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Evaluation of Detailed Tropospheric Chemical Mechanism, MCM v3, using Atmospheric Field Study Data

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No chemical mechanism can be relied upon to give accurate predictions unless it has been evaluated by comparison with experimental data. There are essentially two ways in which a photochemical oxidant model can be evaluated. One relies on the evaluation of individual pollutant compounds, separately. In the case of gas-phase chemical mechanisms, this means evaluating the predictions of the mechanism against results of environmental chamber experiments. Another approach compares the predictions of the complete model against field data taken during a historic ozone pollution episode.

The present study consisted in the evaluation of several schemes of the quasi-explicit chemical model Master Chemical Mechanism version 3 (MCM v3). Firstly the MCM v3 schemes were evaluated using environmental chamber data by adaptation of MCM v3 with inclusion of a chamber-dependent auxiliary mechanism. In this first step Butane degradation mechanism included in MCM v3 was evaluated using Statewide Air Pollution Research Center (SAPRC) at the University of California environmental chamber datasets on the photo-oxidation of butane and its degradation products, methylethyl ketone (MEK), acetaldehyde (CH_3CHO) and formaldehyde (HCHO), in conjunction with an initial evaluation of the chamber-dependent auxiliary mechanisms for the series of relevant chambers. Isoprene and its degradation products, methacrolein (MACR) and methylvinyl ketone (MVK) were also evaluated and refined (already published). The representation of alkene degradation in MCM v3 was also evaluated, using environmental chamber data on the photo-oxidation of ethene,

propene, 1-butene and 1-hexene (submitted to publication). The degradation mechanism of monoterpenes, α-pinene and β-pinene in MCM v3, were sequentially evaluated and refined still with basis on published Chamber experimental data.

The present communication will be focused in a second phase of this study. This phase consisted in the incorporation of the MCM v3 into a Photochemical, one layer, Trajectory box Model (PTM) using a Lagrangian approach. The PTM was used to evaluate and intercompare the original and adapted versions of MCM v3, (resulting from refinements provided by the first step studies), at normal environmental conditions, in the polluted boundary layer atmosphere.

The PTM was applied to a real situation in the Portuguese west coast, during an ozone summer episode, by following the air mass transported by sea breeze, from the coast line (Aveiro) to a location, approximately 65 kilometres inland, (Covelo). The PTM was applied during the period of June 28 to July 1 2001, using meteorological and air quality data, obtained from a field campaign, which consisted in simultaneous measurements at three locations, oriented in-line with the sea breeze penetration inland.

The selected area domain of the study was small enough to allow a good characterization of natural and anthropogenic emissions. The time domain of this field application is in same order of those used in chamber runs, evaluated in the first part of this study. The starting time of the first daily wind trajectory takes place after that the breakdown of nigh time inversion results in a well mixed in boundary layer.

The results allow to compare the predictions of the complete model against field data, both for ozone and oxygenated gaseous organic species, and to infer about the effects of model adaptation (resulting of chamber intercomparisons) to ambient conditions for which the model was developed. Particular emphasis is placed on the ability of the mechanism to describe distributions of specific organic oxygenates observed in the field campaign.