The Greek/German "Helmholtz European Partnership for Technological Advancement" (HEPTA) project was positively evaluated 2019 by the Helmholtz Association. The project starts in September 2020 with the Aristoteles Thessaloniki University and the Karlsruhe Institute of Technology as principal partners.

The HEPTA focusses on the topic "air quality" as a central challenges in all joint research and training activities. In three focal points, "atmospheric physics", "biomass" and "smart cities", only themes that are directly related to air quality can be addressed. In this context, climate change is considered as an overarching game changer. For the joint research about 12 PhD-positions are implemented – the following chapters shortly describe the thematic focus in the three (above mentioned) focal points.

HEPTA Topic 1: Biomass

[Towards better air quality in the cities via utilization of CO_2 neutral fuels and hydrogen]

Project group: Prof. Dr.-Ing. Jörg Sauer (KIT), Prof. Dr.-Ing. Angeliki Lemonidou (AUTh)

The contribution of IKFT in close collaboration with AUTH on the topic biomass valorization will focus on the development of novel catalysts and thermochemical processes for the conversion of syngas to pure hydrogen and high-performance liquid fuels. Due to their composition and chemical structure these fuels inherently lead to cleaner use in the combustion engines and thus to improved exhaust gas quality. Starting material is residual dry or moist biomass. For the conversion of biomass to syngas, the process of hydrothermal gasification in supercritical water will be further developed. The other important path to generate syngas from biomass is pyrolysis-gasification and gas cleaning as realized in the already developed bioliq process. The main experimental work will be performed in the framework of the following four sub-topics.

Pure H_2 from waste biomass via gasification in supercritical water
The target of Sub-topic 1 is to generate pure hydrogen from wet waste biomass (sludge, aqueous waste streams). The raw product gas from SCWG will be cleaned (removal of Sulphur compounds and Tars) and then the carbon containing species (CH_4-CxHy) will be reformed (catalytically) to syngas. The option of sorption enhanced reforming for simplifying the reaction-separation sequence will be also explored. A subsequent fine cleaning step will generate the end product. Part of the work will be performed at AUTh in the Laboratories of Prof. Lemonidou.

Gasoline from biomass via oligomerization of olefins
The target of Sub-topic 2 is to synthesize gasoline by oligomerization of sustainable olefins in the range of C_2-C_4. Different catalysts and supports will be investigated at varying operating conditions and feed compositions. Depending on the selectivity of the catalyst, fractions of renewable Diesel and Jet-Fuel can also be obtained. The produced fuels will be analyzed regarding relevant fuel properties like octane rating and are supposed to meet the required standards. There is a strong thematic connection with the Sub-topic 3.

Selective catalytic hydrodeoxygenation of biomass derived polyols towards lower olefins
The aim of this PhD is the development of new catalysts and process options for the production of C3-C4 mono and dio-olefins to be used as monomers for the oligomerization towards gasoline. Residual biomass is an excellent source of polyols (e.g glycerol, the by product of biodiesel production). The complete deoxygenation in the presence of hydrogen while preserving the C-C bonds and the C=C formed can only be tackled in the presence of active and selective catalysts. The scientific objectives of the work include the development of catalysts mostly based on transition metal-oxides with mild hydrogenation activity, their characterization and testing using high pressure batch and continuous flow reactors operating under trickle bed conditions. Kinetic and mechanistic studies on the best performing catalyst(s) will complement the work. (Sub-topic 3, thematic connected with Sub-topic 2)

Catalytic hydrotreatment of biomass-derived oxygenated compounds towards liquid transportation biofuels
The main objective of the work is the development of advanced catalytic technologies for the hydrotreatment (hydrogenation, hydrodeoxygenation, hydroisomerization) of biomass-derived streams (model compounds and real feeds), including pyrolysis or liquefaction bio-oils, lipids extracted from micro-algae or furan-based side streams, towards high quality hydrocarbon (in gasoline, diesel, aviation fuel range) or oxygenated (MF, DMF, etc.) liquid transportation fuels. The research workplan will include synthesis and characterization of bifunctional supported metal nano-catalysts and their evaluation in lab- and micro-pilot scale high pressure catalytic hydrogenation reactors.

HEPTA- Topic 2: Atmospheric Physics

Project group: Prof. Dr. P. Braesicke (KIT), Prof. Dr. X Y (AUTh)

The composition of the atmosphere is an important boundary condition for human life. It determines the air we breathe and the environmental conditions we encounter, e.g. the radiation (UV in particular) we experience when we are outside. For a sustainable and safe future, we require the best possible knowledge of these boundary conditions, including also the long-lived greenhouse gases (GHGs) as drivers of climate change. Therefore, we suggest a number of research projects that will strengthen our knowledge in this area in a mutual beneficial partnership between AUTh and KIT. Even though the envisaged PhD projects can only cover a small area of this large research field (here: ozone and UV changes, and variability of GHGs), we will follow a seamless approach – in terms of temporal and spatial scales and by confronting models with observations.

Environmental effects of the future evolution of UV and visible solar radiation arising from projected changes in atmospheric composition

The project will use data from the CMIP6 and/or CCMI-type experiments, including ICON-ART simulations performed at KIT, to determine the future evolution of UV and visible radiation, considering the full range of factors i.e. ozone, clouds and aerosol distribution. With the application of appropriate weighting functions (or action spectra), the effects on (a) ecosystems (including urban environments), (b) human health (e.g. Vitamin-D, erythema), and (c) agriculture (crops), will be studied on global scale, focusing also on regional scales where applicable. Moreover, the expected effects on air quality through changes in the photolysis rates of NO_2 and ozone (due to changes in UV-Vis radiation) in the presence of aerosols will be quantified. Effects of area-related climate changes and potential risks (e.g. polar vs mid latitudes) will be examined. A complementary project will look at ozone and UV forecasts on “weather” time scales using the same model (ICON-ART), but in a different configuration. The validation of the modelling system benefits from such a seamless approach, because modelled ozone and UV can be validated with a wealth of station data for the present day. This validation will allow improved climate simulations with ICON-ART that in turn can be used in the assessment cycle used above.

Variability of greenhouse gases in SE Europe

The project will study the variability of the greenhouse gases concentrations in SE Europe using measurements of solar infrared radiation. This will include systematic long-term FTIR measurements of column averaged mixing ratios of CH_4, CO_2, H_2O and CO, which will be collected in Thessaloniki in collaboration with KIT. There are no systematic measurements in the area and this will be a first attempt to study inter- and intra-annual variability of GHG concentrations. In addition, the measurements will contribute to the validation of current (S5P-TROPOMI) and planned (S4 and S5) satellite products. During the project short-term campaigns will be organized with additional spectrometer(s) in order to make emission estimates of GHGs for specific areas of interest in Greece.

This first project work package will be complemented with high resolution modelling of GHG variability using a configuration of ICON-ART. Here, we have the unique opportunity to test existing inventories and the interaction between transport regimes and variability. The model will be confronted with local / regional observations (with a focus on Greece and the Mediterranean). Novel methodologies to characterize the modelled and observed variability spectra will be explored and (where required) inventories will be corrected. This is a unique opportunity for improved observational and modelling systems to assess GHG budgets.

HEPTA-Topic 3: Smart Cities

[Towards better modelling and measurement for smart cities]

Project group: Prof. Dr. X. Ntziachristos (Auth), Prof. Dr. Michael. Beigl/Dr. Till Riedel (KIT)

Cities are a major factor in meeting sustainable development goals. New smart city technologies significantly contribute to this direction but their engineers need reliable models to quantify total benefits. At the same time, fundamental research on modelling traffic, aerosol concentrations, meteorology, energy use and climate in urban areas is currently undergoing a major change. On one hand, the number of environmental and other sensor networks is increasing which leads to vastly growing amounts of data (internet of things / big data). On the other one, the capability of modeling small scale effects of pollutants distribution and transformation in the atmosphere is growing due to available high-performance computing. This leads to new opportunities for future Smart City engineering (meeting mobility, energy, and information demands and resilience against health and infrastructural threads). The current research landscape in the area of modelling (be it emissions, meteorology, transport or energy) is developing in two major directions: simulation-based modelling and measurement-based regression ("inverse modelling"), each of which has its own advantages and disadvantages. Both, simulation-based and measurement-based approaches complement each other. For instance, the measurement-based approach can identify undetected sources of emissions or account for unforeseen rapid changes in activity, and the emission-based approach can compensate for uncertainties and blind spots. The calibration and validation of measurements with other measurements or models, as well as the calibration and validation of models with measurements become more difficult or even impossible with increasing complexity and granularity.

The aim of this project is to compare and combine both approaches based on use cases: Simulating concentrations from emissions with dispersion models, and predicting emissions from concentrations with inverse modeling. To achieve a simultaneous model validation and sensor calibration to estimate exposure, e.g. data driven quality metrics and validation methodologies should be developed, that address problems with feedback loops.

One interesting aspect is the massive use of low-cost sensors. Rather than treating them as measurement equipment (in the sense of DIN-1319), low-cost mass deployed sensor networks can inform model changes and represent valuable input parameters for inverse modelling. Open questions include placement and deployment strategies to maximize the information gain from such networks. Novel ways to incorporate such uncertain signals that can also stem from other data sources, like induction loops or mobile phone data, is an important challenge towards better understanding of mobility and behaviour resulting in energy use and related emissions. Besides the classical approaches for model-assimilation, novel methods of artificial intelligence may play a key role in inverse and hybrid modelling. They support or replace classical simulation models for sensor data with proxy-models (e.g. neural networks or gaussian process regression) which have a much better scaling behaviour. The long-term goal of the cooperation should be to develop a fundamental methodology to combine small scale measurement networks and small-scale modeling approaches in a way that they mutually compensate for their weaknesses and combine their strengths to create a comprehensive, emission- and measurement-data-based modelling approach.

A specific application of the new methodological framework can be done under the recent initiative of the Global Atmosphere Watch Program of the World Meteorological Organization (WMO-GAW) for the study of the effects of the COVID-19 lockdown measures on emissions and air quality. The recent COVID-19 lockdowns and reduced activity levels offer an ideal test case, first, to validate the methodology proposed and, second, to demonstrate its applicability for policy assessment and planning of urban-scale mitigations, as well as the deployment of nature-based solutions.

The project invites PhD proposals towards those topics focusing on simulation, inverse modelling, distributed measurement, and machine learning primarily for air quality and climate aware mobility but also related to adjoining fields like decentralized energy consumption, urban planning, and production in urban areas as key factors towards sustainable development.