SMART|AtmoSim_*Lab*

Letter of Intent for the foundation SMART|*Lab* within the project

Atmospheric Measurements and Simulations

(AtmoSim)

Executive Summary of Science Case and Organizational Structure

Science:	Fundamental and Applied Research: Measurement and simulation of atmospheric processes
Science Impact:	Understanding and forecast atmospheric processes
SMART|*Lab* Issue:	Measurement and Simulation of atmospheric processes
Technology:	Application of specific analytical techniques, as well as numerics of forward and inverse modeling to atmospheric processes
Technology Impact:	Novel methodologies and analytical techniques, as well as new methods of modelling will be applied to atmospheric processes
Partner:	Tbilisi State University (TSU) and Institute of Energy and Climate Research Troposphere (IEK-8) (Jülich) Georgia: Dr. Giorgi Jibuti (Head of the Lab), Prof. Bezhan Chankvetadze, Prof. Ramaz Botchorishvili Jülich: Prof. Andreas Wahner, Prof. Astrid Kiendler-Scharr, PD Dr. Hendrik Elbern
Project Timeline:	Start January 1, 2018 Duration 5 years, with option for additional 5 year extensions
Total Budget:	For the first 5 years 580.000 Euro (five-hundred-and-eighty thousand Euro)

Date/Place: June, 2017, Tbilisi

For
Forschungszentrum Jülich (FZJ), Germany
and Institute of Energy and Climate Research
Troposphere (IEK-8)

Sebastian M. Schmidt
Board of Management FZJ

Andreas Wahner
Director at IEK-8

For
Ministry of Education and Sciences of Georgia,
and the Ivane Javakhishvili Tbilisi State
University (TSU)

Aleksandre Jejelava
Minister of Education and Science of Georgia

George Sharvashidze
Rector at TSU

Scientific Case

1. Novelty of research, goals and objectives

1.1 Actuality of the problem and research novelty

Understanding complex atmospheric processes is a keystone for proper modeling and forecasting changes in the chemistry of the atmosphere in order to improve air quality. Clear example of this is the healing of the ozone "hole" over the Antarctic region after advancements in measuring techniques (such as development of the electron capture detector to measure chloro-fluorocarbons (CFCs)) showing a direct reverse correlation between CFC's and ozone concentration in the stratosphere. Based on this finding, the Montreal Protocol was signed about three decades ago limiting or forbidding the use of CFC's. Recent studies showed, as predicted by the models, that the ozone layer is actually healing and full recovery is expected in the middle of this century.

Air has a direct impact on the quality of life and on human health. That is the reason why it is very important to deepen the knowledge about the processes taking place in the atmosphere. This can be done by developing new methods and techniques for measurement, as well as by developing mathematical methods for the evaluation and modeling of the acquired data.

1.2 Research subject and objectives

Chemical processes in the atmosphere are very diverse and complex. The time-scales of these processes vary from milliseconds to centuries. Some of the organic contaminants are oxidized fairly quickly, but some of them stay in the atmosphere rather long and cause various harmful effects. The main source of the volatile organic compounds (VOC) contamination is biogenic in nature. Anthropogenic pollutants, such as NOx, CO, CO_2 define very often the photochemical pathways, for example, the ozone production rate. The latter is increasing inside the troposphere, especially near urban areas, due to the increase of e.g. traffic emission. Whereas stratospheric ozone shields harmful UV radiation from the sun, increasing ozone concentration in the troposphere is a direct threat to human health because of its toxicity.

The assimilation of data and the creation of suitable models of local atmospheric processes help to evaluate and forecast pollutants on a regional scale as well as on a global scale by defining boundary conditions for the proper inclusion of regional models into global ones.

It is important to note that air quality monitoring programs are just starting in Georgia. Until now, most of the analysis was performed in foreign laboratories. This is not a robust and flexible way to measure pollution dynamics and, based on that information, to create local atmospheric models. A local state-of–the-art laboratory will help to resolve this issue.

2. Research methods and expected outcomes

2.1 Concepts

Due to the complexity of atmospheric chemistry, and due to the fact, that pollutant concentrations vary between parts per million in volume (PPMv) to parts per trillion in volume (PPTv) levels, their measurement is challenging. For precise observation of different pollutants in ambient air it is necessary to use a variety of analytical techniques and methods. For the analysis of VOC's, the Gas Chromatography-Mass Spectrometric method is favorable, because this method in principle gives the most complete set of different VOC's in atmospheric samples. For the determination of the

enantiomeric composition of certain VOCs, a GC-MS method with specially designed capillary columns is required.
The commonly used way to measure the NO and NO_2 content in ambient air is the chemiluminescence method (reaction of NO with ozone).
There are several ozone detection methods available. Chemiluminescence and electrochemical methods are widely used due to their sensitivity and speed of analysis. For CO, CO_2, CH_4 and water vapor content, the cavity ringdown spectroscopic (CRDS) method is used.
Beside various gases, very important part of the atmosphere are aerosols. These are different solid or liquid particles which are present in ambient air and have a big impact on air quality. There are different techniques to measure the particle content in air, for example PM-2.5 and PM-10 (particulate matter with less than 2.5 and 10 micrometer diameters, respectively, in the air usually presented in micrograms per cubic meter). Certified filter samplers and mass balances are used to measure the particle content.
To integrate data collected from different measurement techniques into a larger context, for example the interpolation of local data onto larger regions or the prediction of future trends, it is necessary to develop numerical methods for data assimilation as well as methods for forward and reverse modelling.

2.2 Implementation and expected impact

One of the aims of the project will be measuring the concentration of air pollutants in Georgia (such as VOC's NOx, CO, CO_2 etc.). Based on this information a photochemical coordinate system (which shows estimate ozone production based on its precursors) will be used to estimate possible impacts for air quality.
The data will also be used to feed a local atmospheric pollution model for the forecasting of future trends and the assimilation of regional data into global models. The results will be published in international journals and reported on international conferences. They will also be the basis for official monitoring and legislative initiatives of the government and will help to plan actions for the avoidance of harmful air pollution.

3. Additional information about the project

3.1 Feasibility and structure of the international team

3.1.1 German group

The Institute of Energy and Climate: Troposphere (IEK-8) is a leading institution worldwide in the field of atmospheric research. In fact, the world calibration centers for ozone (WCCOS) and NOx (WCC-NOx) are hosted by the IEK-8. The institute has a large scientific infrastructure, for example the large atmospheric simulation chamber SAPHIR ("Simulation of Atmospheric Photochemistry In a large Reaction chamber"). It is also using air-based platforms like Zeppelin NT (to study the Planetary Boundary Layer), HALO (a high altitude and long range research aircraft), as well as mobile laboratories, and develop unique tools for atmospheric research. The IEK-8 is involved in many local and international atmospheric research programs, such as ESM (Earth System Modelling, HGF), EUROCHAMP 2020 (European Infrastructure for Atmospheric Simulation Chambers), urban Climate Under Change (BMBF project involving IEK-8 high resolution mobile measurements), Nano-PLOT (the use of ceramic nano-particles equipped with organic dispersions as highly efficient separation media for gas chromatography), PEGASOS (Pan-European Gas-

AeroSOls-climate interaction Study), ZEPTER (Airship measures cleansing power of atmosphere), IAGOS (In-service Aircraft for a Global Observing System and so on).
The Research Center Jülich has close scientific contacts with many of the surrounding universities in Germany (Aachen, Bochum, Bonn, Cologne, Düsseldorf, Essen, Erlangen-Nürnberg, Münster, Wuppertal) and cooperates with leading laboratories worldwide.

3.1.2 Georgian group

Full Professor Dr. Bezhan Chankvetadze, Academician of the Georgian National Academy of Sciences and head of the Chair of Physical and Analytical Chemistry of TSU, has great experience in the development and the application of miniaturized methods for chemical analysis. His major research area is separation science (chromatography, capillary electrophoresis and capillary electrochromatography), especially applied to the separation of enantiomers of chiral compounds in the liquid phase. Many of his products are patented and commercialized by US, Japanese and German companies and are used worldwide. The current collaboration with IEK-8 involves preliminary studies to the development of nano-particle based chiral columns for gas chromatography, as well as preliminary measurement of some pollutant levels in ambient air of Tbilisi
Professor Ramaz Bochorishvili has long term experience of the collaboration with IEK-8 in the field of the development of numerical methods for 4D-Var data assimilation and forward and reverse modeling of atmospheric processes.
Dr. Giorgi Jibuti has experience working in the field of instrumental methods for application to atmospheric research. He had several stays for the advancement of scientific exchange at the Jülich Research Center and is already involved in a test project for the observation of pollutants to explore the photochemical regime of ambient air in Tbilisi.

4. Description of the SMART|AtmoSim_*Lab*

4.1 General concept of SMART|*Labs*

The idea of smart (SMART: Science, Medicine, Applied Research and Technology) labs implies the establishment of relatively small, well equipped and maintained modern laboratories. Such labs are supposed to contribute to different fields of fundamental and applied science within the framework of international collaborations. The main objectives of such labs can only incorporate a few ideas at a time and they may change dynamically. The laboratory and its staff should be able to efficiently switch from one activity to another and to also contribute to neighboring directions of research and developments using its infrastructure. Therefore, smart labs need to be supplied with modern equipment and tools. These goals set additional requirements for the location where such labs will be situated, and also general technical requirements and regulations must be satisfied. Although the main purpose of the smart labs is its engagement in research projects involving a young generation of students (Bachelor, Master and PhD) inducing a large educational impact. The best sites for such laboratories will thus be near or at universities. This will facilitate interest of students and will motivate them to participate in ongoing projects where they will have an opportunity to gain knowledge in modern experimental techniques and to improve their scientific skills.

4.2 Research objectives:

The **SMART|AtmoSim**_*Lab* introduces a wide range of opportunities for young researchers to develop their research skills in co-operation with internationally recognized leaders in the field. During the long-term project, new methodologies and analytical techniques should be developed to obtain information on atmospheric pollutants. The study of the local photochemical regime in Georgia will be conducted and numerical methods of data assimilation and modelling will be developed. Laboratory equipment for measurement and data analysis will be installed in the local Georgian lab.
SMART|AtmoSim_*Lab* with Georgian scientists and students with collaboration of IEK-8 will plan, perform, and analyze experimental data. The main focus of experiments will be:

- Development and application of specific analytical techniques for atmospheric process:
  - performing R&D on enantioselective processes of gas-phase chiral pollutants in the environment;
  - development and application of micro- and nano-analytical techniques for the observation of atmospheric trace compounds.
  - development of mini and smart drones for sampling and analyzing atmospheric and ambient pollutants.
  - Development of micro- and nanosensors for atmospheric pollutants with enhanced specificity and limit of detection.
- Numerics of forward and inverse modelling of atmospheric models:
  - performing research and development (R&D) on the discretisation of icosahedral grids;
  - performing R&D on data assimilation with adjoint atmospheric modelling, including preconditioning and minimisation for variational methods and further afield;
  - performing R&D on numerical solution of stochastic differential equations of atmospheric processes

4.3 General requirements and laboratory equipment

Taking all issues mentioned above into account, the future **SMART|AtmoSim**_*Lab* should satisfy the following demands:
Required area:

- Laboratory and office space in total up to 60 m^2

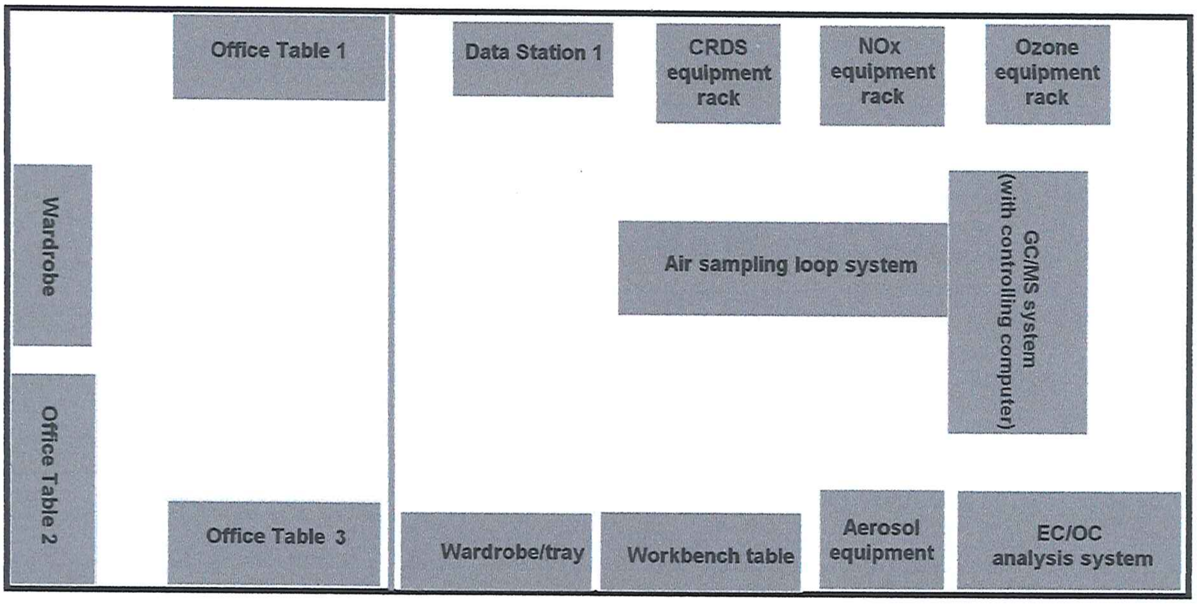
Main technical requirements for laboratory area are following:

- Light, clean and dry room (≈7000 euro, renovation and furniture TSU contribution)
  supplied with heating and air ventilation and conditioning systems; (≈5000 euro TSU contribution)
- Water supply and a tap must be available.
- Grounded mains sockets for electrical supply plus separate grounding wire must be available.
- There should be one non-interruptible power supply (UPS) dedicated for the laboratory (with minimum power of 10 KW). Thus, separate electrical lines and sockets must be provided;(≈4000 euro TSU contribution)
- Local area network to interconnect PCs and experimental equipment (with minimum link of 100 Mbit/s) and access to the internet (unlimited, with minimum upload/download speed of 10 Mbit/s);
- Steel and plastic tube support system over the lab: at 2.5 m height from the floor along the walls and middle of the laboratory for easy and secure access of air samples. (1000 euro TSU contribution)

- Ambient air sampling system, desired to be on top of the building.(3000 euro TSU contribution)
- The laboratory will be equipped with expensive experimental apparatus. Therefore, it should be protected by security systems.

The preliminary distribution of the laboratory area
(see the sketch below):

- Rack for CRDS equipment (CO, CO_2, CH_4)
- Rack for NOx equipment
- Rack for the O_3 equipment
- Table for data stations (PC's) for above mentioned equipment
- Place for EC/OC analysis system
- 3 Office table with PC (one for mathematical simulations)
- Lockable wardrobes, tray
- 2 table for GC/MS system and its PC
- Workbench table GC/MS system (with controlling computer)



4.4 Resources and budget

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The main infrastructure of the laboratory will be provided by the Tbilisi State University (TSU).

There are two additional parts for the demand of resources: personnel (see below), which will be provided by Georgian side, and equipment: the start-up laboratory equipment with total value of **100.000 Euro** (see list of the equipment given in section 4.6) will be covered by Georgia.

The additional demands for laboratory resources will be supplied by Forschungszentrum Jülich (IEK-8) as a donation.

The **tentative** budget (for **5 years** period) is as follows:

• Head of the lab (**PI**): 250.00 EUR per month × 60 = 15.000 EUR (This is on-top salary to basic salary at the main job)

• Deputy Head of the lab (**PI**): 200.00 EUR per month × 60 = 12.000 EUR (This is on-top salary to basic salary at the main job)

3 Postdoctoral students: 150.00 EUR monthly 3 x 60= 27.000 EUR

• 3 PhD students: 120.00 EUR monthly 3 x 60=21.600 EUR
• 3 Master student(s): 60.00 EUR monthly 3 x 60 =10.800 EUR
• Travel money: 7.000 EUR per year × 5 = 35.000 EUR
• Other goods and services: 10.720 EUR per year × 5 = 53.600 EUR (Consumables, instrument re-pair, small instrument acquisition and other activities necessary for laboratory operation).
• Start-up equipments: 100.000 EUR × 1 = 100.000 EUR

Total budget (Georgia-External Source): 275.000 EUR
From FZJ 285. 000 EUR

In summary, the total (**tentative**) budget for the first 5 years will be **500.000 €**, with contributions from:

☐ **Georgia-External Source: 275.000 € Financing of the SMART|AtmoSim_*Lab* and its operation**

☐ **TSU Contribution 20 000 € (For laboratory room renovation and furniture)**

☐ **IEK-8 of FZJ: 285.000 €** (* (* **Estimated indirect contributions, comprising of:** Instruments for Smartlab at TSU, the scientific project and infrastructure at FZJ and travel expenses of Jülich scientists to Georgia.

The amount Euro 285.000 represents the estimated expense of the instruments listed in Table 1 and provided by German side, as well as the expenses of their shipment to Georgia. This amount does include training and infrastructure expenses provided to Georgian scientists in Jülich, as well as travel expenses for German scientists to Georgia.

Table 1 Major Instruments for SMART|AtmoSim_*Lab*

Agilent GC/MS ≈100 000 Euro	Georgia-External Source
Elementar PrecisION IRMS ≈160 000 euro	On later stage
Pyrolytic interface between GC and IRMS ≈ 40 000 euro	On later stage (possibly Jülich can provide one)
Custom gas tubing ≈8 000 Euro	Germany (Jülich)
Liquid nitrogen Dewar flask ≈1500 Euro	Germany (Jülich)
Silicometal Tubing with fittings ≈4000 Euro	Germany (Jülich)
GC custom sample introduction system ≈3000 Euro	Germany (Jülich)
Custom sampling controller ≈10 000 Euro	Germany (Jülich)
GC column DB1 120m ≈1800 Euro	Germany (Jülich)
10X silicometal cans ≈20 000 Euro	Germany (Jülich)
Calibration standard ≈5000 Euro	Germany (Jülich)
Picarro CRDS (CO, CO_2, CH_4) ≈90000 euro	Germany (Jülich)
NOx Chemiluminescence (EcoPhysics) ≈90000 euro	Germany (Jülich)
Ozone monitor ≈25000 euro	Germany (Jülich)
EC/OC analyzer ≈10 000 euro	Germany (Jülich)
Aerosol monitor PM-10, PM-2.5 (sample collector, mass balance) ≈15000 euro	Germany (Jülich)

Shipment of Instruments from Germany to Georgia (Tbilisi, CIP) ca. Euro 1.700,00 will be taken over by Germany (Jülich). Custom formalities will be arranged and custom fee will be paid by TSU: