Evaluation of acetone absorption bands for breath analysis in the UV and IR region with optical sensors

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Introduction

Being a young and highly promising research field, **breath analysis** is still facing severe obstacles regarding daily application in clinics and doctor's offices. One of them is a missing technical approach allowing cost efficient and small reliable sensor systems, which furthermore enable real time analysis of one or multiple breath constitutents of interest, so called biomarkers.

One approach to fullfil these requirements are optical sensor technologies. However, prior to the development of optical sensors for gas analysis, applicable absorption lines of the target analyte have to be determined. Especially the gas matrix of human breath exhale is rather complex and hence, needs detailed examination regarding potential cross sensitivites and interference suppresion techniques.

This poster deals with optical interference analysis and simulation for **acetone** detection. Furthermore, exogenous substances, present in ambient air in clinics have been considered, too.

High abundant breath constituents

Human breath exhale is a complex measurement matrix consisting of a variety of gaseous molecules. The following molecules have been identified by literature research since they were mentioned frequently [1-5] and have an abundance above 50ppbV. If applications in clinical environment are planned, exogenous substances, emmited from cleaning agents and disinfectants, have to be considered, too.

Molecule	Concentration [ppmV]	Altered concentration in disease state [ppmV]	Literature
Nitrogen	780,000	-	[1],
	744,000	-	[6] pp. V/101
Oxygen	160,000	-	[1], [7],
	136,000 – 160,000	-	[6]
Water	50,000	-	[1],
	50,000 – 63,000	-	[6]
Carbondioxide	50,000	-	[1],
	45,000	-	[7], (p. 943)
	40,000 – 53,000	-	[6] (Wikip)
Argon	10,000	-	[1], [6]
Carbonmonoxide	0.4 – 0.8	-	[8],
	1.14 – 1.37	13.6 – 19.3 (recent exposure to CO, smoking)	[9]
Methane	3 – 8	Rise of 10 ppmV to baseline (SIBO)	[8], [10]
Hydrogen	ppmV range	Rise of 20 ppmV to baseline (SIBO)	[3], [10]
Ammonia	0.425 – 1.800	Up to 14.7 ppmV unhealthy (end-stage renal failure)	[11],
	0.050 – 0.150	-	[8],
	0.628	-	[12]
Dinitrogenmonoxide	0.080 ± 0.017 (male) 0.177 ± 0.055 (female)	0.246 ± 0.087 ppmV (elevated NO_2- in gastric juice, linked to gastric cancer risk)	[13]
Isoprene	0.118 ± 0.068	< 0.014 ppbV as cut-off value for fibrosis	[14], [15],
	0.037	-	[12],
	0.022 – 0.234	-	[16]
Methanol	0.461	Change due to food intake	[17], [18],
	0.261	-	[12],
	0.238	-	[19]
Ethanol	0.196 ± 0.244	Change due to food intake	[20], [21],
	0.187	-	[12],
	0.027 – 0.153	-	[16]
Carbonylsulfid	0.096 ± 0.193	0.637 ± 0.377 ppmV (after lung transplant rejection)	[22], [23]
Acetone	0.3 – 0.9	128 ± 23.6 ppmV (children on ketogenic diet)	[16], [24]
	0.297	-	[12],
	0.144 – 0.732	-	[19],
	0.392 ± 0.085	-	[25],
	0.120 – 0.728	-	[26],
	0.177 – 3.490	-	[26],
	0.280 – 1.269	-	[26]

Table 1: Main components of breath for healthy humans and in diseased state. SIBO = Small Intestinal Bacterial Overgrowth. Literature sources attached to poster.

Substance	Expected max. concentration range [ppmV]
Ethanol	2.5 (99.22 nmol/L)
1-propanol	1.7 (65.78 nmol/L)
Isopropyl alcohol	5.4 (212.69 nmol/L)
Formaldehyde	0.6 (max. long term exposition limit in Germany)

Table 2: Expected maximum breath concentrations of disinfectants and cleaning agents in ambient air of clinics. Literature sources attached to poster [27-30].

Aceton spectra

Aceton has four major peaks in the infra-red region between 1-10µm and one broad absorption band around 278nm due to a forbidden n→p* transission.

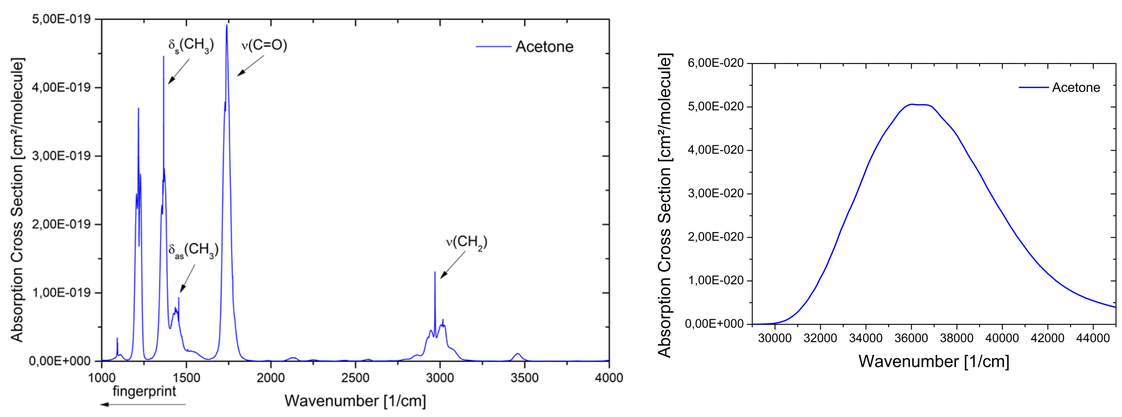


Figure 1: (left) FT-IR acetone spectrum from PNNL database and (right) carbonyl absorption band of acetone in the UV region [31].

Optical interference analysis

Measured FT-IR data from the PNNL database, HITRAN data and the Spectral Atlas of the MPI Mainz were consulted to receive the raw data of spectra from acetone and other constitutents in the IR and UV region. A selfwritten LabVIEW tool was used to simulate and analyse different mixtures to obtain promising wavelength regions for optical acetone detection.
Since water was identified to have a high interference potential in the **IR region** due to its concentration around 5%V the baseline of the FT-IR water measurements were compared to simulated HITRAN data. The left part of figure 2 indicates that most of the baseline is actually smooth and less fluctuating, especially around 1200 cm^{-1}.

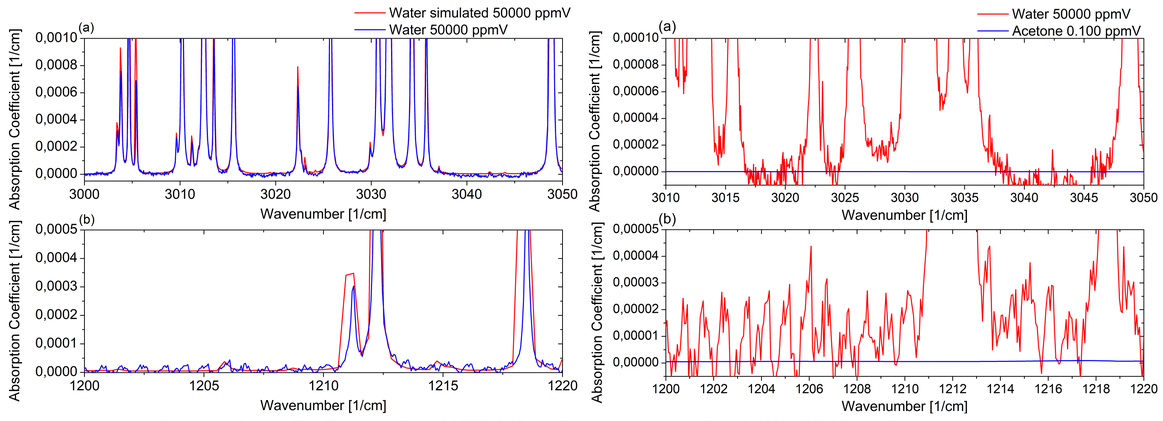


Figure 2: (left) Simulated HITRAN data compared to PNNL FT-IR data and (right) simulation of 50,000ppmV water with 0.1ppmV acetone.

Besides water and a few endogenous substances especially the exogenous substances are interfering strongly in the IR region. For a better visualization acetone was also simulated at 1ppmV and 0.5ppmV.

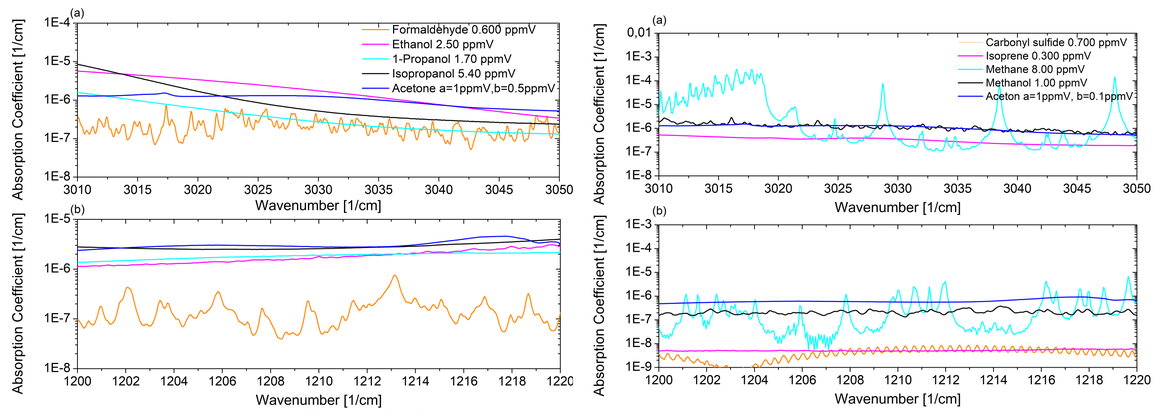


Figure 3: Simulation of worst case concentrations of (left) exogenous and (right) endogenous breath constituents.

The **UV region** looks much less crowded. Only molecules with a carbonyl group like aldehydes or ketones absorb around 278nm, thus only formaldehyde has an absorption profile in this region.

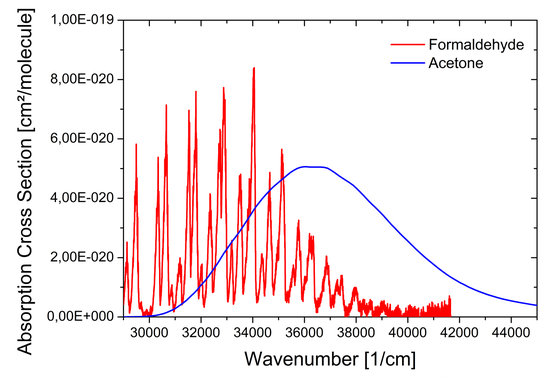


Figure 4: Absorption cross section of acetone and formaldehyde around 278nm.

Results:

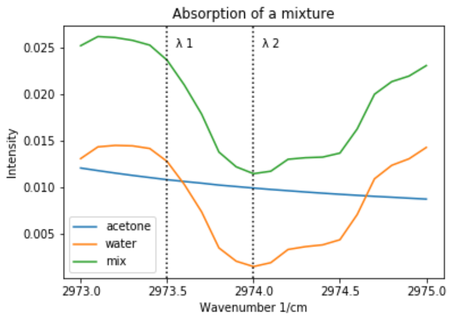
1. The most promising regions in the IR are **3023.75 – 3024.5cm^{-1}** and **3040 – 3042cm^{-1}** as well as **1204.5 – 1208cm^{-1}**
2. The exogenous substances have the strongest interference potential
3. Less interference at 1200cm^{-1}
4. Data treatments like linear regression are unavoidable in the IR region
5. In the UV region, only formaldehyde is expected to interfere

Conclusion

To allow sub ppm detection of acetone in human breath exhale in the IR region, cross sensitivity suppression techniques have to be applied since especially the absorption bands of the exogenous substances strongly overlap with the acetone bands.

Multiple measurements at different wavelengths combined with linear regression or similiar post processing methods might pave the way for reproducable breath acetone measurements in the IR region.

In contrast, the absorption peak in the UV region offers an elegant solution to avoid interferences and is recommended to be considered as well.



$$S = \sum S_i = \sum c_i * X_i(\lambda_j)$$

$$S(\lambda_1) = c_{Ac}X_{Ac}(\lambda_1) + c_{H2O}X_{H2O}(\lambda_1)$$
$$S(\lambda_2) = c_{Ac}X_{Ac}(\lambda_2) + c_{H2O}X_{H2O}(\lambda_2)$$

Figure 5: Concept of a linear regression method to compensate cross sensitivites.

References

The list of the references can be found in the attached folder!

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