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An algorithm for variational data assimilation of contact concentration measurements for atmospheric chemistry models

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Contact concentration measurement data assimilation problem is considered for convection-diffusion-reaction models originating from the atmospheric chemistry study. High dimensionality of models imposes strict requirements on the computational efficiency of the algorithms. Data assimilation is carried out within the variation approach on a single time step of the approximated model. A control function is introduced into the source term of the model to provide flexibility for data assimilation. This function is evaluated as the minimum of the target functional that connects its norm to a misfit between measured and model-simulated data. In the case mathematical model acts as a natural Tikhonov regularizer for the ill-posed measurement data inversion problem. This provides flow-dependent and physically-plausible structure of the resulting analysis and reduces a need to calculate model error covariance matrices that are sought within conventional approach to data assimilation. The advantage comes at the cost of the adjoint problem solution. This issue is solved within the frameworks of splitting-based realization of the basic convection-diffusion-reaction model. The model is split with respect to physical processes and spatial variables. A contact measurement data is assimilated on each one-dimensional convection-diffusion splitting stage. In this case a computationally-efficient direct scheme for both direct and adjoint problem solution can be constructed based on the matrix sweep method. Data assimilation (or regularization) parameter that regulates ratio between model and data in the resulting analysis is obtained with Morozov discrepancy principle. For the proper performance the algorithm takes measurement noise estimation. In the case of Gaussian errors the probability that the used Chi-squared-based estimate is the upper one acts as the assimilation parameter. A solution obtained can be used as the initial guess for data assimilation algorithms that assimilate outside the splitting stages and involve iterations. Splitting method stage that is responsible for chemical transformation processes is realized with the explicit discrete-analytical scheme with respect to time. The scheme is based on analytical extraction of the exponential terms from the solution. This provides unconditional positive sign for the evaluated concentrations. Splitting-based structure of the algorithm provides means for efficient parallel realization.

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