

CEAM CONTRIBUTION TO JRA2

EUPHORE team, Mike Pilling, Ian Barns, Jens Hjorth

amalia@ceam.es

The JRA2 activity of the EUROCHAMP project deals with the development of oxidants mechanisms and their evaluation against chamber experiments in the EUROCHAMP installations as well the development of techniques that could improve the mechanistic modelling of atmospheric reaction. CEAM contribution to this activity could be summarized in 3 main topics:

1. Carbonyl formation in the photo-oxidation of benzene and toluene.

The methodology of SPME can be applied to the determination of carbonylic intermediates in the degradation of atmospheric precursors with O-(2,3,4,5,6)-pentafluorobenzyl-hydroxylamine (PFBHA) applied on the fibre for in situ derivatisation of carbonyls. It is especially sensitive for dicarbonyls and particularly, dialdehydes, which determination poses an analytical challenge. This analytical methodology can introduce a substantial improvement in mechanistic development since it can potentially enable to obtain reaction profiles of dicarbonylic compounds and isomeric discriminated quantitative determination of unsaturated dicarbonylic intermediates.

2. Improving the mechanisms for aromatics (nitrophenols)

The possible contribution of nitroaromatic compounds to forest decline created the impetus for the study of their atmospheric behavior. The photolysis of 2-nitrophenol with natural sunlight has been studied in the European smog photoreactor (EUPHORE) under different conditions. The effects of the presence and the absence of NO_x and also an OH radical scavenger on the aerosol and ozone formation from the photolysis have been investigated. One of the main results is the high aerosol yield (30 – 56 %) obtained from the photolysis reaction, demonstrating that 2-nitrophenol photolysis is a potentially important contributor to the SOA formation observed from the photooxidation of aromatic hydrocarbons. Increasing our understanding of the chemical behavior and properties of these compounds, their physico-chemical processes and their products is vital for properly assessing their role in pollution and climate change.

3. Development of Chamber modelling tools

In this contribution, a graphical interface created for the modeling of the chemical mechanisms studied in simulation smog chamber is presented. The work was carried out in collaboration with the University of Leeds and supervised by Professor M. J. Pilling. The interface is based on the Open Source MCM Box Model developed in FORTRAN at the University of Leeds. It avoids the direct modification of the model code by the user and enables an easy configuration of its parameters. It covers the setting of the experimental conditions (species, chemical mechanism, initial concentrations, photolysis frequencies, environmental conditions, etc), model parameters (start time, number of steps and step size, data interpolation method, etc) and sensibility analysis tests as a Rate Of Production Analysis (ROPA) of the species of interest established by the user. To develop the graphical interface two main programs were used; Anjuta 1.2.4a (<http://www.anjuta.org>) and Glade 2.12.1 (<http://glade.gnome.org>).