

## Statistical analysis of chamber VOCs emission data

Romain, AC\*, Degrave, Ch\*, Nicolas, J,\* Lor. M\*\*,  
Vause. K\*\*, Dinne. K\*\*, Maes. F\*\*\*, Goelen, E\*\*\*

*HEMICPD partners*

- \* *Ulg, Department of Environmental Sciences and Management, (Belgium)*
- \*\* *BBRI*
- \*\*\* *VITO*



- Created in 1973 (FUL), Ulg since 2003  
Ulg, Arlon campus
- Teaching and research on environmental topics
- 5 research units
- **Environmental monitoring: Polluted Atmosphere team + spin-off**

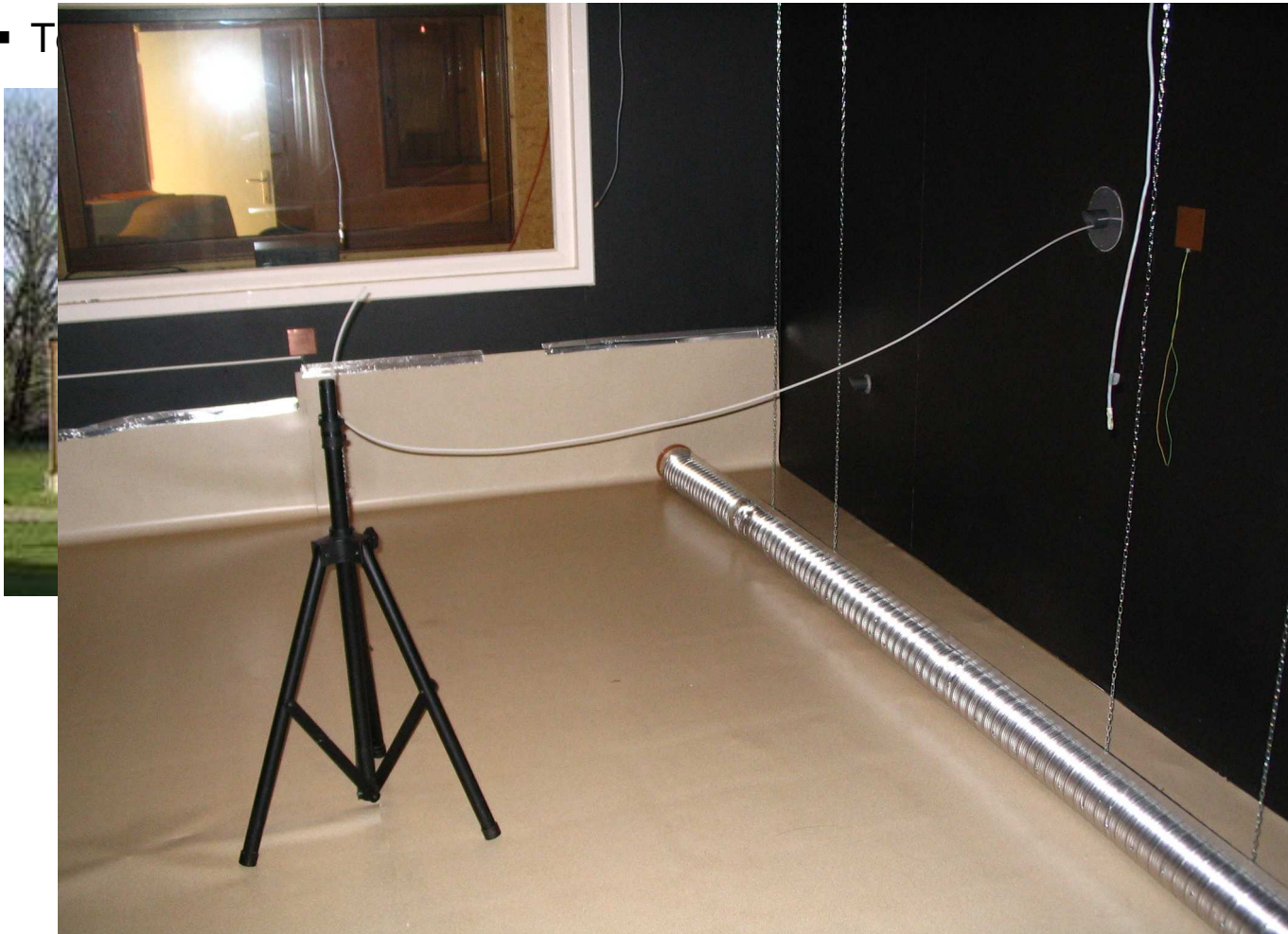


***Our goal: Developing tools & methods of gathering and processing of environmental data to help the decision maker***

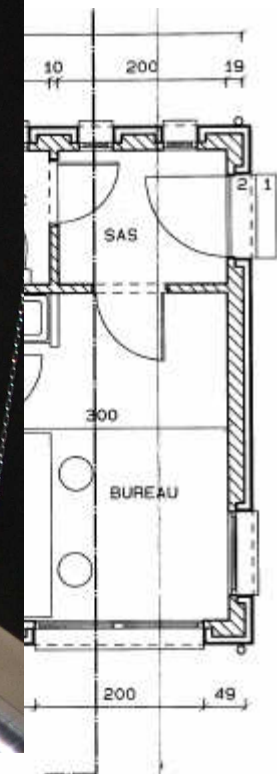
Principal topics:

- environmental off-odour measurements (*see next ULg presentation*)
- e-nose technology (member of ISOCS)

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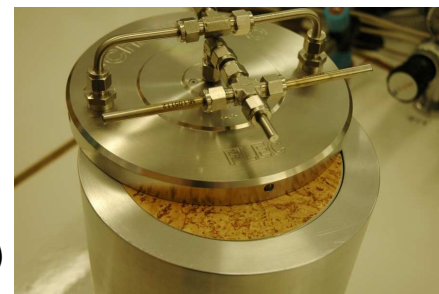
- Test of a large chamber (50m<sup>3</sup>), no labelled “emission chamber” (near-real life conditions)
    - 8 materials : 4 flooring and 4 insulation materials (glass wool uncovered, gypsum board covered, glass wool, polystyrene glued to a gypsum board, wood wool glued to expanded polystyrene)
    - sampling after **3**, **7** and **28** days for VOC's and aldehydes measurements
    - influence of height of chamber air collection
    - electronic nose tests
  - TD-GC-MS analyses of VOC's emissions collected from various emission chambers (*ISO 16000- CEN/TC351*, ULg, VITO and BBRI, *see Vito presentation*)
  - Development of an instrument and a methodology for odour intensity measurement dedicated for materials, first results (*see scd ULg presentation*)
  - Preliminary tests of e-nose technology for indoor application (*see scd ULg presentation*)
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- **VOC data treatment to compare the emission chambers of each partner**

## One of the project goals: comparison of the chambers

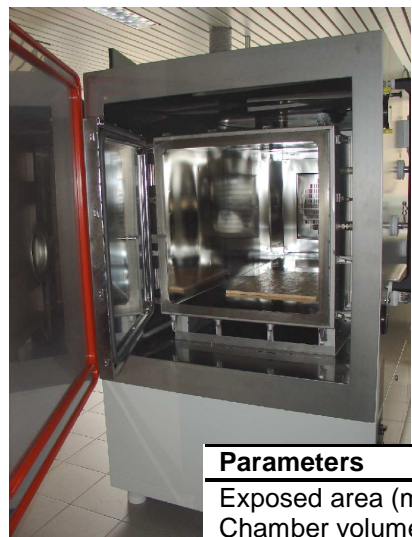


**μ-chamber**  
(BBRI)

**FLEC**  
(VITO&BBRI)

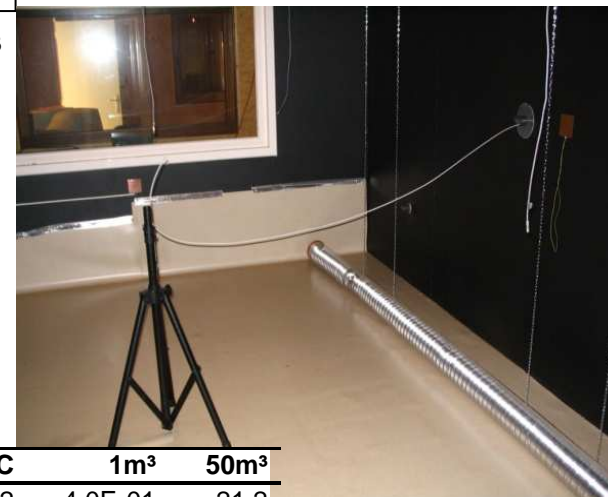


**4 test chambers**



**1 m³**  
(VITO)

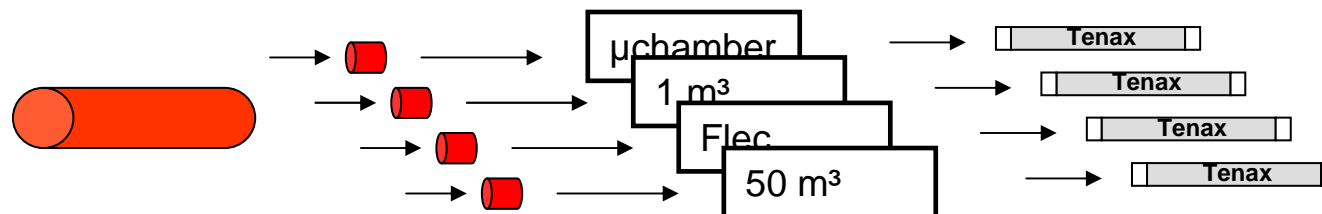
**50 m³**  
(ULg)



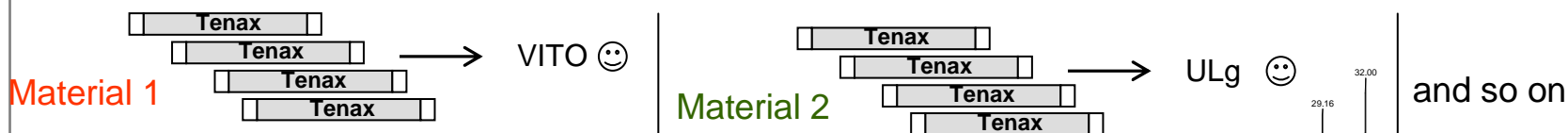
Parameters	μ-CTE	FLEC	1m³	50m³
Exposed area (m²)	1.3E-03	1.8E-02	4.0E-01	21.2
Chamber volume (m³)	3.2E-06	3.5E-05	1	50.5
Load factor (m²/m³)	401	506	0.40	0.42
Air flow rate (L/min)	0.03	0.3	8.3	883
Exchange rate (h⁻¹)	491	514	0.498	1.05
Area specific air flow rate (m³/m².h)	1.23	1.02	1.25	2.50

## Methodology to compare the chambers

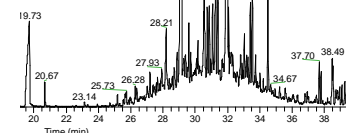
- Tests with **4 floor covering** material samples; insulating materials are in process of being analysed
  - 4 chambers with the same material
- 4 floor coverings:
- Material 1: PVC floor covering
  - Material 2: PVC floor covering
  - Material 3: Carpet
  - Material 4: Linoleum
- samples of the same flooring material **distributed to each chamber** (for each partner)  
located at the same time in each chamber (**samples of same age**)



- Sampling after 3, 7 and 28 days
- TD-GC-MS analyses randomly by each partner (same analytical conditions)



- Screening COV's: exhaustive analysis of each chromatogram (*see VITO presentation*)





## How to compare so many chromatograms ?

**First sample**, first sampling day, 4 chambers: **6** comparisons

**First sample**, second sampling day, 4 chambers: + 6, **12**

**First sample**, third sampling day, 4 chambers: + 6, **18**

**Second sample**, first sampling day, 4 chambers: + 6, **24**

**Second sample**, second sampling day, 4 chambers: + 6, **30**

**Second sample**, third sampling day, 4 chambers: +6, **36**

1m<sup>3</sup>

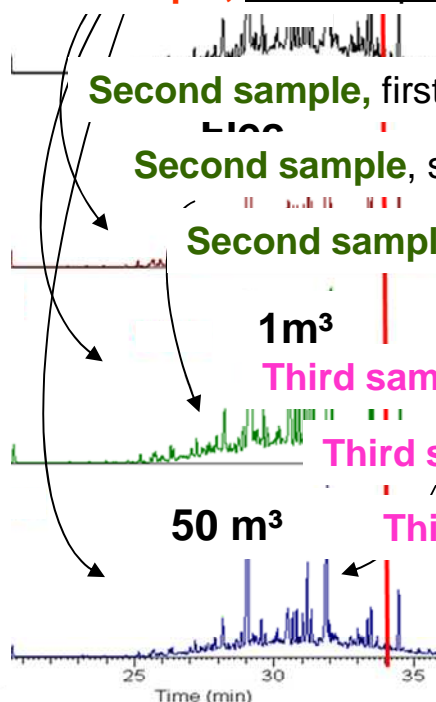
**Third sample**, first sampling day, 4 chambers: + 6, **42**

**Third sample**, second sampling day, 4 chambers: + 6, **48**

50 m<sup>3</sup>

**Third sample**, third sampling day, 4 chambers: + 6, **54**

**Fourth sample**, first sampling day, 4 chambers: + 6, **60**



+....: more than 70 comparisons??

## How to compare so many chromatograms ?



**Comparison by global visualisation not possible**



**Comparison by global data processing possible**



Multivariate statistical techniques:

**Principal component analysis (PCA)**

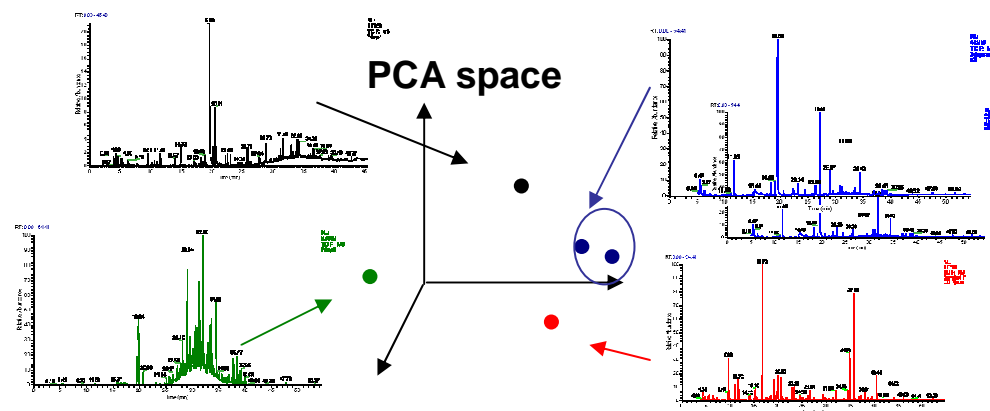
*[PCA explanation on a poster]*

PCA highlights, in one shot, differences or similarities between data sets,  
reduces numerous variables (compounds) to two or three,.. keeping max info

Tool to compare fast, easily and objectively the whole data  
taking into account samples, chambers and days



In the PCA space, a chromatogram is a dot in a 2 or 3 dimensions plot



**If the points are close, they are similar: same chromatograms profiles**

Input variables used for this analysis: **chemical families**

instead of COV's compounds

- For a statistical analysis, many variables (numerous compounds) require ideally many data (chromatograms),
- All GC peaks not recognizable,
- Various isomers for the hydrocarbons families (i.e. uncertainty on the name 1-methyl-.... or 3-methyl-....?)
- Chemical family belonging of the compounds easy to qualify even if the exact name of the compound not

## PCA inputs

Chamber	Day	Sample	Organic acid	Alkane	Alkene	Alcohol	Aldehyde	Aromatic	Ketone	CycloAlkane	Ether	HAP
1 m <sup>3</sup>	3	sample 1	4	21	2	3	7	48	2	5	8	0
1 m <sup>3</sup>	28	sample 1	2	34	2	4	2	43	2	5	5	1
50 m <sup>3</sup>	3	sample 1	2	30	1	1	21	26	2	8	2	1

### Variables used:

10 chemical families specific of the 4 materials tested

carboxylic acids, alkanes, alkenes, aromatics, ketones, aldehydes, alcohols, ethers, HAPs,  
cycloalkanes

Compounds present in all the samples database, merged with chemical family category

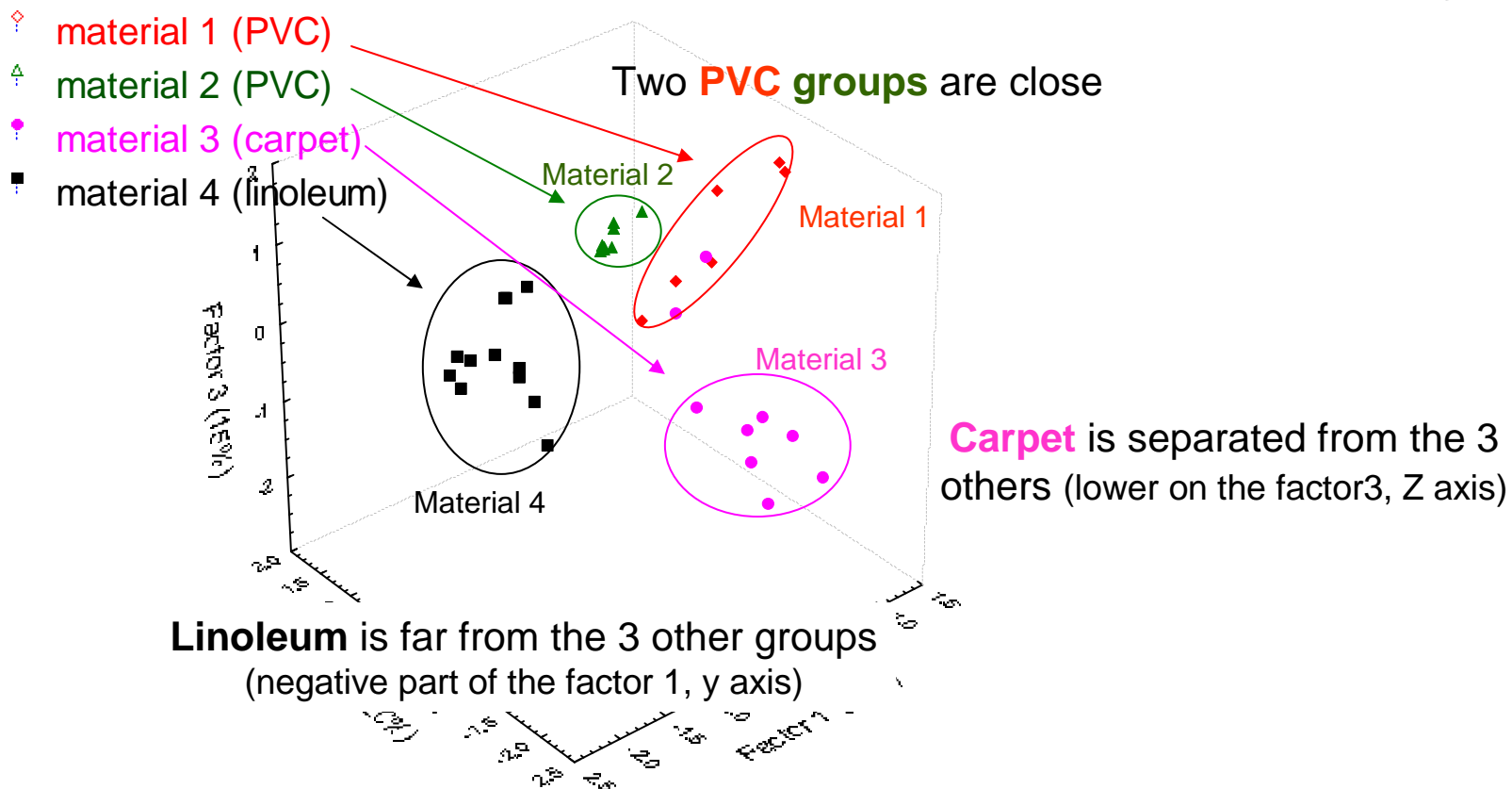
### Data set:

39 reliable observations (relative abundance in percentage for each chromatogram, total  
for the 10 families considered = 100%)

Flec	3	sample 4	19	0	7	0	70	4	0	0	0	0
Flec	7	sample 4	26	0	11	0	63	0	0	0	0	0
Flec	28	sample 4	27	0	8	0	65	0	0	0	0	0
50 m <sup>3</sup>	3	sample 4	8	0	0	0	25	0	0	0	0	0
50 m <sup>3</sup>	7	sample 4	8	0	0	0	26	0	0	0	0	0
50 m <sup>3</sup>	28	sample 4	4	0	0	0	9	0	0	0	0	0
1 m <sup>3</sup>	3	sample 4	13	0	7	0	55	10	15	0	0	0
1 m <sup>3</sup>	7	sample 4	8	0	4	0	69	8	12	0	0	0
1 m <sup>3</sup>	28	sample 4	11	0	16	0	56	5	12	0	0	0
50 m <sup>3</sup>	3	sample 4	11	5	1	5	76	0	0	0	0	0

## PCA results

1st question: Are the 4 materials identified?

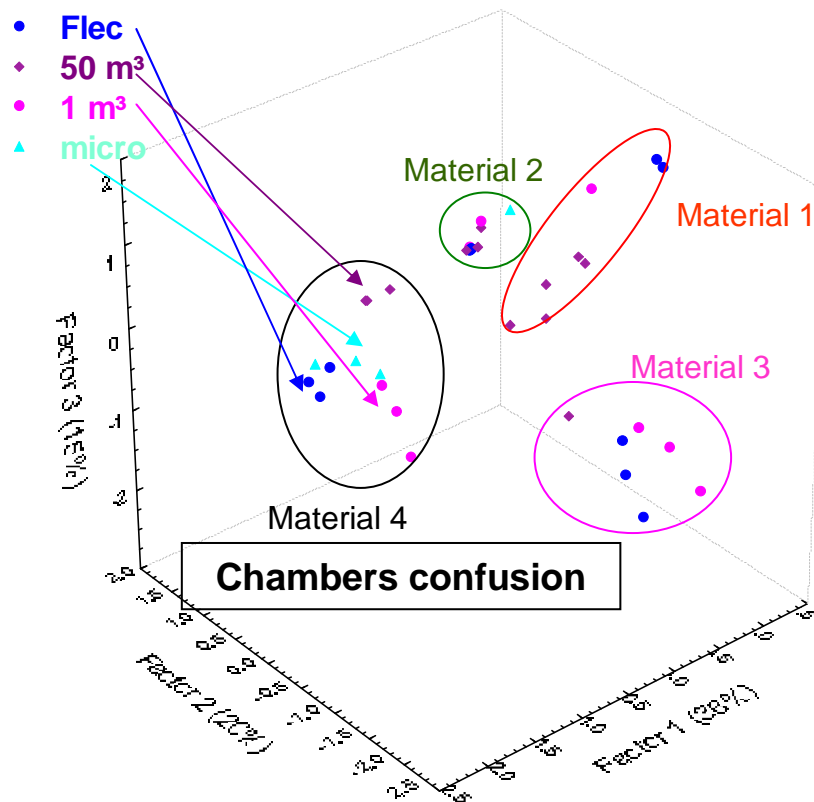


→ **YES**, even if 2 data of material 3 are confused with material 1

the real size chamber had a higher VOC background than the other ones

## PCA results

*Scd question:* Is there an influence of the emission chambers



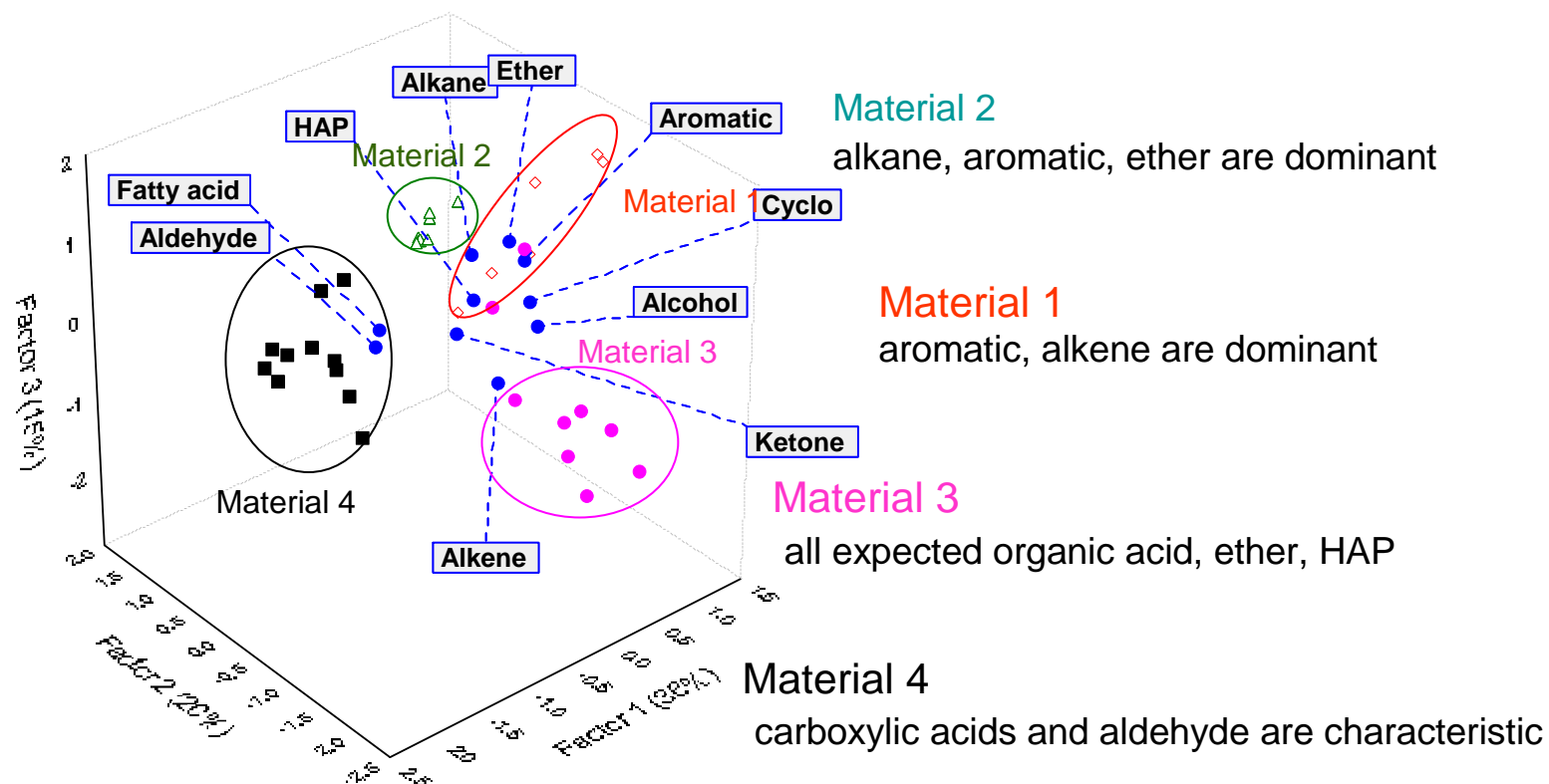
no separation of the chambers (**real size chamber** in the middle for material 1 and 3)

→ NO, the chambers don't influence the chemical profile results (proportion of families)

## PCA results

3rd question: Which chemical families specific of the materials?

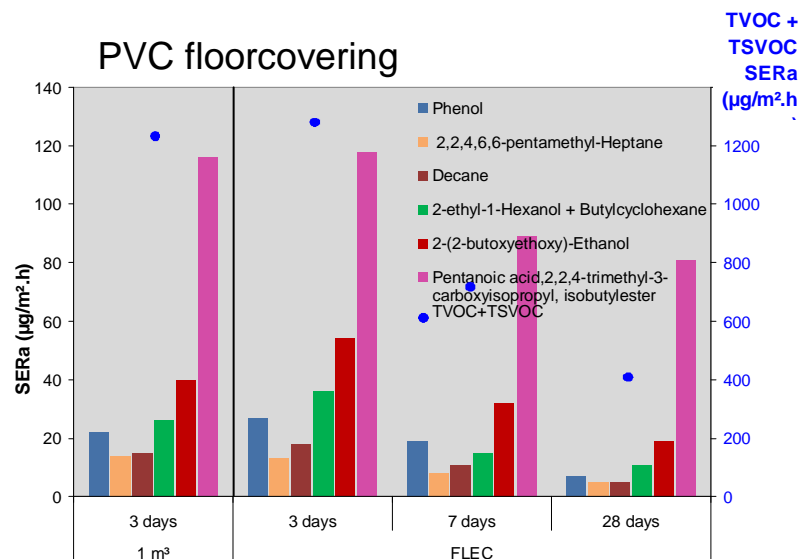
Same plot but addition of the 10 variables “chemical families” (loadings in PCA terms)



→ Global and fast explanation of the data (materials) separation

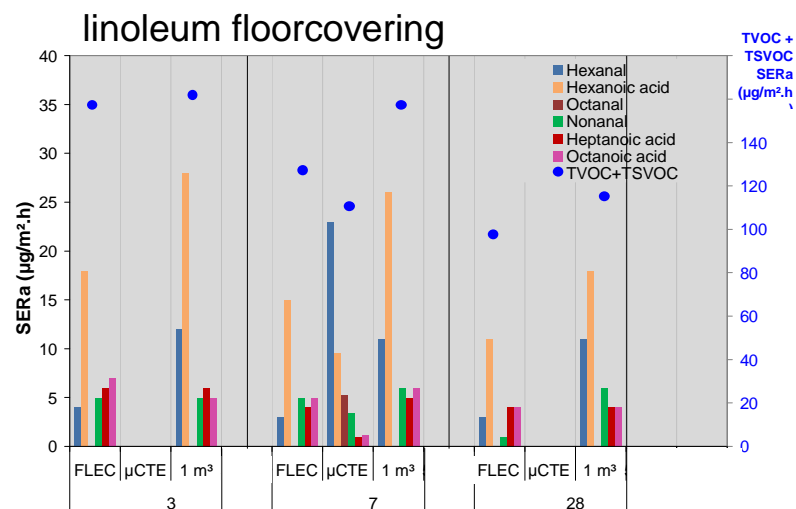
For instance:

(Ongoing work, First results)



### For 1m³ and Flec

- comparable SER results
- same composition



### For 1m³, Flec and µchamber

- comparable SER results
- similar composition
- “tuning” work needed for µchamber (ongoing)



- Qualitative and chemical families relative abundance information: **no distinction between emission chambers**, same behaviour

Results obtained in a real size chamber in less controlled conditions are similar to the ones realised in standard emission chamber: good news for **labo** → **field extrapolation**

- First quantitative results: same behaviour for Flec and 1 m<sup>3</sup> chambers,  $\mu$ chamber results similar (treatment in process), comparable results for large size chamber but higher background.

(Ongoing data treatment on SER values (on TVOC's, on compounds, on chemical families))

- No influence of the sampling procedure
- Multivariate data processing like PCA:  
easy tool to evaluate, in one shot, results analysis and various parameters
- Output for the chamber choice, selection of  
the most rapid, less material consumption, no expensive, easy to manipulate and control (simple), able to manage different tests simultaneously (for instance, "Flec" type chamber good compromise: VOC analyses and sensory tests)

## Co-workers:

**BBRI:** *Marc, Kevin and Karla*

**VITO:** *Frederick and Eddy*

## Polluted atmosphere team:

In particular: Christophe, Jacques, Roland, Maria Elisabete, Laurent,  
Cédric, Catherine

results mentioned in this presentation are funded by



Thanks for your attention