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Chemical 4D-variational tropospheric data assimilation on multiple scales

A. Strunk and H. Elbern

Rhenish Institute for Environmental Research at the University of Cologne

Forecast skill of tropospheric chemical regimes is dominated mainly by the knowledge of emission scenario, which is of highly variable spatial scale and usually not sufficiently exact ascertained. To this end the presentation adresses the requirement to join emission rate coefficients and model state parameters in a common optimisation space on different horizontal resolutions using the grid nesting technique. Further, the radius of influence attributable to observations must also be adapted to the special situation.

The Eulerian mesoscale-α chemistry transport model EURAD-CTM (EURopean Air Dispersion pollution model) with the RADM2 (Regional Acid Deposition gas phase Mechanism 2) has been extended to an adjoint model version, which forms the kernel of the 4D-variational algorithm (4D-var). New estimates for the underlying covariance matrices have been coded. For the initial value background error covariance matrix a diffusion technique has been introduced to provide a feasible operator having now the possibility to model influence radii of the observations. An emission rate background error covariance matrix has been designed by analysing the source categories of EMEP-emission-inventories.

Within the presented work the combined optimisation of initial state and emission rates has been applied and will be compared to single initial state and emission rate optimisation.

Two different model adaptions to measurement campaigns will be shown:

1. CONTRACE/SPURT (two air borne campaigns focusing on the chemical situation in the free troposphere/lower stratosphere) with a vertical refinement of the upper model layers.

2. VERTIKO (vertical transport within the atmospheric boundary layer over com-

plex terrain) with three nested grid levels using a nesting factor of five.

Satellite data, air borne data and in situ observations have been assimilated. GOME/SCIAMACHY NO_2 tropospheric columns and GOME tropospheric ozone profiles from a neural network approach were available from space borne data. Additionally available operational European measurements have been used as observation data. Assimilated species were O_3, NO, NO_2, SO_2, CO, H_2O_2 and HCHO.
Key result is that both grid refining and emission rate optimisation are especially crucial features for improved forecast of primary emitted species. In both air borne experiments the 4D-var system demonstrates that initial model states can be found to simulate a very good, partly excellent agreement with the observations. The presentation assesses the improved forecast skill and discusses the benefits from the variational assimilation scheme with respect to traditional air quality simulation.