

BIOSOA

Biogenic Influences on Oxidants and Secondary Organic Aerosol: theoretical, laboratory and modelling investigations

DURATION OF THE PROJECT
15/12/2010 – 15/12/2014

BUDGET
1.156.978 €

KEYWORDS

Secondary organic aerosol; tropospheric composition; oxidative capacity; biogenic; isoprene; monoterpenes

CONTEXT

Due to their large emissions (~1000 megatons per year globally), biogenic volatile organic compounds (BVOCs) released by plants play a key role in air quality and in the climate system. Their atmospheric oxidation is a large source of secondary organic aerosol (SOA), an important component of fine particulate matter; it also strongly impacts tropospheric ozone and the oxidising capacity of the atmosphere, and therefore the abundance of important greenhouse gases like methane. Large uncertainties remain, however, regarding (1) the influence of isoprene, the major BVOC at the global scale, on the abundance of hydroxyl radicals (OH), (2) the pathways leading to key SOA constituents from major BVOCs, and (3) the magnitude of the SOA source contributed by the different BVOCs.

PROJECT DESCRIPTION

Objectives

Building on two projects of the previous SSD program (IBOOT and BIOSOL, 2006-2010), we propose to conduct laboratory, theoretical and modelling investigations in order to better understand and quantify the role of BVOCs as a source of SOA and as a major factor influencing the oxidation capacity of the atmosphere. This project aims to provide a better scientific basis for decision-making, especially at the international level, since the effects of pollutant emission controls on e.g. air quality cannot be determined without a better understanding of the BVOC oxidation and biogenic SOA formation processes.

The specific objectives of BIOSOA are

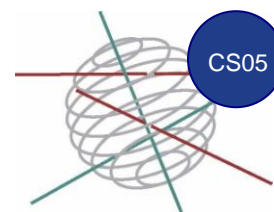
1. to assess the impact of isoprene emissions on the abundance of oxidants,
2. to gain insight into the chemical pathways leading to key chemical SOA constituents from the oxidation of BVOCs,
3. to quantify the contribution of specific BVOCs to the organic aerosol,
4. to assess the impact of BVOC emissions on organic aerosols at the global scale.

Methodology

- Laboratory experiments will be conducted (UA, IFT) to elucidate the formation mechanisms of key SOA tracers from isoprene and α -pinene found in substantial amounts in ambient aerosols. The structure of unknown SOA tracers from α -pinene will also be elucidated.
- A suitable method will be developed (UA) to estimate the contribution of isoprene and α -pinene to ambient aerosol concentrations. This method will be applied to fine aerosol sampled during field campaigns in Finland, in Hungary and possibly in the Amazon forest.
- A complete gas-phase mechanism for the oxidation of isoprene by hydroxyl radical will be developed (KULeuven), applying the high-level theoretical methods used in earlier work, and evaluated against available laboratory and field data (KULeuven, IASB-BIRA).
- A detailed model of gas/aqueous oxidation chemistry will be developed (IASB-BIRA), based on newly elaborated methods for the thermodynamic properties of SOA constituents, in order to assess the role of in-cloud chemistry on the budget of SOA. This model will be tested against available laboratory and field data.
- A key gas-phase reaction involved in this multi-phase chemistry will be investigated in the laboratory (KULeuven)
- The impact of BVOC emissions on the budget and distribution of SOA will be investigated using a global model (IASB-BIRA). The calculated contributions of different BVOCs will be compared to estimations based on observations of marker compounds.

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INTERACTION BETWEEN THE PARTNERS

A close cooperation between the partners will be essential to the success of BIOSOA. The theoretical and laboratory results obtained at KULeuven will be used in the models of BVOC degradation and SOA formation developed at IASB-BIRA. The evaluation of these models against experimental (field and laboratory) data should provide additional constraints on the theory-based mechanism.

The laboratory experiments on the formation and ageing of SOA tracers will be conducted in a reaction chamber at IFT; chemical analysis of the aerosol samples and interpretation of the results will be made at UA. The global model results will be validated using the relative contributions of different BVOCs to the concentrations of ambient SOA estimated by UA based on marker compound concentrations.

EXPECTED RESULTS

- Better understanding of the processes leading to SOA formation from biogenic precursors, in particular isoprene and α -pinene
- Better quantification of the contribution of the different BVOCs to the concentrations of fine aerosols
- State-of-the-art chemical mechanism for the oxidation of isoprene by OH, evaluated against laboratory data and against field measurements
- State-of-the-art SOA formation model, considering in-cloud chemistry as well as ageing processes, and evaluation of the respective influences of biogenic and anthropogenic emissions on the budget and abundance of SOA.

PARTNERS

Activities

The tropospheric chemistry modelling of IASB-BIRA group contributes to emission modelling, chemical mechanism development and evaluation, SOA formation modelling and global modelling.

The KULeuven group contributes 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.

The UA group focuses on the characterisation of SOA tracers from the photooxidation of isoprene and α -pinene, as well as on the development of suitable methodology based on liquid chromatography/mass spectrometry to assess SOA contributions to ambient fine aerosol.

The IFT group has wide experience with and is well equipped for laboratory smog chamber experiments under simulated atmospheric conditions.

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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>

