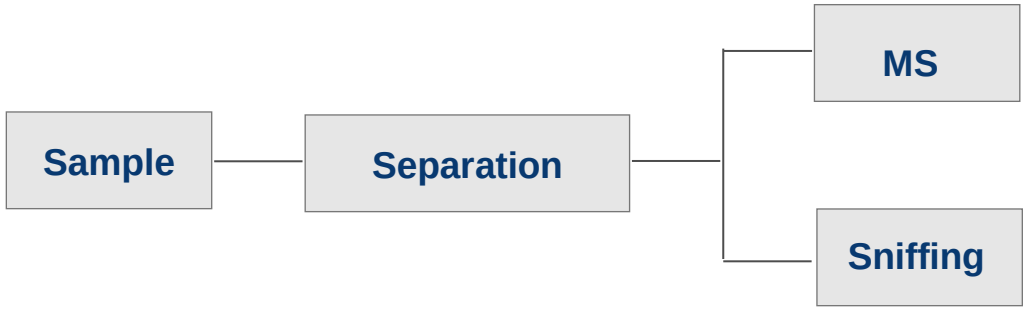
1)Twister EG silicone
Magnetic stirring / 1h

2) Twister PDMS
Magnetic stirring / 1h

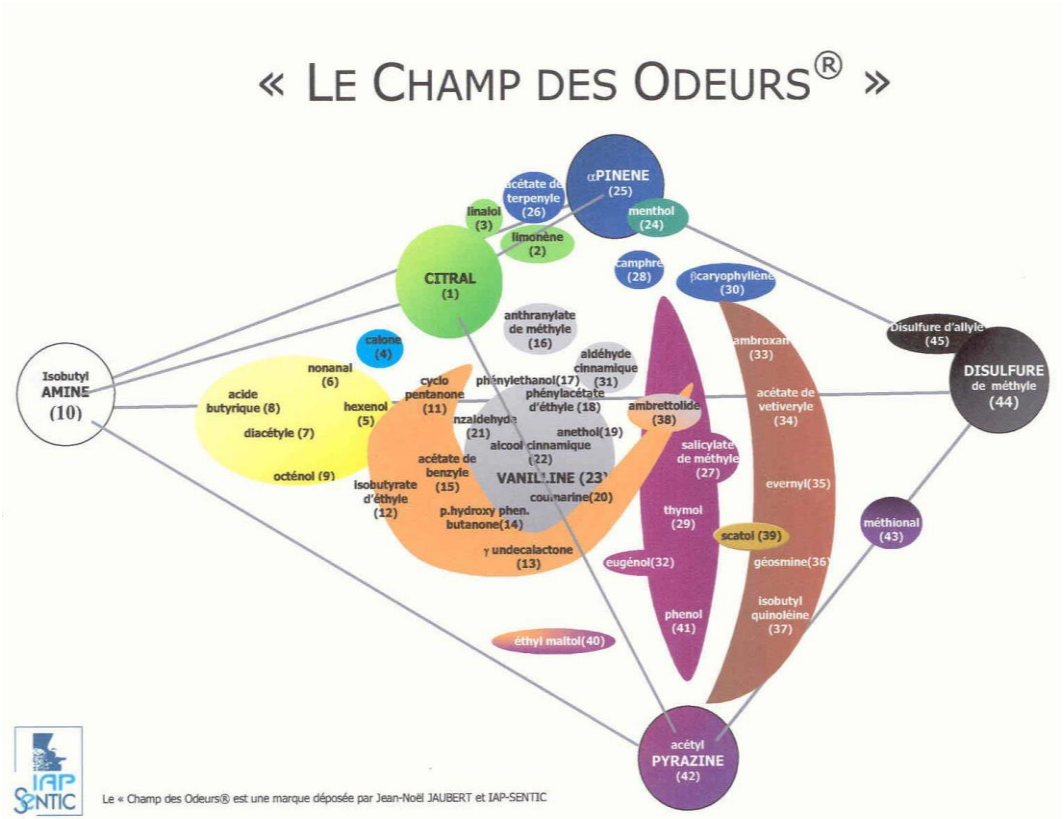


TD-GC-MS-sniffing
(expert panel)

GC-MS-Sniffing analysis



GC-MS-Sniffing analysis :
correlation chemistry/odour



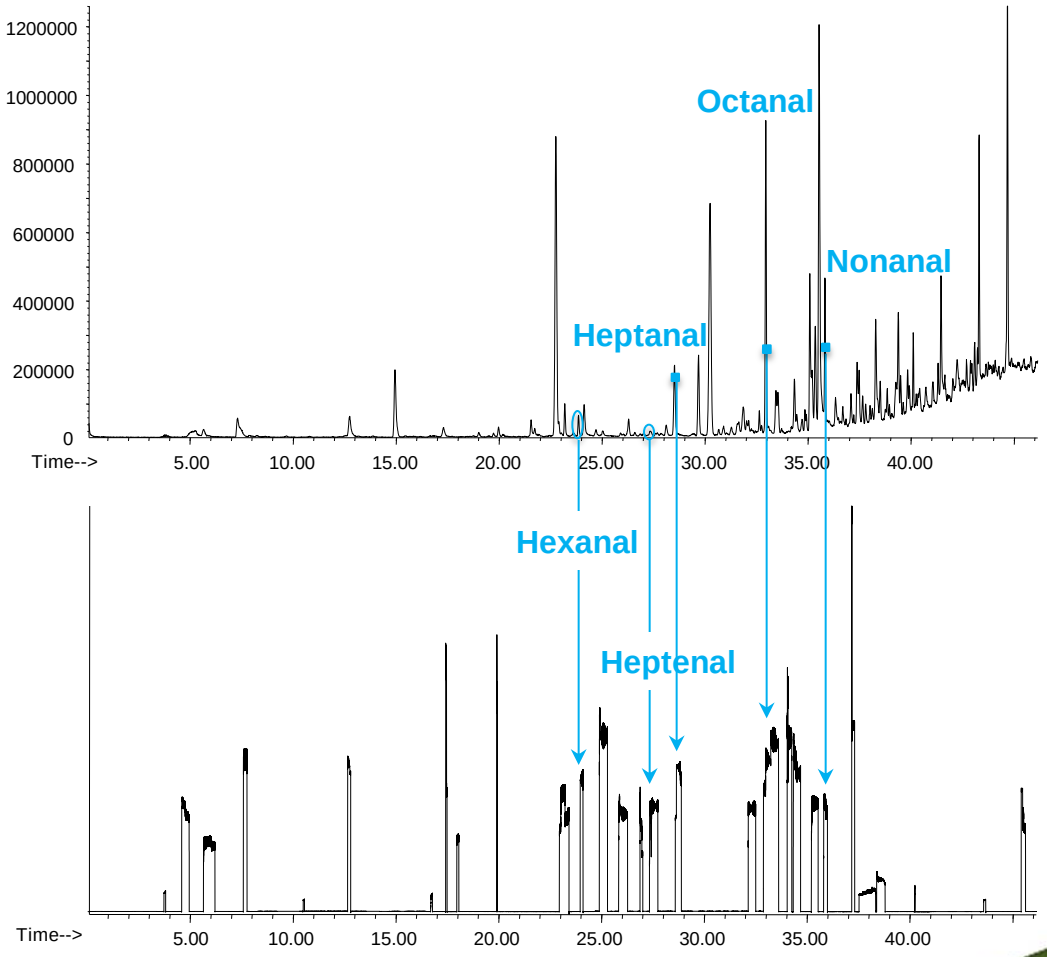
Organisation of the **olfactive space** according to 6 axes (amine, hesperidic, terpenic, sulphured, pyrogenous and sweet)

45 descriptors (references molecules) are used to characterise the odours (qualitative and quantitative analysis based on a relative intensity scale)

Formulation without anti-UV

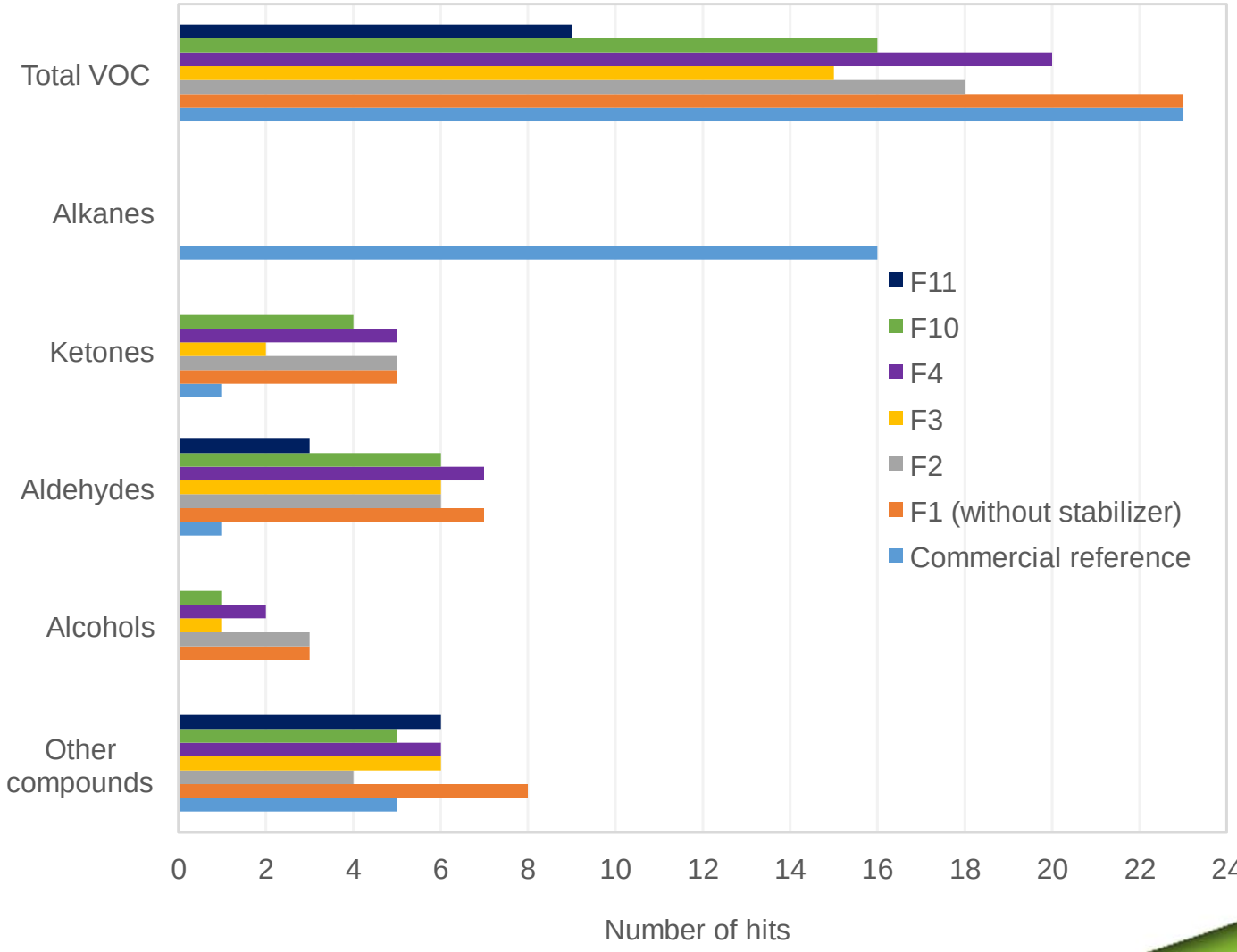
Chemistry

Odour



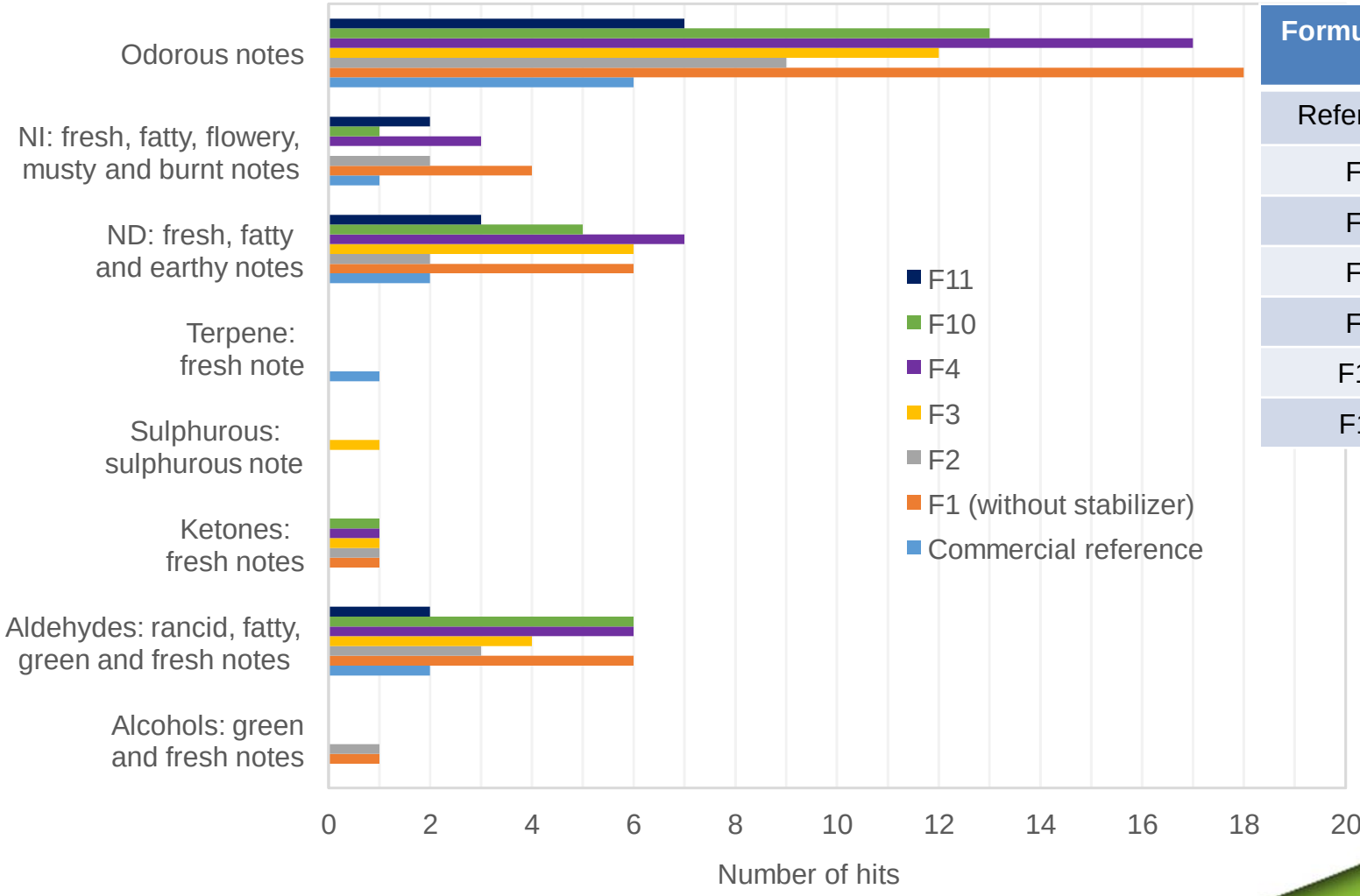
Minor compounds can be responsible of odour !

Comparative study - VOCs



Formulation	Slip agent	Anti UV
Reference	A	1
F1	B	No
F2	B	2
F3	B	3
F4	B	1
F10	C	2
F11	D	3

Comparative study - Odour



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Conclusion of the study

- SBSE coupled with GC-MS-Sniffing is a powerful technique for the identification of organoleptic contaminants in aqueous samples.

- Effect of sunlight exposure of PO on the organoleptic properties. Degradation of slip agents.

- Odorous compounds coming from the stir bars themselves have to be taken into account

GC-Sniffing analysis of EG-PDMS Twisters®

GC-MS-Sniffing analysis of Twister® without extraction step

RT (min)	CAS Nr	Compounds Detected by MS	Field of Odours® references	Evocation	Intensity
5,09		ND	cyclopentanone + diacetyl	solvent/ether +fatty notes	1 + 1,5
5,52		unknown	cyclopentanone	solvent/ether note	1
5,8		ND	acetyl pyrazine	roasted note	1
13,4		ND	diacetyl	fatty note	1
14,87	497-26-7	1,3-Dioxolane, 2-methyl-	cyclopentanone	solvent/ether note	<1
17,24		unknown alcohol	cis-3-hexenol	green note/grass	2
19,94	1663-35-0	2-Methoxyethyl vinyl ether	cyclopentanone	solvent/ether note	2,5
22,73		unknown ether	cyclopentanone	solvent/ether note	2
23,17		unknown ether	acetic acid -->cyclopentanone	pungent--> solvent/ether note	2-->2,5
25,02		unknown acid	acetic acid	pungent note	1
35,38		ND	1-octen3-ol	fresh note/mushroom	2
36,63		ND	phenol	ink	2
39,24		ND	isobutylquinoleine	earthy note, asparagus	1

EG vs PDMS Twister® : numerous solvent/ether notes !

Many thanks to Mrs Anne BORCY

For more information:

Zone industrielle C
Rue Jules Bordet
B-7180 Seneffe
BELGIUM
Tél. +32 64 520 211
Fax. +32 64 520 210
annabelle.cingoz@certech.be
www.certech.be

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