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Sensitivity analysis by the adjoint chemistry transport model DRAISfor an episode in the Berlin Ozone (BERLIOZ) experiment

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Abstract. The Berlin Ozone Experiment (BERLIOZ) was carried out in summer 1998. One of its purposes was the evaluation of Chemistry Transport Models (CTM). CTM KAMM/DRAIS was one of the models considered. The data of 20 July were selected for evaluation. On that day, a pronounced ozone plume developed downwind of the city. Evaluation showed that the KAMM/DRAIS model is able to reproduce the meteorological and ozone data observed, except at farther distances (60–80 km) downwind of the city. In that region, the DRAIS model underestimates the measured ozone concentrations by 10–15 ppb, approximately. Therefore, this study was conducted to detect possible reasons for this deviation. A comprehensive sensitivity analysis was carried out to determine the most relevant model parameters. The adjoint DRAIS model was developed for this purpose, because for this study the application of this model is the most effective method of calculating the sensitivities. The least squares of the measured and simulated ozone concentrations between 08:00 UTC and 16:00 UTC at two stations 30 km and 70 km downwind of the city centre were chosen as distance function. The model parameters considered in this study are the complete set of initial and boundary species concentrations, emissions, and reaction rates, respectively. A sensitivity ranking showing the relevance of the individual parameters in the set is determined for each parameter set. In order to find out which modification in the parameter sets most reduces the cost function, simplified 4-D data assimilation was carried out. The result of this data assimilation shows that modifications of the reaction rates provide the best agreement between the measured and the simulated ozone concentrations at both stations. However, the modified reaction rates seem to be unrealistic for the whole simulation period. Therefore, the good agreement should not be overestimated. The agreement is still acceptable when the parameters in the other sets are modified together. The investigation demonstrates that an analysis of this type can help to explain inconsistencies between observations and simulations. But in the case considered here the inconsistencies cannot be explained by an error in only one parameter set.

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