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Optimization of long-term air quality modelling for Baden-Württemberg (FRG): Part I, annual chemistry-transport modelling using the KAMM/DRAIS model system[1]

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The use of a complex Chemistry-Transport-Model (CTM) like KAMM/DRAIS in studies related to regional long-term air quality requires the classification of meteorological conditions of at least ten years, because the continuous application of such a model over a time period of 10 years or even longer would be too time consuming and too expensive. Therefore, the overall aim of the project is the examination of two different classification methodologies with respect to their practical applicability in the field of long-term air quality studies. The two techniques chosen are "classical" cluster analyses, and Kohonen's Self-Organizing-Map (SOM). Criteria of judgement will be

- the efficiency of a method (handling, computation time, interpretation of classification results),
- and whether the resulting classes are good representatives of the whole spectrum of meteorological conditions.

The last aspect is related to the question whether statistical measures based on the classification agree with those calculated from detailed simulations over a whole period. Such statistical quantities characterizing the long-term air quality are, for example,

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AOT40 and SOMO35. In order to achieve the goal of the project it is not necessary to consider the meteorological conditions over a long period, it is sufficient to take into account a much shorter one, for example one whole year. Therefore, KAMM/DRAIS simulations for the Federal State of Baden-Württemberg (FRG) are performed for the year 2000, calculating hourly concentrations of all 41 RADM2 species. Statistical measures will be derived from the results of this detail simulation. The classifications of the meteorological conditions of the same year are carried out using the simulation results of the large-scale EURAD model. The statistical values are then recalculated based on the known KAMM/DRAIS results of class representatives taking into account the corresponding class frequencies. By comparing the statistical measures, those from the detail simulations and those from the classifications, and considering also its efficiency, the most suitable classification method can be found.

In the talk, the first major part of the project, the KAMM/DRAIS simulations for the year 2000 are described. The results of the simulations are compared with measured data. This comparison is performed in a statistical manner. In addition, AOT40 and SOMO35 values derived from the simulated and the measured ozone concentrations are compared. Qualitatively, the annual cycle of simulated daily mean ozone agrees well with the corresponding observation. This is also valid for the daily ozone maxima. With respect to the annual average of ozone concentration for each of 56 stations, 63% of all cases show deviations less than $\pm$15%, in 86% the agreement between simulation results and observation was better than $\pm$30%. The mean bias between simulated and measured ozone concentrations is -2.6 ppb. This value is averaged over the whole year and all measurement stations and, thus, based on more than 400.000 hourly concentrations. For NO_x, the discrepancies are larger. But taking into account the uncertainties of emission data, the model results are still acceptable. For air quality indices like AOT40 and SOMO35 the deviations from the observations are even larger. Except for a few stations, the model tends to underestimate these quantities. 80% of the AOT40 values for forests and 71% for crops and natural vegetation fall within the deviation interval of $\pm$50%. For SOMO35 the agreement is better, 88% of all cases lie within the 50% range. However, for such statistics the model results are still satisfactory.