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Variational inverse modelling of surface particulates fluxes: a method for emission data quality improvement for CACs and GHGs

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Air pollution dispersion modelling is widely used to study the impact of human activities and weather-related incidents on the concentration of criteria air contaminants. One of the most uncertain inputs to the air pollution dispersion model is source emissions. Also, the sensitivity of receptor sites to the changes of emission sources is of interest. In this study, a four-dimensional variational (4D-Var) data assimilation method was used for inverse modelling of atmospheric PM2.5 in a large city. The modelling platform includes Weather Research and Forecasting (WRF) for meteorological data, Community Multiscale Air Quality (CMAQ) chemical transport model, the backward (adjoint) model (CMAQ-ADJ), which used a detailed bottom-up emission inventory as an input. The study's objective was to analyze the emission file input for PM2.5 using an inverse modelling approach and an optimization procedure. The PM2.5 emission was examined in a 1-week high air pollution episode, using air quality monitoring ground observation data as receptors. The assimilation window was set to 24 hours, and the forward and backward modelling of 9-kilometre spatial resolution was considered for the computational domain.

The results show that both emission inventories are generally underestimated. Comparing base emission rates and optimized emissions indicated that the bottom-up emission inventory contained fewer uncertainties, especially in the high emission regions.

In the central, eastern and southern parts of the city, daily scaling factors (an indication of emission correctness, 1 for being accurate) for weekends varied between 1.67 to 3.06 and for weekdays varied between 0.44 to 2.19. Emissions in the northern and western parts of the city significantly increased after emission inversion, with daily scaling factors ranging from 4.28 to 7.06 and 5.85 to 8.73, respectively. Priory emission rates are derived from top-down emission inventory for neighbouring cities. The study exhibited the effectiveness of the adjoint modelling tool on identifying high emission sources, the impact of neighbouring jurisdictions, and the performance of an analytical tool for improved emission reporting that can be used for both CACs and GHGs.