Dutch Photonics Event

Life Science Trace Gas Research Group

Towards broadband mid-infrared trace gas sensing using a supercontinuum source

Qing Pan

Delft, 10-09-2019

Institute for Molecules and Materials
Radboud University

Need for trace gas sensing

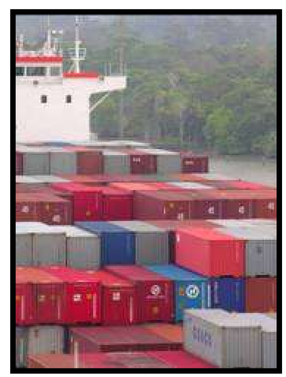
Environmental

Breath analysis

Combustion

Fresh fruit storage

Transport products



Green houses

Purity gases

Need for trace gas sensing

Environmental

Combustion

Fresh fruit storage

Transport products

Green houses

Purity gases

The objective

Reducing storage losses of agro-products

Production North-West Europe:

- Apples: 3.4 million tons
- Pears: 0.9 million tons
- Blueberries: 18000 tons
- Potatoes: 28.6 million tons

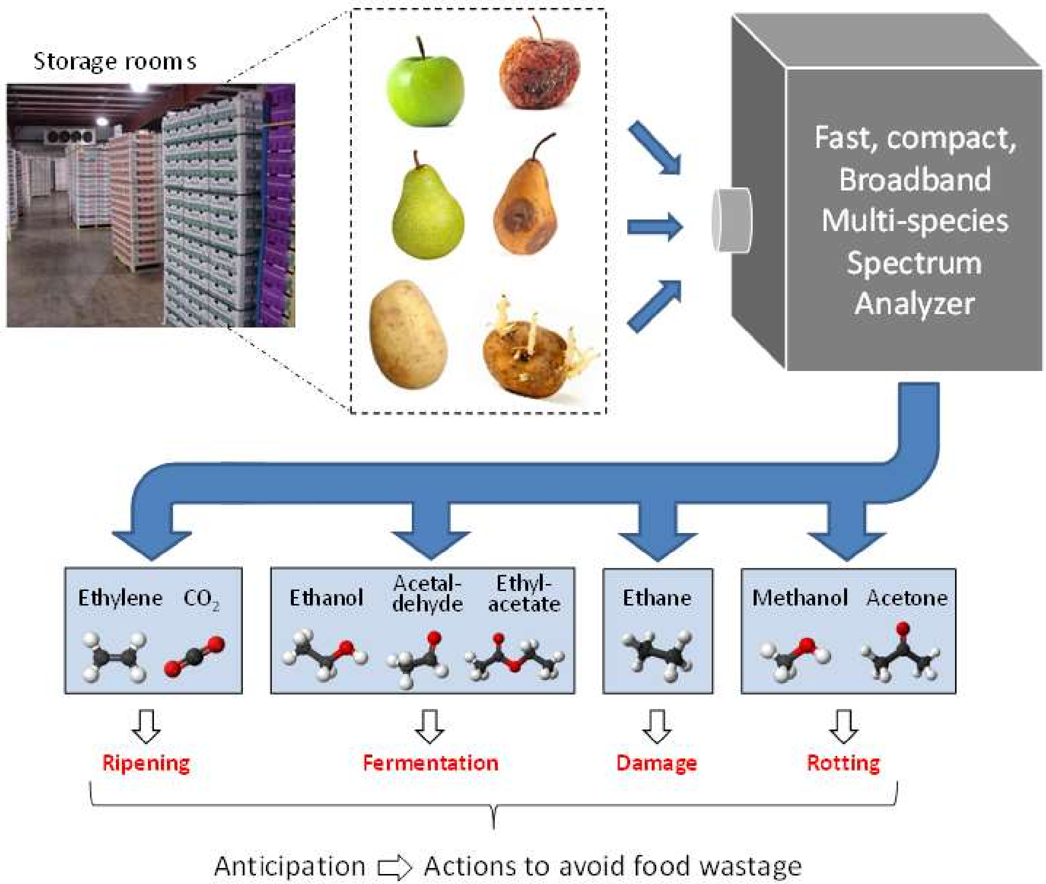
Estimated losses during storage: 3 – 5%

~60k Euro/year/farmer

The QCAP concept

Quality Control of Agro-Products

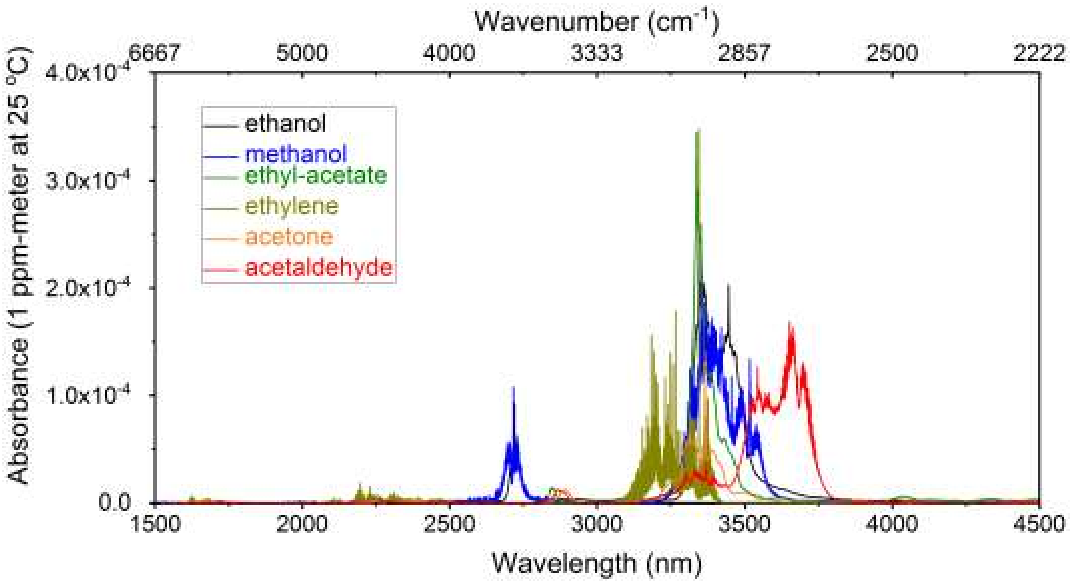
North-West Europe
QCAP
European Regional Development Fund



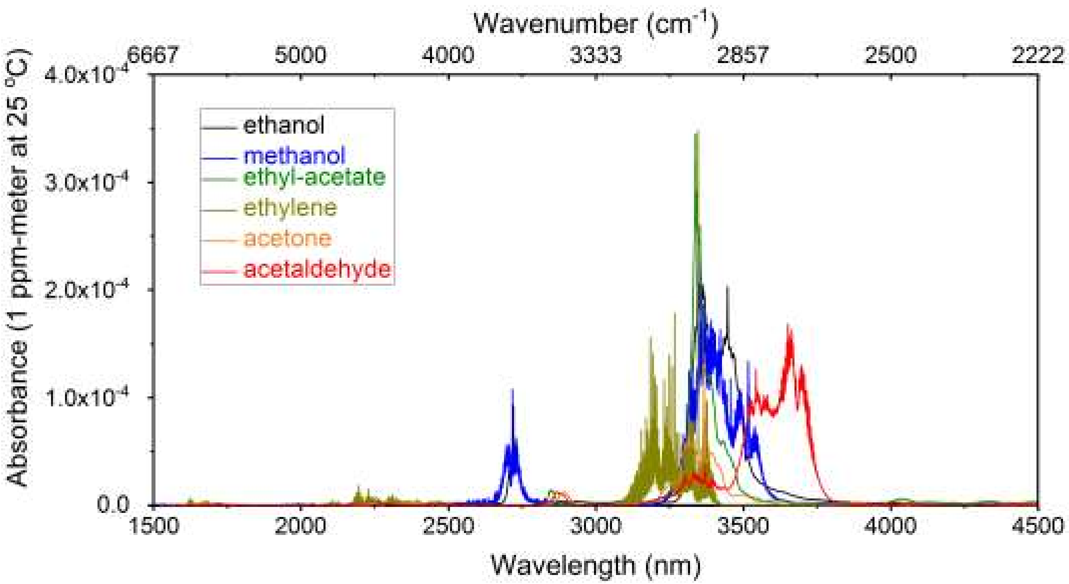
Challenges:

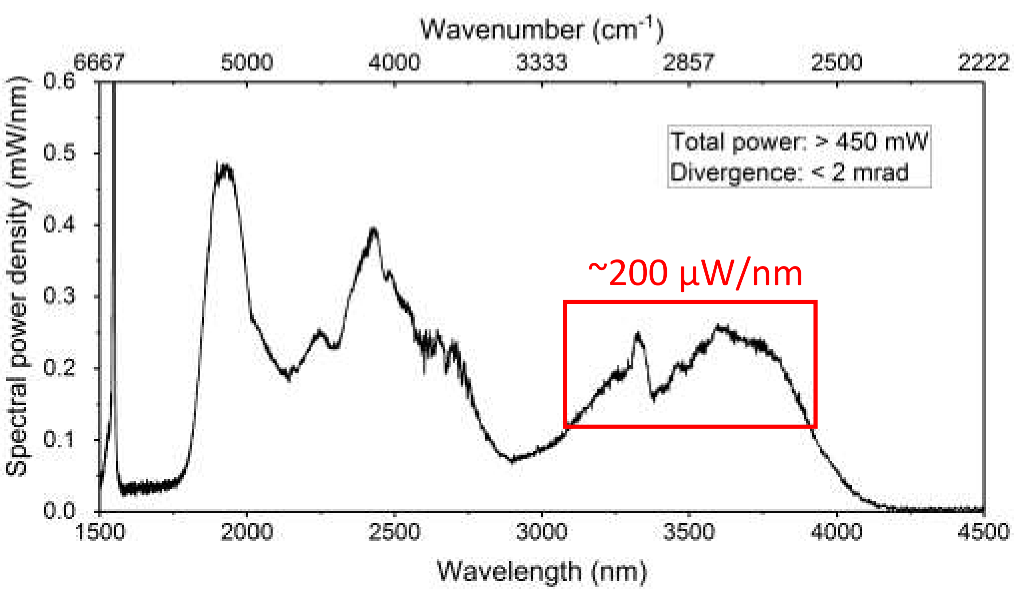
- Multi-species detection
- Sensitivity
- Stability
- Cost

Requirement: broad mid-IR spectral coverage



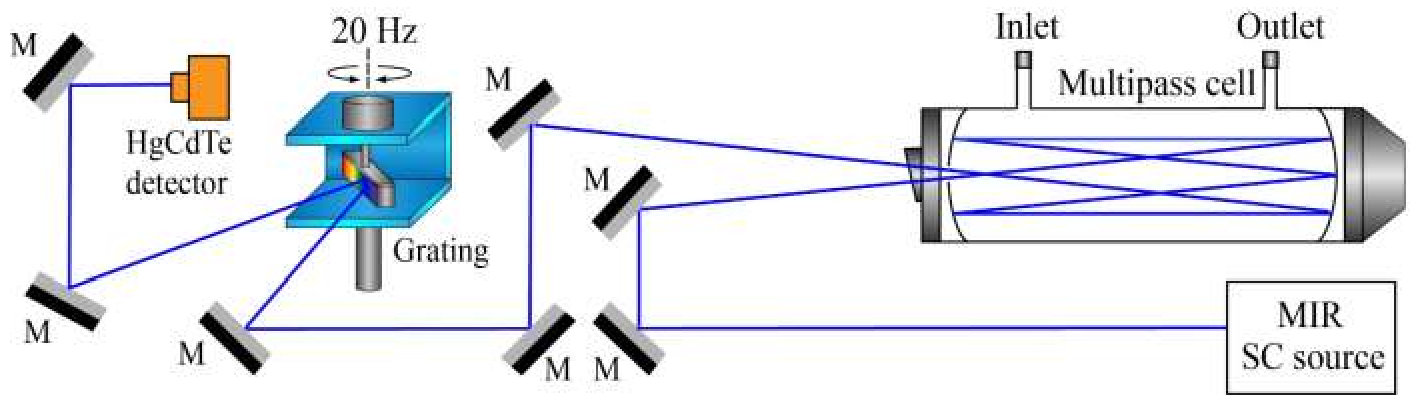
The supercontinuum light source





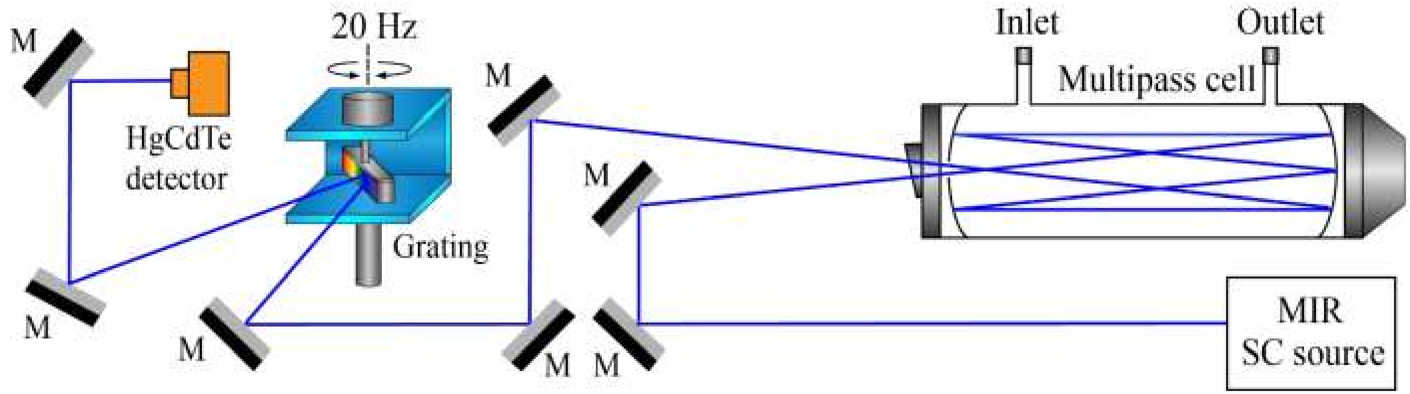
SuperK MIR, NKT Photonics

Supercontinuum + multipass cell

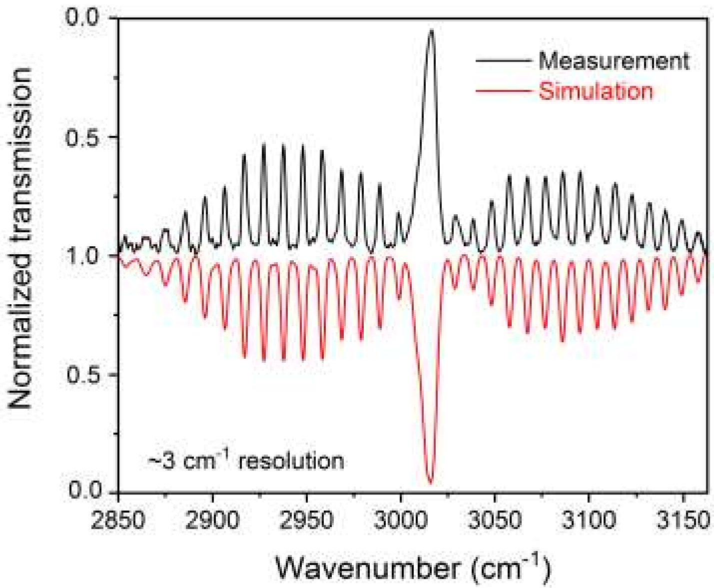


Photodetector (VIGO) specific detectivity: 10^{11} cm·Hz$^{1/2}$/W

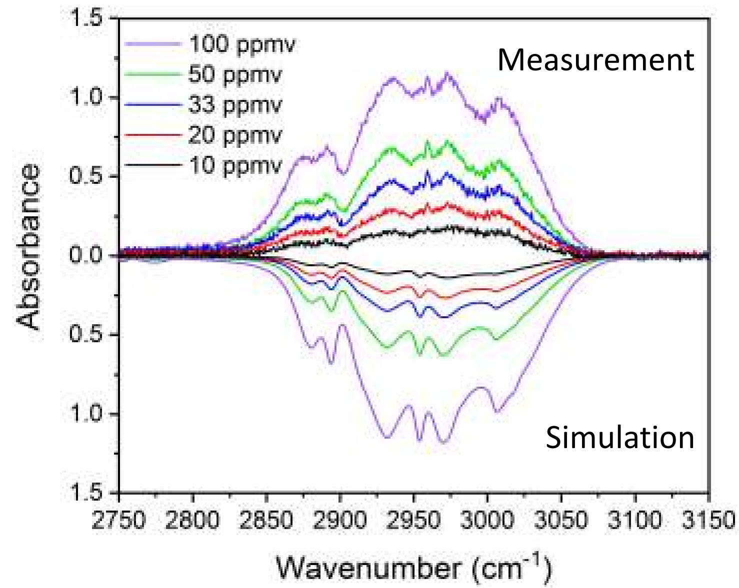
Supercontinuum + multipass cell



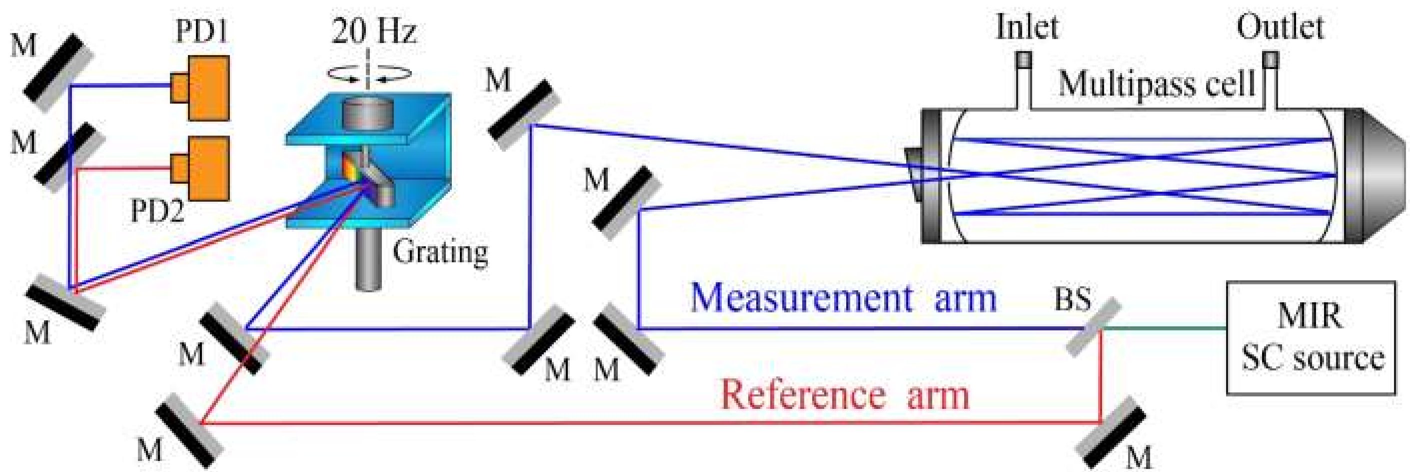
Methane



Ethane



Balanced detection



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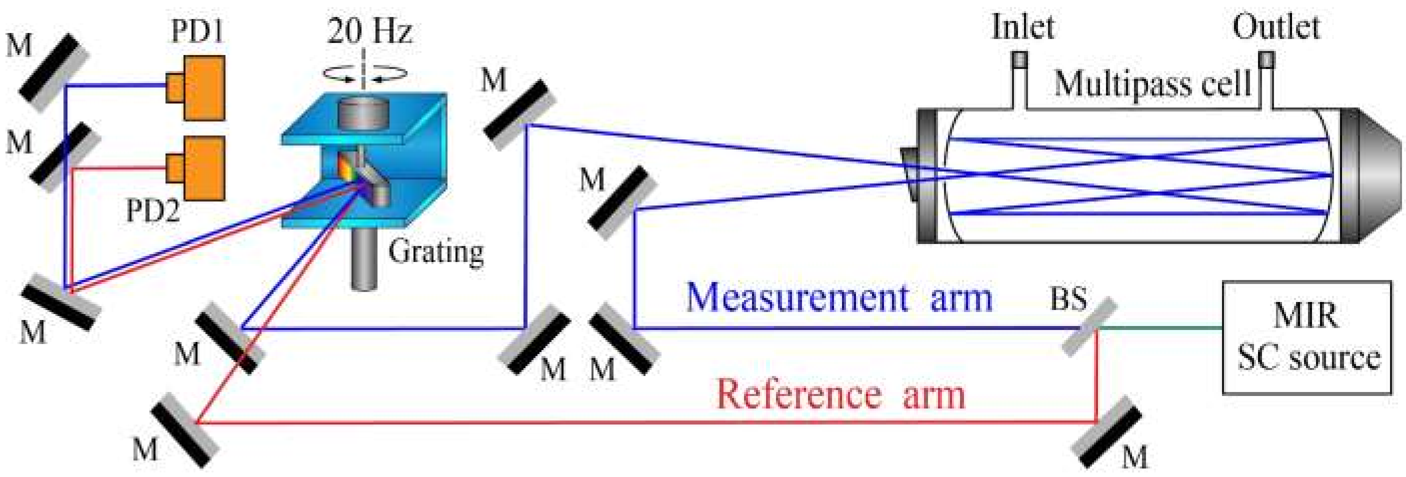
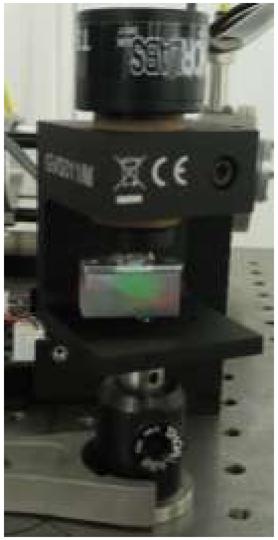
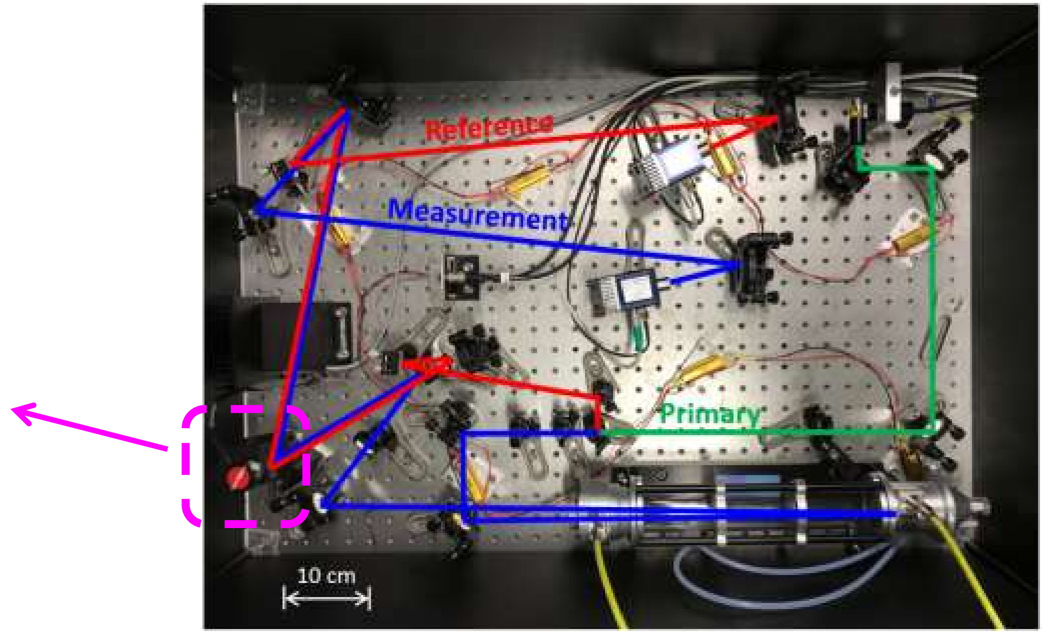
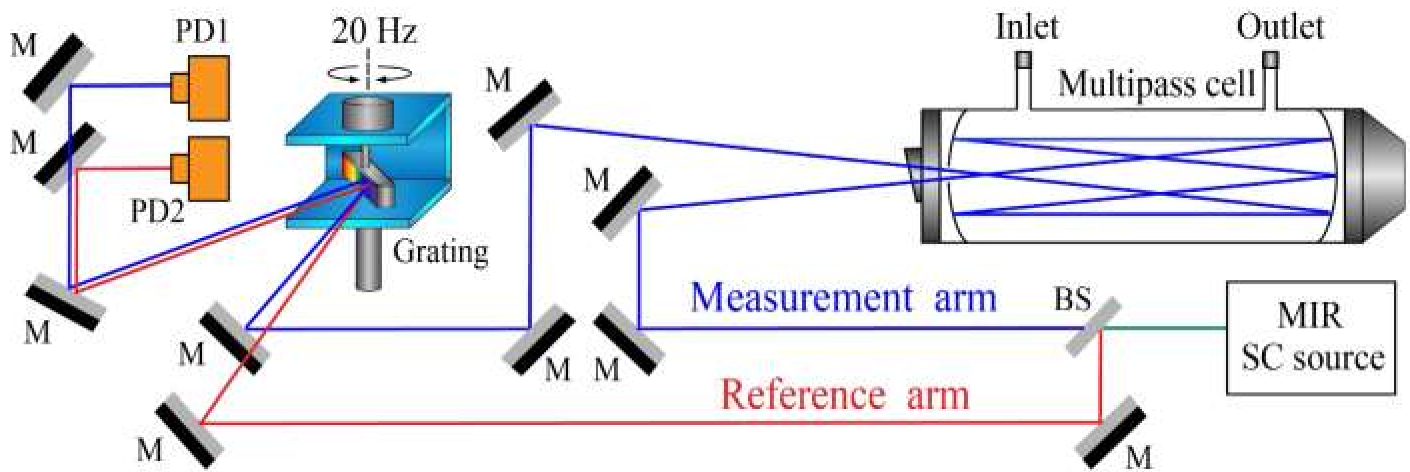
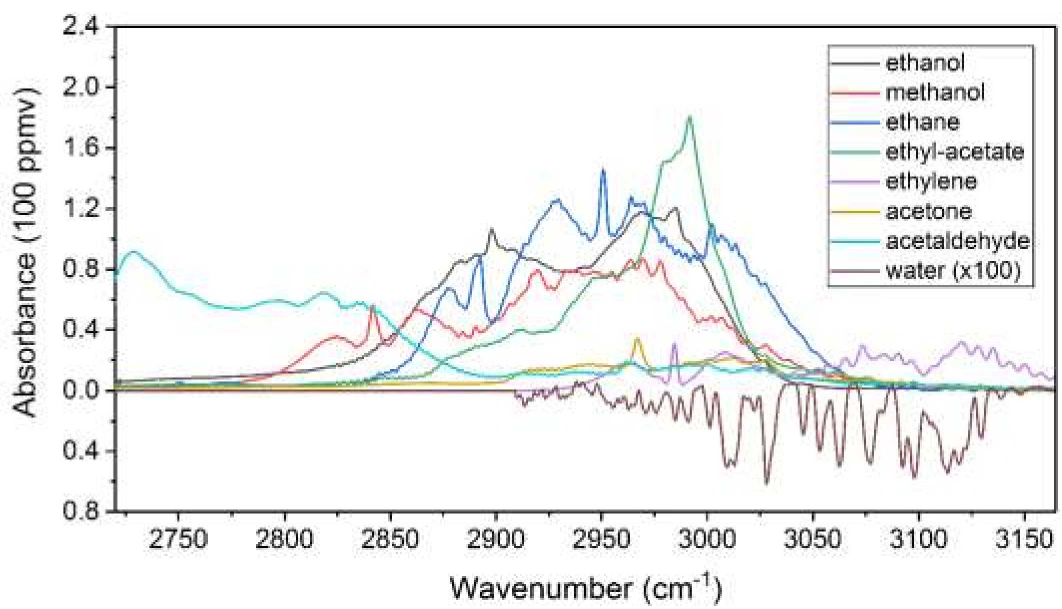






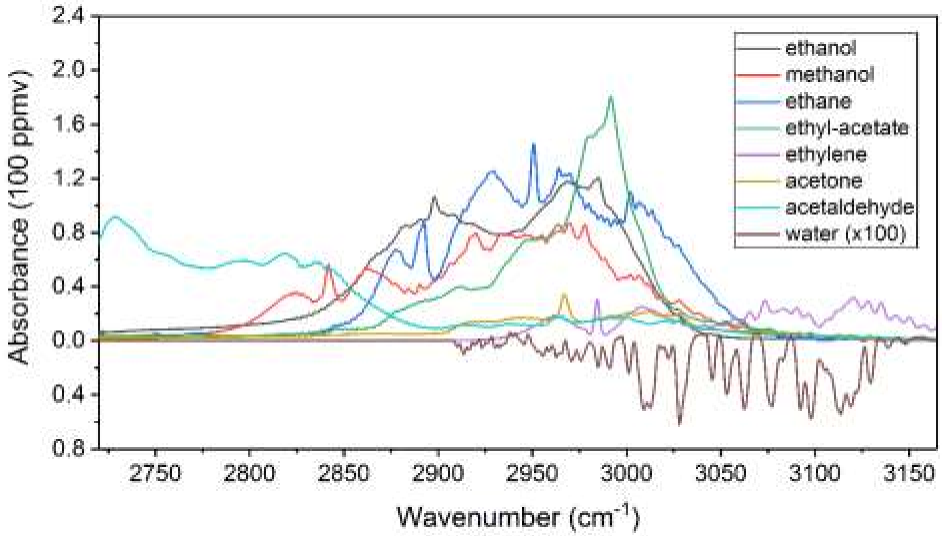
Balanced detection





Broadband multi-species detection

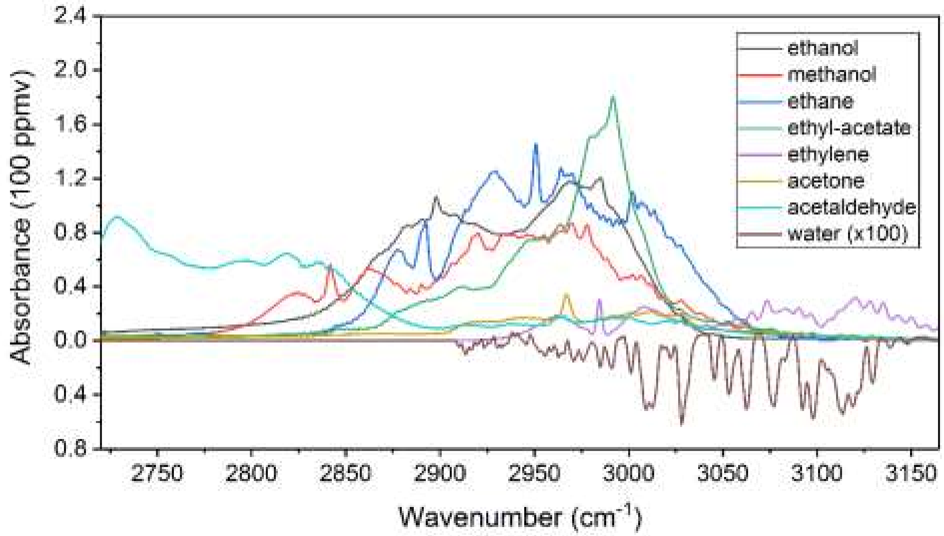
Establish a reference database



$$= \begin{bmatrix} \lambda_1^A & \lambda_1^B & \cdots & \lambda_1^K \\ \lambda_2^A & \lambda_2^B & \cdots & \lambda_2^K \\ \lambda_3^A & \lambda_3^B & \cdots & \lambda_3^K \\ \vdots & \vdots & \ddots & \vdots \\ \lambda_n^A & \lambda_n^B & \cdots & \lambda_n^K \end{bmatrix}_{n \times K} = \mathbf{R}$$

Least-square global curve fitting

$$\boxed{\mathbf{D}_{n\times 1} = \mathbf{R}_{n\times K}\,\mathbf{C}_{K\times 1} + \mathbf{E}_{n\times 1}}$$



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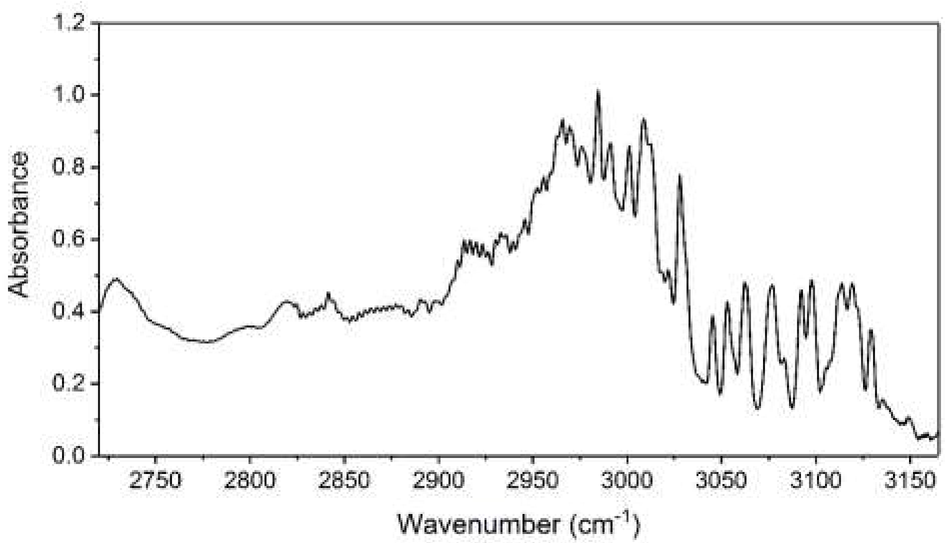
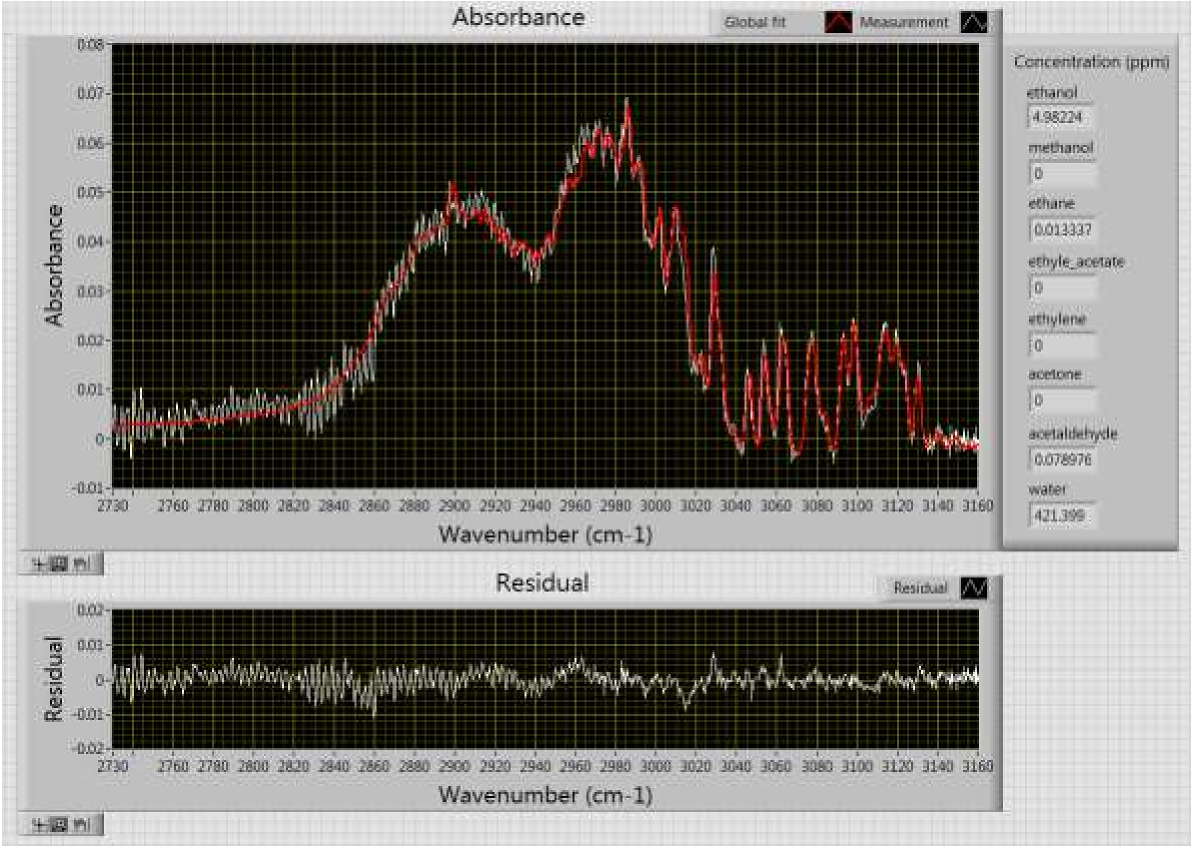


$$= \begin{bmatrix} \lambda_1 \\ \lambda_2 \\ \lambda_3 \\ \vdots \\ \lambda_n \end{bmatrix}_{n\times 1} = \mathbf{D}$$

Real-time data analysis

- Calibrated 5.0 ± 0.1 ppmv ethanol source
- 4.87 ± 0.32 ppmv obtained



System integration and validation

QCAP-1

Pear storage containers

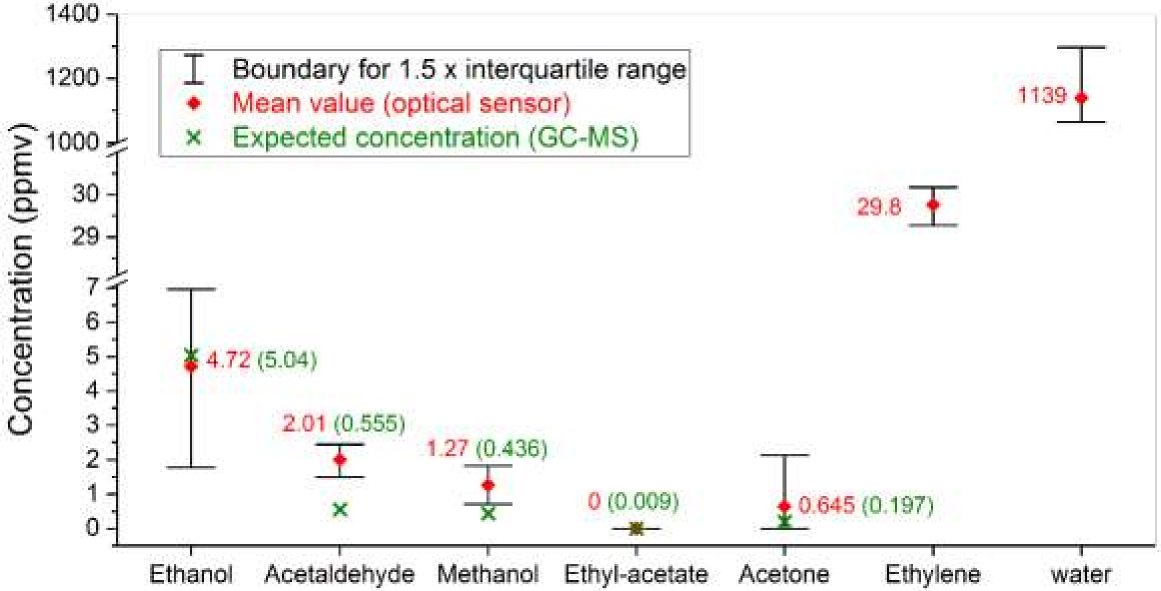
Radboud University

21-Jan-2019

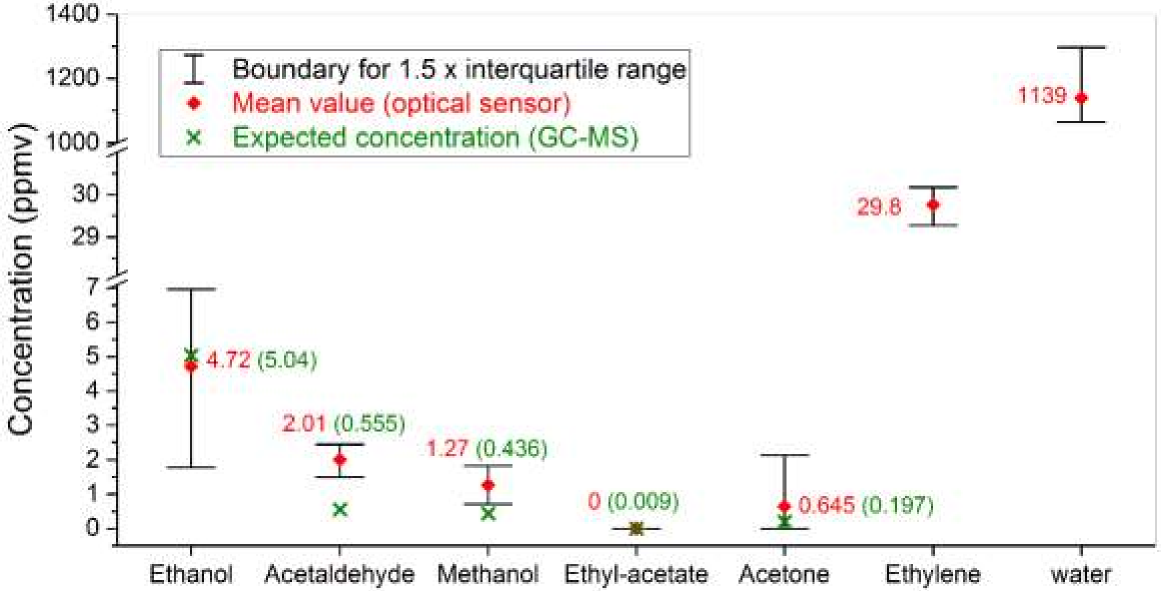
210 km

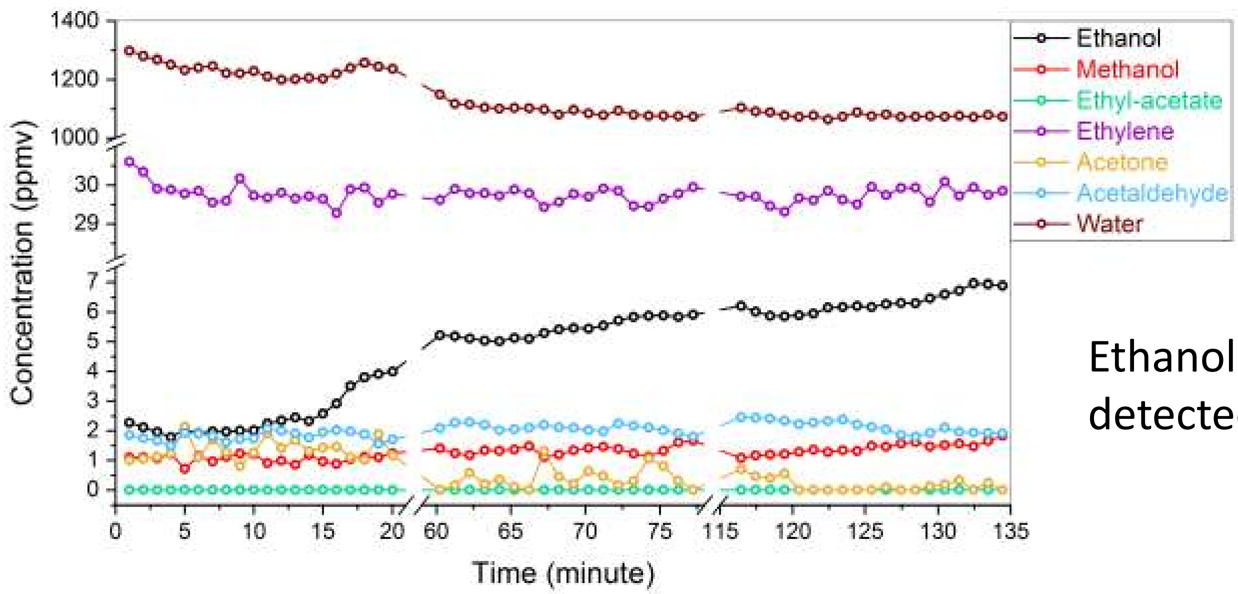
KATHOLIEKE UNIVERSITEIT LEUVEN

Optical sensor vs. GC-MS



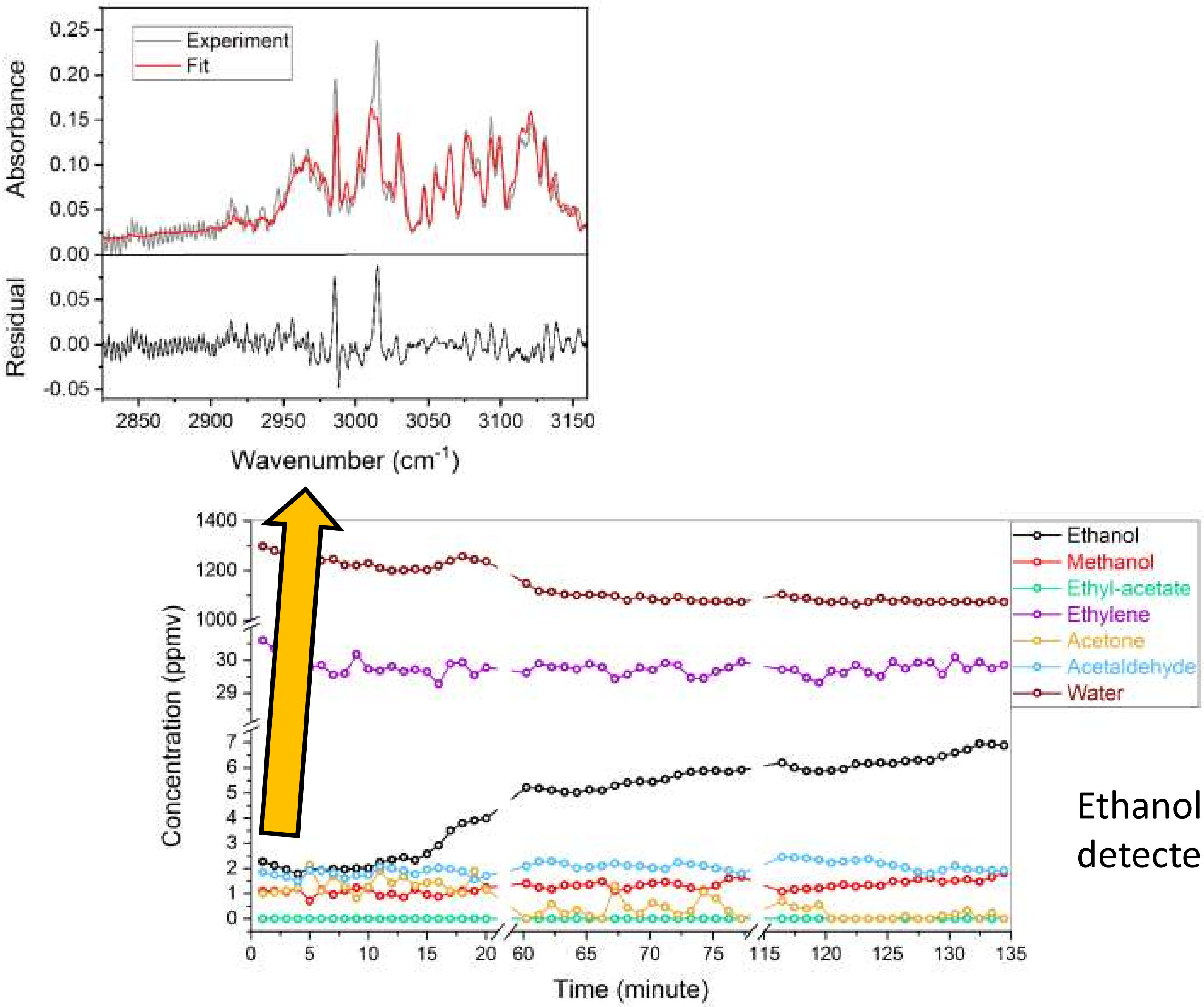
Optical sensor vs. GC-MS





Ethanol emission detected !

Optical sensor vs. GC-MS



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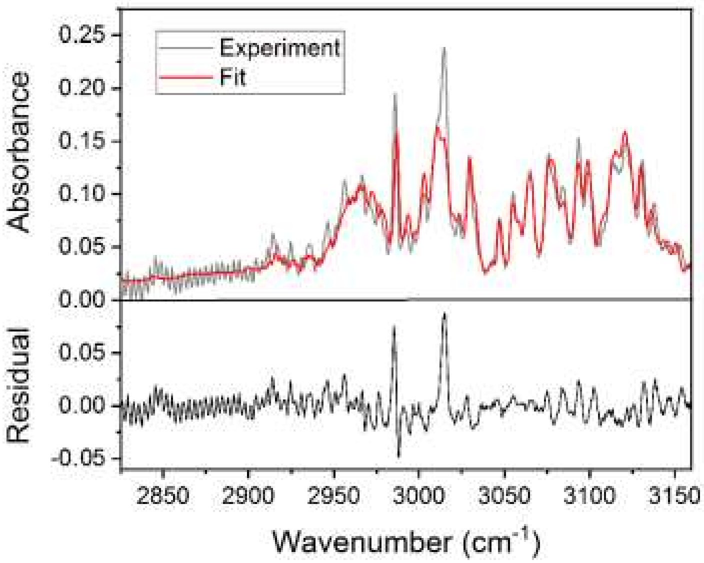
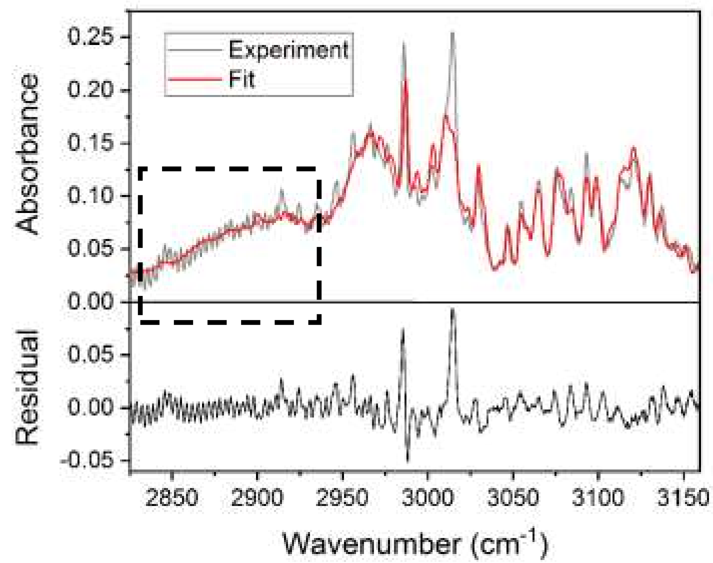
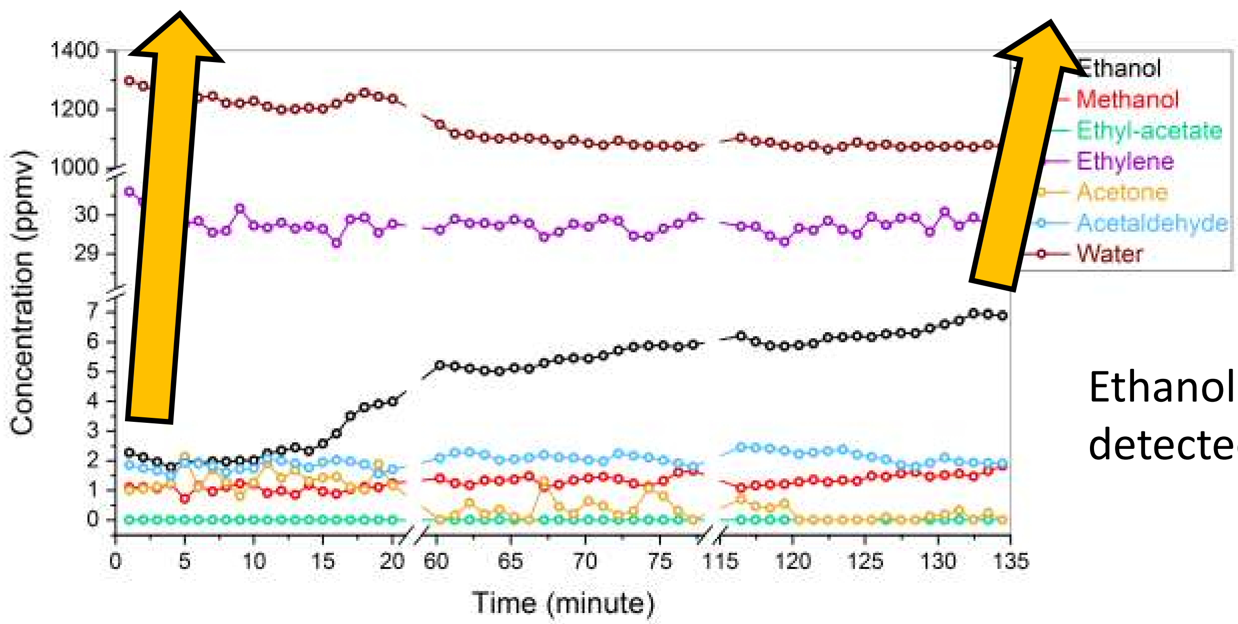






Ethanol emission detected !

More recent field tests

QCAP-2

Installed for blueberries & apples

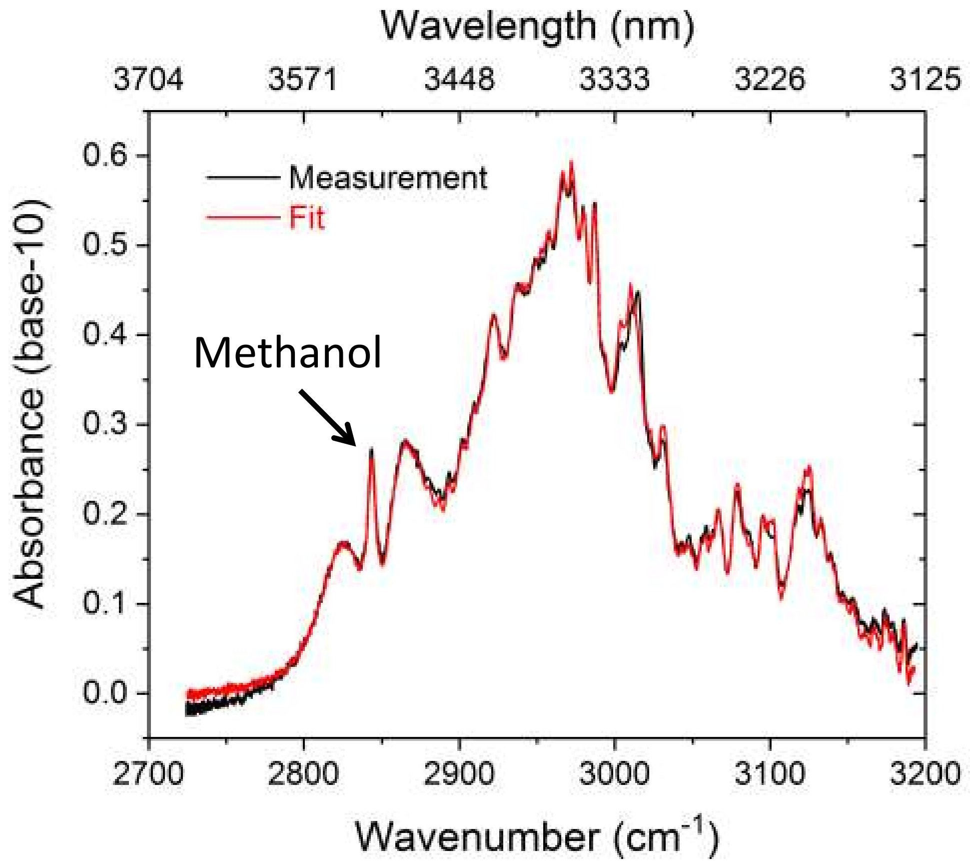
Radboud University

10-July-2019

420 km

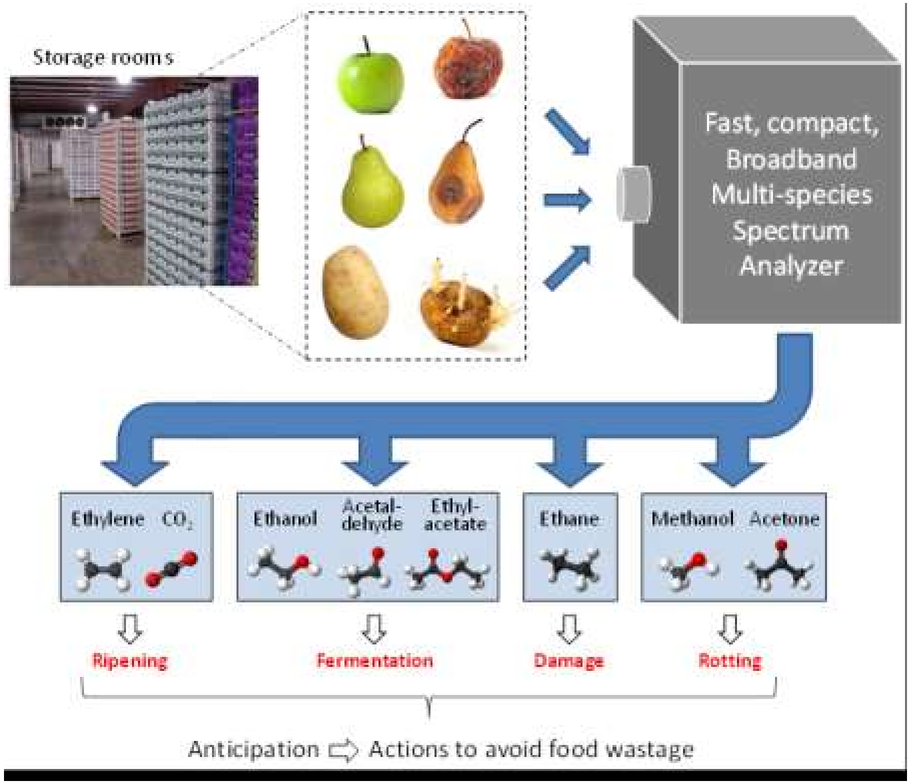
ESTEBURG
OBSTBAUZENTRUM JORK

First measurement of apples (Elstar)



Methanol detected → signature of rotting apples (stored for 1 year)

Summary



- ❖ Supercontinuum light source
  → **broadband** spectroscopy
- ❖ Multipass cell + balanced detection
  → **sub-ppm** sensitivity
- ❖ Global curve fitting
  → **multi-species** detection
- ❖ Automatic operation
  → **continuous** monitoring

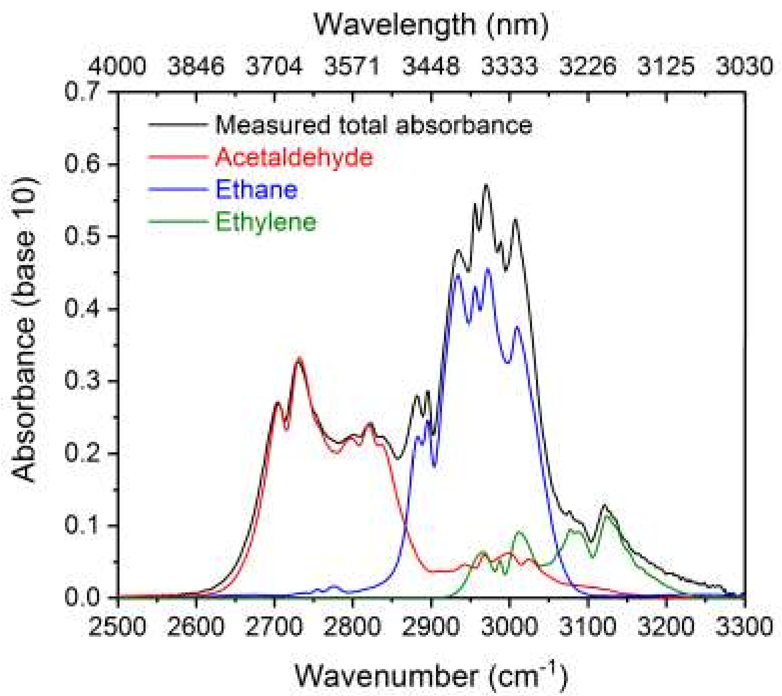
- More information:
  http://www.nweurope.eu/qcap
- Recently published paper:
  Khalil Eslami Jahromi, et al., *Sensors*, **2019**, *19*(10), 2334.

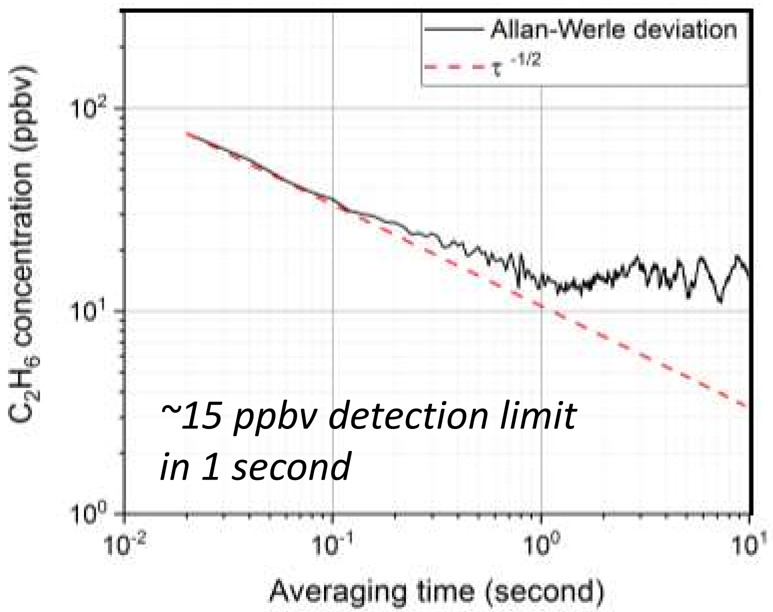
Upconversion: going beyond the horizon

Measuring the mid-IR features in the near-IR

Advantages:

- ❖ Enhanced robustness: no mechanical movement
- ❖ Enhanced photodetector sensitivity: 60% – 80% QE
- ❖ Enhanced detection speed: single-point detector → Si CCD array





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More information @ poster:

"Broadband Multi-species Trace Gas Detection by Upconverting Mid-Infrared Supercontinuum Light into the Near-Infrared"

Recently published paper:

Khalil Eslami Jahromi, et al., *Optics Express*, **2019**, 27, 24469-24480.

Acknowledgements

Life Science Trace Gas Research Group

Frans J. M. Harren

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Interreg North-West Europe QCAP

EUROPEAN UNION

European Regional Development Fund

Project partners:

NKT Photonics the power of light

STOREX CONTROLLED ATMOSPHERE

ESTEBURG OBSTBAUZENTRUM JORK

Censor Sense

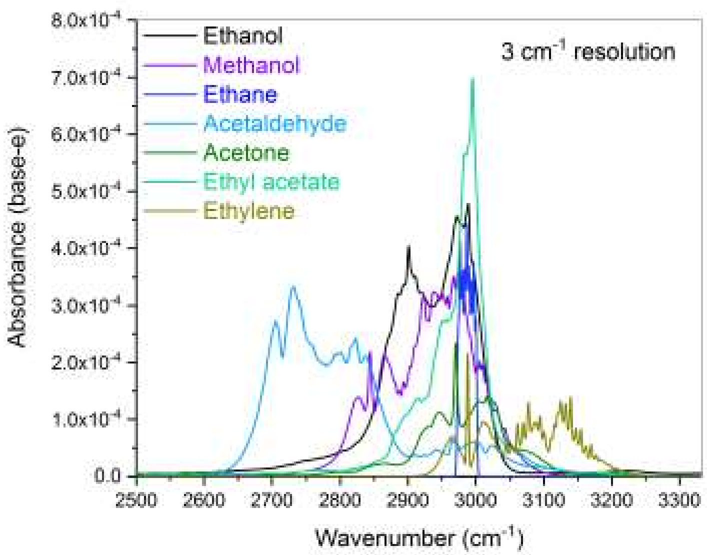
cbT

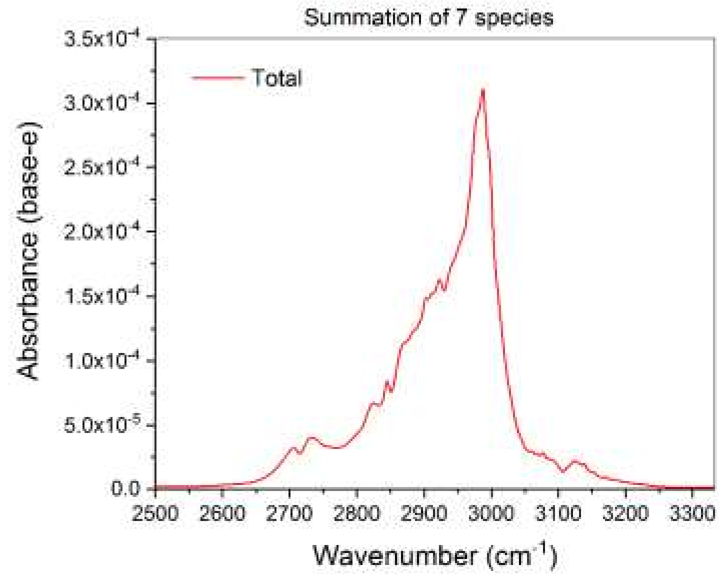
Cranfield Environment and Agrifood

Thank you

Multi-species detection

→ Non-negative least square curve fitting





$$
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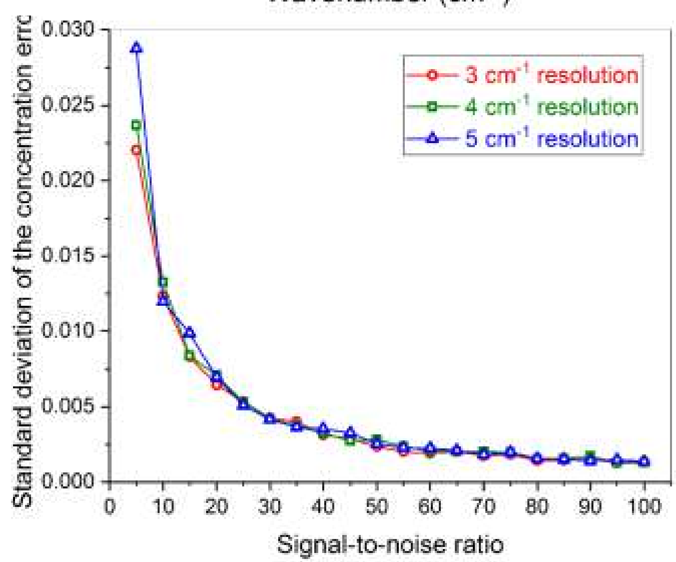
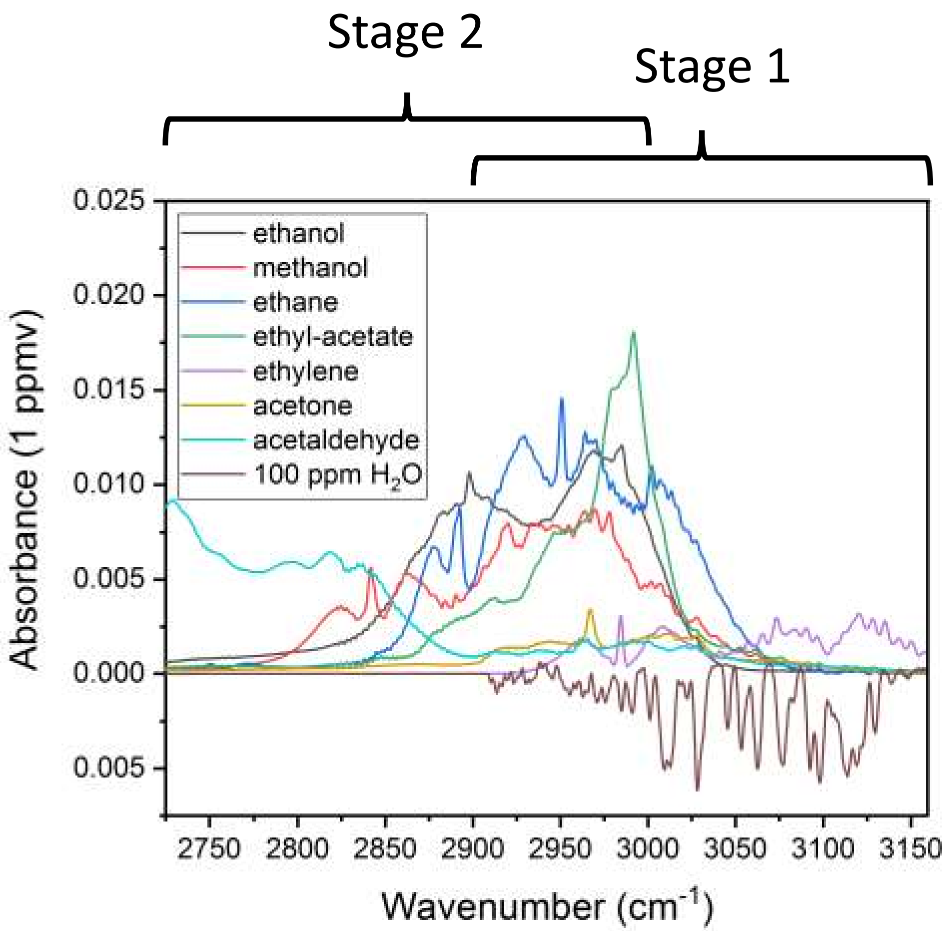
$$

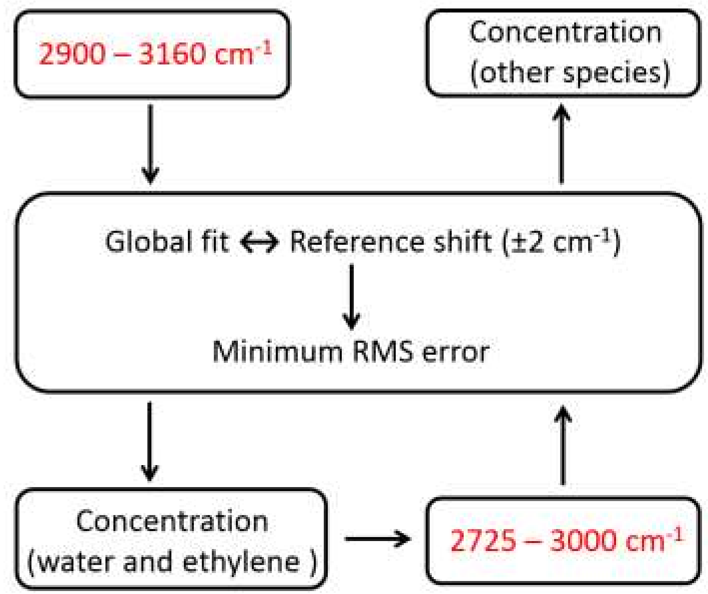
$$
\mathbf{D}_{n \times 1} = \mathbf{R}_{n \times K}\, \mathbf{C}_{K \times 1} + \mathbf{E}_{n \times 1}
$$



In practice, two-stage curve fitting



Fitting algorithm



Evaluation with a calibrated gas mixture

Dominating

Gas mixture composition

Compound name	Calibrated concentration (ppmv)	Diluted concentration (expected, ppmv)
Ethylene	5000 ± 25	~19.5
Ethanol	100 ± 0.5	~0.39
Acetaldehyde	100 ± 5	~0.39
Methanol	100 ± 1	~0.39
Ethyl-acetate	100 ± 1	~0.39
Acetone	100 ± 0.5	~0.39
1-propanol	100 ± 1	~0.39
2-butanone	100 ± 5	~0.39
Propylene	100 ± 1	~0.39
Propionaldehyde	100 ± 5	~0.39

Not included in the reference database

Evaluation with a calibrated gas mixture