AT03

IBOOT

Impact of Biogenic emissions on Organic aerosols and Oxidants in the Troposphere

DURATION OF THE PROJECT
Phase 1: 15/12/2005 – 14/12/2007
Phase 2: 15/12/2007 – 31/01/2010

BUDGET
685.568 €

KEYWORDS
Biogenic emissions, secondary organic aerosols, VOC oxidation mechanisms, troposphere, ozone, oxidizing capacity of the atmosphere

CONTEXT

This project aims to better understand and quantify the impact of Biogenic Organic Compounds (BVOC) on air quality and the climate system (aerosols and the greenhouse gases ozone and methane). It will therefore support policy making at the international level (e.g. IPCC) as well as at the Belgian federal level. Detailed degradation mechanisms for important BVOC compounds (the mono- and sesquiterpenes) will be developed based on advanced theoretical techniques, and implemented in a large-scale model order to assess their impact in the atmosphere. The mechanisms and the model will be validated by laboratory and field observations, including measurements performed in the BIOSOL project.

PROJECT DESCRIPTION

Objectives

Our general objectives are
1) To estimate the impact of biogenic organic compounds in the atmosphere
2) To establish the photochemical degradation mechanism and aerosol formation potential of several mono- and sesquiterpenes

More specifically, we aim to
1) Provide experimental constraints on the oxidation mechanism and aerosol formation potential of two sesquiterpenes by ozone
2) Develop a comprehensive model describing the gas-phase oxidation and the aerosol formation resulting from the degradation of important terpenes
3) Assess the impact of these terpenes on tropospheric ozone and organic aerosols at the global scale
4) Determine the impact of the reactions of organic oxygenated compounds in the upper troposphere

Methodology

1) Conduct oxidation experiments of two sesquiterpenes, β-caryophyllene and α-humulene, in a large reactor (International partner MPI-Mainz), where both gaseous and particulate compounds from their reaction with ozone will be analyzed, and the aerosol yields, sizes and CCN (Cloud Condensation Nuclei) activities will be determined. The influence of the reaction conditions (e.g. temperature) will be investigated
2) Use the most advanced theoretical methods to develop the predictive tools (Structure-Activity Relationships or SARs) needed for the development of comprehensive degradation mechanisms for terpenes and other compounds (KULeuven). Develop such mechanisms for selected monoterpenes and sesquiterpenes. The pathways leading to the formation of key low-volatility compounds will be elucidated. These mechanisms could serve as a basis to develop template mechanisms for other terpenes
3) Develop a model for the partitioning between the gaseous and particulate phase of the products of mono- and sesquiterpenes oxidation, based on state-of-the-art prediction methods of their thermodynamic properties. Couple this model to a "box" model for the gas-phase degradation of selected mono- and sesquiterpenes (IASB-BIRA). Validate this coupled model by confrontation with laboratory measurements in various conditions. Determine the extent to which the observed aerosol formation can be reproduced with or without parameterizations for heterogeneous reactions
4) Implement a simplified version of this model in a global chemistry-transport model of the atmosphere, and determine the impact of terpenes emission on the budget and distribution of oxidants and organic aerosols (IASB-BIRA)
5) Determine the temperature and pressure-dependent rates and products of the reaction of a number of oxygenated organic compounds with OH and/or HO2 radicals, using advanced theoretical methods, and assess the impact of these compounds in the atmosphere (KULeuven)

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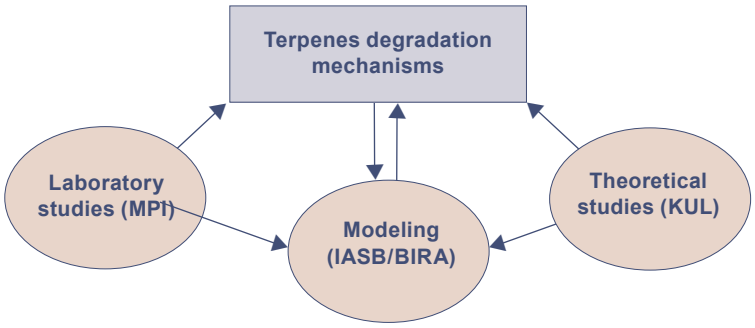
INTERACTION BETWEEN THE PARTNERS

Research results from both KULeuven and the International partner MPI will be needed to design the terpene degradation mechanisms. These mechanisms will be introduced in the model developed at IASB-BIRA, which will be validated using laboratory data obtained within this project (by MPI) as well as from previous studies.



EXPECTED RESULTS AND/OR PRODUCTS

Our research results will be disseminated through publications in international journals, communications at international conferences, and our web site. Furthermore, valorization activities will include

1) the development of a website for Structure-Activity Relationships (SARs) which will include pedagogical tools, a discussion of the methods, the chemical kinetic datasets as well as their statistical analysis. A program will be developed for the automatic application of the SARs,
2) workshop/school on mechanism development, in collaboration of the BIOSOL project and under the auspices of the INTROP programme of the NSF, and
3) data submission to international databases (e.g. within the European Network for Atmospheric Composition Change (ACCENT)).

PARTNERS - ACTIVITIES

IASB-BIRA
has a long tradition in atmospheric research, which is one of its major tasks. A large part of the scientific work performed is devoted to the stratosphere and troposphere through laboratory, modelling and atmospheric monitoring activities.

The laboratories of KULeuven
involved in this project contribute to chemical kinetics of elementary gas phase reactions, as well as to the application of high-level quantum chemical methods to solve chemical problems, including reaction mechanisms and reaction kinetics.

Research of the International partner MPI
focuses on ozone and the role of radicals in photo-oxidation mechanisms which play a central role in the self-cleansing capacity of the atmosphere. MPI develop highly sensitive instrumentation to measure trace gases, and uncover the photochemical reaction chains.

CONTACT INFORMATION

Project Website:
www.oma.be/TROPO/IBOOT/Home.html

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Follow-up Committee

For the complete and most up-to-date composition of the Follow-up Committee, please consult our Federal Research Actions Database (FEDRA) by visiting http://www.belspo.be/fedra or http://www.belspo.be/ssd

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