H2020

REQUIREMENTS FOR FLAIR SENSOR SYSTEM

FLAIR - FLying ultrA-broadband single-shot InfraRed Sensor
GA732968

Deliverable Information	
Deliverable Number: 2.1	**Work Package:** 2
Date of Issue: 29/03/2018	
Document Reference: 732968-FLAIR-D2.1-Requirements for FLAIR Sensor System	
Version Number: 2.0	
Nature of Deliverable: R	**Dissemination Level of Deliverable:** PU
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Keywords: UAV; IR sensor; air pollution; natural disasters	

Abstract:
Deliverable 2.1 contains the information regarding the requirements for sensors to be used in the FLAIR project. These requirements were elaborated by the members of the consortium during Task 2.1. This report contains a description of the main functionalities of the sensor system, and the target molecular species and concentrations.

Document History

Date	Version	Remarks
02/02/2017	0.1	Skeleton
27/02/2017	1.0	Elaboration of the deliverable text
06/03/2017	1.1	Final version
29/03/2018	2.0	Final revised version (as requested by PO and experts)

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Executive Summary

Deliverable 2.1 contains the information regarding the requirements for sensors to be used in the FLAIR project. These requirements were elaborated by the members of the consortium during Task 2.1. This report contains a description of the main functionalities of the sensor system, and the target molecular species and concentrations.

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List of Acronyms

Acronym	Meaning
IR	Infrared
MDC	Minimum Detectable Concentration
TRL	Technology Readiness Level
UAV	Unmanned Aerial Vehicle
WP	Work Package

Table 1 – List of acronyms.

1 Introduction

In task 2.1, the system requirements for the FLAIR sensor system are defined with respect to the main objectives of the project, which are summarized below for convenience (sub-objectives can be found in the project description in the Grant Agreement):
O1: Sensor prototype development for cost effective, compact, highly sensitive and selective ul-tra-broadband real-time molecular trace gas detection of several species simultaneously in a complex mixture from their infrared (IR) absorption fingerprints. Target TRL: 4
O2: FLAIR sensor mounted on a UAV for pervasive (large area covering) sensing. Target TRL: 4
O3: Airborne detection of relevant molecular gases and fine particles emitted into the atmosphere by human activities as well as natural processes by flying the sensor mounted on the modified UAV along well-defined trajectories. Target TRL: 5

The system requirements for the FLAIR sensor shall serve as a guideline and benchmark for the entire sensor development process. These requirements include:
a) A definition of the main functionalities of the sensor system with respect to the objectives above. This set of functionalities mainly focuses on the spectrometer system and its interfaces with the UAV system. Technical specifications related to the UAV system will be covered in another deliverable document (D2.2).
b) The identification of target gases, which are relevant for atmospheric processes, health effects and global climate, and that are released into the atmosphere by natural events (i.e. volcano eruptions, wildfires, animals, unexplored hydrocarbon reservoirs, etc.) or by human activities (transport exhausts, industrial and residential emissions, etc.). Furthermore, this list lays the ground for the demonstrations foreseen in WP6. More specifically, WP6 includes two applications: (i) the measurement of carbon dioxide (CO2) and methane (CH4) which are evaluated during UAV flights on well- defined horizontal and vertical routes at the Beromünster tall tower, and (ii) the observation of gaseous and particulate species near Härkingen, a rural site next to a major motorway in central Switzerland.

2 Procedure

This report was established by the participants listed in the table above, as foreseen in the project description under the lead of EMPA. More specifically, the following steps were taken:

- establishment of a first structure and draft (19.12.2016)
- feedback by all participants (17.01.2017)
- teleconference with the participation of RU, EMPA, SA, NIT, CSEM (23.01.2017)
- second draft (27.01.2017) and feedback by all participants (10.02.2017)
- final report (submitted 24.03.2017)
- final revised report including recommendations from first review meeting (29.03.2018)

3 Main functionalities of the sensor system

The sensor system that will be developed in O1 is meant to cover the spectral windows 2-5 µm and 8-12 µm. Covering both spectral windows simultaneously within the same instrument constitutes a serious technical challenge. Therefore, the strategy adopted by the consortium for fulfilling objectives O1-O3 is to develop two distinct instruments with different TRLs for both spectral windows:

i) A first instrument covering the 2-5 µm window will be developed and tested onboard an UAV up to TRL 5, according to objective O3 and corresponding demonstrations foreseen in WP6.
ii) A second instrument covering the 8-12 µm window will be developed and tested only in a laboratory environment with a target TRL 3-4. The main technical challenge for this system lies in the development of a NIR supercontinuum source operating in this wavelength range, which will constitute a major advancement in the field.
A more technical description of these functionalities will be provided at the end of WP2 within the deliverable document D2.3.
In the following paragraphs, if not specified, we will refer to the first instrument i).

3.1 Sensing functionalities

- Real time, simultaneous detection of gases at concentrations specified in section 4.
- The applied sensing technique is highly selective and the response to interfering gases such as water is negligible.
- Better resolution can be achieved at lower pressure. Studies for designing a pumping system targeting 50-100 mbar will be performed in WP3 and WP4.
- The ideal and targeted sensor sampling rate is 10 Hz, however, a sampling rate of 1 Hz is sufficient for most applications.
- The spatial resolution of the airborne measurements is limited by the residence time of the air sample in the sensor system rather than by the sampling rate of the sensor. For a typical cruise speed of the UAV (80km/h) and a realistic residence time of 2 seconds, a spatial resolution of 50 meter can be achieved.
- Additional and complementary measurements of atmospheric fine particles are measured using diffusion charging and electrical detection as well as light absorption technologies that are commercially available.

3.2 Electronic and mechanical interfaces

- Such interfaces will strongly depend on the type of UAV that will be used (most probably AR3 NetRay). Specifications and guidelines will be provided in deliverable document D2.2.
- The spectrometer will be designed using professional software, Zemax and Solidworks, in order to provide a technical drawing for a compact and robust system prototype that will fit the available payload volume of the UAV, together with the fine particle detector.
- Ideally, the data generated by the sensor shall be transferred to the ground with a dedicated datalink, otherwise it will be stored and retrieved once the UAV has landed. These different possible scenarios will be studied and described in D2.3.

4 Target species and concentrations

The expected detection sensitivity in terms of the minimum detectable concentration (MDC) of the ultra-broadband IR sensor developed within FLAIR was calculated for a wide range of gases. This was done for an absorption wavelength range between 2-5 micrometer assuming a minimum detectable absorption of $\Delta P/P=10e-4$ and an absorption length of 20 meters at a gas pressure of 1 bar. The details of the calculation and the obtained MDCs are provided in the Annex.
The table below lists the potential target gases. It evaluates their importance in various application fields. Furthermore, it contains the typical range of atmospheric concentrations

and our judgement about their relevance for atmospheric observations in general as well as for the demonstration applications in WP6.

For any meaningful application, the FLAIR sensor system must be sufficiently sensitive for detecting the target gas of interest. Therefore, the table below contains a column stating the expected feasibility of the FLAIR sensor for detection of the target gases at typical atmospheric concentrations based on the above mentioned sensitivity calculations.

Table 2 - Target species and concentrations

Domain/Sources	Gas	Mixing Ratio	Relevance[1] (+/o/-)	Usefulness of Mobile Measurement[1] (+/o/-)	Relevance for WP6	Comments
Air Quality	NO_2	0.1-100 ppbv[2]	+	+	✓	MDC 11 ppbv[3]
	NO	0.1-100 ppbv	o	+	✓	MDC 172 ppbv[3]
	CO	0.1-10 ppmv[2]	o	+	✓	MDC 1 ppbv[3]
	NH_3	0.1-100 ppbv[4]	+	+	✓	MDC 14 ppbv[3]
	SO_2	0.1-50 ppbv[2]	-	o	-	MDC 88 ppbv[3]
	O_3	1-100 ppbv[2]	+	+	✓	MDC 2 ppbv[3]
	C_6H_6	0.1-10 ppbv[2]	+	o	✓	MDC 9 ppbv[3]
	BaP	0.1-10 ppbv[2]	+	o	✓	unknown
Climate	CO_2	400-2000 ppmv[5]	+	+	✓	MDC 0.1 ppbv[3], explicitly stated in GA, WP6
	CH_4	2-20 ppmv[5]	+	+	✓	MDC 1 ppbv[3], explicitly stated in GA, WP6
	N_2O	0.3-1 ppmv[5]	+	+	✓	MDC 135 ppbv[3], small atmospheric variation
	SF_6	0.1-10 pptv[5]	+	-	✓	
Ship Emissions	SO_2	unknown	+	+	✓	MDC 88 ppbv[3]
	CO_2	> 10000 ppmv	+	+	✓	MDC 0.1 ppbv[3]
Volcanic Eruptions	SO_2	unknown	+	+	✓	MDC 88 ppbv[3]
Wildfires/Biomass Burning	CO	≈ 1-100 ppmv	o	+	✓	Emission ratio 66.4 mmol/mol CO_2 [6]; MDC 1 ppbv[3]
	C_2H_3N	0.01-100 ppbv[7]	o	+	✓	Emission ratio 0.0082 mmol/mol CO_2 [6]; MDC 31 ppbv[3]
Agricultural Emissions	NH_3	1-500 ppbv	+	+	✓	Expected mixing ratio over managed agricultural land; background 1-10 ppbv; MDC 14 ppbv[3]

(1) based on expert judgment

(2) EEA (2016) Air quality in Europe — 2016 report, European Environmental Agency, doi:10.2800/413142

(3) MDC: Minimum detectable concentration, see Annex

(4) Fagerli, H. and W. Aas (2008). Trends of nitrogen in air and precipitation: Model results and observations at EMEP sites in Europe, 1980-2003. Environmental Pollution 154(3): 448-461

(5) IPCC (2013). Climate Change 2013: The Physical Science Basis. Contribution of Working Group I to the Fifth Assessment Report of the Intergovernmental Panel on Climate Change (eds Stocker, T. F. et al.). Cambridge Univ. Press, New York, USA

(6) Christian, T. J., B. Kleiss, R. J. Yokelson, R. Holzinger, P. J. Crutzen, W. M. Hao, B. H. Saharjo and D. E. Ward (2003). Comprehensive laboratory measurements of biomass-burning emissions: 1. Emissions from Indonesian, African, and other fuels. Journal of Geophysical Research-Atmospheres 108(D23)

(7) Muller, M., B. E. Anderson, A. J. Beyersdorf, J. H. Crawford, G. S. Diskin, P. Eichler, A. Fried, F. N. Keutsch, T. Mikoviny, K. L. Thornhill, J. G. Walega, A. J. Weinheimer, M. Yang, R. J. Yokelson and A. Wisthaler (2016). In situ measurements and modeling of reactive trace gases in a small biomass burning plume. Atmospheric Chemistry and Physics 16(6): 3813-3824

5 Summary and conclusions

A high level description of the main functionalities of the system is given. This will serve as a guideline and benchmark for the entire sensor development process. A more detailed description of the sensor system with its subsystems and different interfaces will be provided in deliverable document D 2.3.

Based on the analysis of the expected sensitivity of the FLAIR sensor system and the relevance of the identified feasible gases for atmospheric observation, it is suggested that the flight tests within WP6 will focus on CO_2, CH_4, CO and O_3. A more detailed evaluation of the performance with respect to expected observations will be provided in D 2.4.

Owing to their spectral signature and atmospheric relevance, N_2O and SO_2 have been identified as additional potential target gases for sensor characterization, optimization and validation. Furthermore, NH_3 and HCl may be investigated in dedicated laboratory tests because they have strong spectral characteristics and are relevant in many environmental and industrial processes.

6 Annex

Calculation of the minimum detectable concentration

The transmission/absorption of monochromatic light in a gas atmosphere is expressed by the Beer-Lambert law as:

$$I = I_0 e^{-\alpha(\nu)}, \qquad \alpha(\nu) = \sigma \cdot n \cdot L = S \cdot g(\nu, \nu_0) \cdot n \cdot L$$

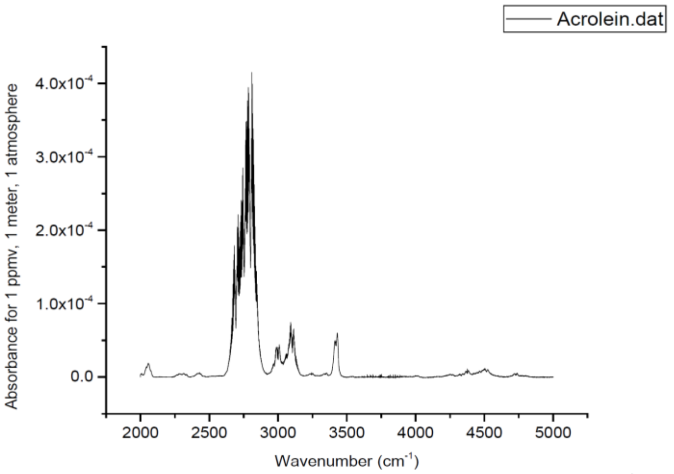
I: intensity after transmission
I_0: initial light intensity
$\alpha(\nu)$: absorbance
σ: absorption cross section of a photon
n: density of the molecules (molecules per unit volume)
L: optical path length
S: line strength connecting ground and excited states
$g(\nu, \nu_0)$: normalized line shape function (Gaussian, Lorentzian)
υ: laser frequency
ν_0: frequency line center molecule

If $\alpha \ll 1$, then according to this approximation: $e^x \approx 1 + x$, we can obtain:

$$I = I_0(1 - \alpha) \Rightarrow I_0 - I = I_0\alpha \Rightarrow \Delta I = I_0\alpha$$

From the noise level of the instrument: $\alpha_{min} = \dfrac{\Delta I_{min}}{I_0}$

A typical α_{min} will be: 10^{-4} . The minimum detectable absorption is: MDA = $\alpha_{min}/\sqrt{B}$ with a detection bandwidth B of 1 Hz: MDA=10^{-4}. Using the HITRAN and PNNL database we can calculate the absorbance α. If we define a Signal-to-Noise-Ratio (SNR) we can calculate the minimum detectable concentration (MDC).



Example: Using the PNNL, for acrolein the maximum absorption peak with 1 ppmv mixing ratio and 1 m path length at 1 atmosphere pressure is (see Figure): $\alpha_{max} = 4 \times 10^{-4}$.

For a 20 m path length: $\alpha_{max} = 80 \times 10^{-4}$. Using •, the minimum detectable concentration with a SNR =1 becomes:

$$\text{MDC} = \frac{\text{SNR} \times 1\ \text{ppmv}}{\alpha_{max}/\text{MDA}} \Rightarrow \text{MDC} = \frac{1 \times 1\ \text{ppmv}}{80 \times 10^{-4} / 1 \times 10^{-4}} = 12.5\ \text{ppbv}$$

* [LEL]: lower explosive limit

The color code of the column indicating the Minimum detectable concentration spans the range from low (green) to high MDC (red).

Name of Gas	Wavenumber Maximum Absorption (cm-1)	Wavelength Maximum Absorption (micrometer)	Minimum detectable concentration (ppbv) MDA=1E-4; l= 20 m, p= 1 bar, SNR=1	Data Source	Immediately Dangerous to Life or Health Concentrations (IDLH)
1_1_2_2-Tetrachloroethane	2966	3,37	30,49	PNNL	100
1_1_2-Trichloroethane	2974	3,36	24,27	PNNL	100
1_1-Dichloroethane	2996	3,34	5,75	PNNL	3000
1_1-Dimethylhydrazine	2775	3,60	3,42	PNNL	15
1_3-Butadiene	3089	3,24	18,32	PNNL	2000 ppmv [LEL]*
1-Nitropropane	2988	3,35	7,14	PNNL	1000
2-Butoxyethanol	2970	3,37	0,02	PNNL	700
2-Ethoxyethyl acetate	2875	3,48	4,42	PNNL	500
2-Hexanone	2969	3,37	3,82	PNNL	1600
2-Nitropropane	2966	3,37	8,70	PNNL	100
Acetaldehyde	2740	3,65	12,20	PNNL	2000
Acetic acid	3582	2,79	4,55	PNNL	50
Acetic anhydride	3033	3,30	51,55	PNNL	200
Acetone	2970	3,37	14,71	PNNL	2,500 ppmv [LEL]
Acetonitrile	3017	3,31	31,25	PNNL	500
Acrolien	2809	3,56	12,50	PNNL	2
Acrylonitrile	3043	3,29	151,52	PNNL	85
Allyl alcohol	2878	3,47	17,24	PNNL	20
Allyl chloride	3003	3,33	35,71	PNNL	250
Ammonia	3335	3,00	14,49	HITRAN	300
Ammonia anhydrous	3335	3,00	15,87	PNNL	300
Aniline	3048	3,28	8,33	PNNL	100
Arsine	2127	4,70	0,65	PNNL	3
Benzene	3047	3,28	8,93	PNNL	500
Benzyl chloride	3045	3,28	12,82	PNNL	10
Boron trifluoride	2338	4,28	33,33	PNNL	25
Butyl acetate	2973	3,36	2,50	PNNL	n-Butyl acetate: 1,700 ppmv [LEL]
Carbon dioxide	2363	4,23	0,12	HITRAN	40000
Carbon dioxide	2363	4,23	0,14	PNNL	40000
Carbon disulfide	2179	4,59	15,63	PNNL	500
Carbon monoxide	2173	4,60	0,75	HITRAN	1200
Carbon monoxide	2173	4,60	0,96	PNNL	1200
Chlorobenzene	3081	3,25	10,20	PNNL	1000
Chloropicrin	2925	3,42	70,42	PNNL	2
Cumene	2973	3,36	2,50	PNNL	900 ppmv [LEL]
Cyclohexanone	2945	3,40	1,67	PNNL	700

Cyclooctane	2930	3,41	0,96	PNNL	2000
Diacetone alcohol	2983	3,35	3,33	PNNL	1,800 ppmv [LEL]
Diborane	2519	3,97	1,79	PNNL	15
Dichlorofluoromethane (Freon-21)	3024	3,31	11,76	PNNL	15000
Diethylamine	2969	3,37	3,57	PNNL	200
Difluorodibromomethane (Freon-12B2)	2232	4,48	38,46	PNNL	2000
Diisopropylamin	2971	3,37	1,61	PNNL	200
Dimethyl sulfate	2968	3,37	6,41	PNNL	7
Dimethylamine	2792	3,58	5,15	PNNL	500
Dipropylene glycol methyl ether	2989	3,35	2,91	PNNL	600
Ethyl acetate	2995	3,34	5,99	PNNL	2,000 ppmv [LEL]
Ethyl acrylate	2995	3,34	5,81	PNNL	300
Ethyl alcohol (Ethanol)	2989	3,35	7,09	PNNL	3,300 ppmv [LEL]
Ethyl benzene	2975	3,36	4,35	PNNL	800 ppmv [LEL]
Ethyl bromide (Halon-2001)	3022	3,31	9,84	PNNL	2000
Ethyl formate	2998	3,34	5,92	PNNL	1500
Ethyl mercaptan	2988	3,35	5,88	PNNL	500
Ethylamine	2968	3,37	5,10	PNNL	600
Ethylene oxide	3066	3,26	0,59	PNNL	800
Formaldehyde (Methanal)	2779	3,60	2,17	HITRAN	20
Formaldehyde monomer	2778	3,60	1,92	PNNL	20
Formic acid (and some dimer)	2778	3,60	1,95	PNNL	30
Hydrogen bromide	2636	3,79	5,68	HITRAN	30
Hydrogen chloride	2963	3,37	0,70	HITRAN	50
Hydrogen chloride anhydrous	2963	3,37	0,95	PNNL	50
Hydrogen cyanide	3337	3,00	1,61	HITRAN	50
Hydrogen cyanide (prussic acid)	3340	2,99	2,24	PNNL	50
Hydrogen fluoride	4076	2,45	0,17	HITRAN	30
Hydrogen fluoride anhydrous	4076	2,45	0,27	PNNL	30
Hydrogen sulfide	3746	2,67	128,21	HITRAN	100
Hydrogen sulfide	3746	2,67	222,22	PNNL	100
Isoamyl alcohol	2965	3,37	2,43	PNNL	500
Isobutyl acetate	2976	3,36	2,94	PNNL	1,300 ppmv [LEL]
Isophorone	2965	3,37	2,53	PNNL	200
Isopropyl acetate	2987	3,35	3,42	PNNL	1800
Methane	3068	3,26	0,85	HITRAN	
Methane	3086	3,24	1,04	PNNL	
Methyl acetate	2965	3,37	10,42	PNNL	3,100 ppmv [LEL]
Methyl acrylate	2964	3,37	11,42	PNNL	250
Methanol	2982	3,35	7,92	PNNL	6000
Methyl bromide	3061	3,27	12,47	PNNL	250

Methyl chloride	2966	3,37	34,72	PNNL	2000
Methyl formate	3008	3,32	9,52	PNNL	4500
Methyl iodide	2970	3,37	19,92	PNNL	100
Methyl mercaptan	2947	3,39	13,66	PNNL	150
Methyl methacrylate	2963	3,37	7,30	PNNL	1000
Methylamine	2962	3,38	10,20	PNNL	100
Morpholine	2831	3,53	2,65	PNNL	1,400 ppmv [LEL]
n-Amyl acetate	2970	3,37	2,84	PNNL	1000
Naphthalene	3068	3,26	4,39	PNNL	250
n-Butyl alcohol	2968	3,37	3,82	PNNL	1,400 ppmv [LEL]
n-Butylamine	2968	3,37	3,88	PNNL	300
n-Heptane	2935	3,41	1,88	PNNL	750
n-Hexane	2965	3,37	2,08	PNNL	1,100 ppmv [LEL]
Nickel carbonyl	2058	4,86	0,07	PNNL	2
Nicotine@50C	2979	3,36	2,81	PNNL	0.75 ppmv
Nitric acid anhydrous	3552	2,82	1,71	PNNL	25
Nitric oxide	3741	2,67	172,41	PNNL	100
Nitrobenzene	3083	3,24	15,87	PNNL	200
Nitrogen dioxide	2918	3,43	10,00	HITRAN	20
Nitrogen dioxide	2918	3,43	11,36	PNNL	20
Nitrogen trifluoride	2695	3,71	751,88	PNNL	1000
Nitromethane	2964	3,37	54,05	PNNL	750
Nitrous oxide	3742	2,67	135,14	HITRAN	100
Octane	2933	3,41	1,45	PNNL	1,000 ppmv [LEL]*
o-Toluidine	3035	3,29	10,53	PNNL	50
o-Xylene	2948	3,39	7,76	PNNL	Xylene (o, m, p isomers): 900 ppmv
Ozone	2123	4,71	2,38	HITRAN	5
Phenol	3656	2,74	4,55	PNNL	250
Phosphine	2380	4,20	1,52	HITRAN	50
Propane	2968	3,37	1,68	PNNL	2,100 ppmv [LEL]
p-Xylene	2936	3,41	6,69	PNNL	Xylene (o, m, p isomers): 900 ppmv
Pyridine	3088	3,24	12,11	PNNL	1000
sec-Amylamine	2966	3,37	2,55	PNNL	2000
sec-Butyl alcohol	2973	3,36	3,60	PNNL	1,400 ppmv [LEL]
Styrene (monomer)	3095	3,23	10,87	PNNL	700
Sulfur dioxide	2517	3,97	76,92	HITRAN	100
Sulfur dioxide	2511	3,98	87,72	PNNL	100
tert-Butyl acetate	2987	3,35	3,14	PNNL	1,500 ppmv [LEL]
Tetrachloroethylene	2494	4,01	917,43	PNNL	150
Vinyl toluene	3024	3,31	9,35	PNNL	400