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Variational fine-grained data assimilation schemes for atmospheric chemistry transport and transformation models

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The paper concerns data assimilation problem for an atmospheric chemistry transport and transformation models. Data assimilation is carried out within variation approach on a single time step of the approximated model. A control function is introduced into the model source term (emission rate) to provide flexibility to adjust to data. This function is evaluated as the minimum of the target functional combining control function norm to a misfit between measured and model-simulated analog of data. This provides a flow-dependent and physically-plausible structure of the resulting analysis and reduces the need to calculate model error covariance matrices that are sought within conventional approach to data assimilation.

Extension of the atmospheric transport model with a chemical transformations module influences data assimilation algorithms performance. This influence is investigated with numerical experiments for different meteorological conditions altering convection-diffusion processes characteristics, namely strong, medium and low wind conditions. To study the impact of transformation and data assimilation, we compare results for a convection-diffusion model (without data assimilation), convection-diffusion with assimilation, convection-diffusion-reaction (without data assimilation) and convection-diffusion-reaction-assimilation models.

Both high dimensionalities of the atmospheric chemistry models and a real-time mode of operation demand for computational efficiency of the algorithms. Computational issues with complicated models can be solved by using a splitting technique. As the result a model is presented as a set of relatively independent simple models equipped with a kind of coupling procedure. With regard to data assimilation two approaches can be identified. In a fine-grained approach data assimilation is carried out on the separate splitting stages [1,2] independently on shared measurement data. The same situation arises when constructing a hybrid model out of two models each having its own assimilation scheme. In integrated schemes data assimilation is carried out with respect to the split model as a whole. First approach is more efficient from computational point of view, for in some important cases it can be implemented without iterations [2]. Its shortcoming is that control functions in different part of the model are adjusted independently thus having less evident physical sense. With the aid of numerical experiments we compare the two approaches.

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