

WP6 JRA2

Development of common techniques for the use of chamber measurements in model development and evaluation

WP6.1 Gas phase processes

WP leader Mike Pilling, University of Leeds

WP6.2

Aerosol process modelling

Thermodynamics, particle formation, transformation, ageing, multiphase chemical reactions

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JRA2 WP6.1: Overview

to design and test methods that facilitate the use of chambers both to evaluate chemical mechanisms, and, in particular, the master chemical mechanism (MCM) and to provide new information to develop it further, by filling in the gaps in our understanding



Objectives

- To continue the development and dissemination of a database of rate parameters and mechanisms for elementary reactions involving oxygenated species, based on chamber measurements and other sources.
- To develop a model, based on the master chemical mechanism (MCM) for the atmospheric oxidation of volatile organic compounds, to enable the design of chamber experiments and the analysis of chamber data, through model / experiment comparisons.
- To carry out experiments in chambers across the consortium specifically designed to test and develop the model and the comparison methodology.
- To develop metadata, based on semantic web methodologies, to provide an easily used method to describe the chamber modelling process, and facilitate archiving of the modelling and of its conclusions.
- To provide a searchable database of model / measurement comparisons and conclusions and to facilitate the use of the database by MCM developers.



Tasks (+ partners and deliverable times)

- **Task 1** *Continued development of a database for oxygenated compounds.*(CNRS-ICARE) (Continuing)
- **Task 2** *Creation of a computer model that can be used across all chambers investigating gas phase mechanisms.* (LEEDS, CEAM, FZJ) (Code, Month 12)
- **Task 3.** *Testing of the model / experiment comparison methodology* (BUW, FZJ, CEAM, UBT, UCC,CNRS-ICARE, PSI ,LEEDS) (Protocol - month 18; activity reports and publications - continuing)
- **Task 4.** *Development and implementation of a modelling database* (LEEDS, CEAM, FZJ) (Report, month 30)
- **Task 5.** *Evaluation of a lumped mechanism, based on the MCM.* (LEEDS) (Protocol, computer model, month 36)

Milestones

6.1.1 Computer model for use in experimental / model comparisons in M12. Verified through use by consortium in analysis of chamber data.

6.1.2 Searchable database for experiment / model comparisons in M30. Verified through transfer of analyses of chamber modelling experiments.

