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Inverse modeling of emissions for local photo-oxidant pollution: testing a new methodology

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For local chemistry-transport models, surface emissions are the input data to which the output concentrations are the most sensitive. They are nevertheless poorly known, mainly because their high spatiotemporal variability makes it very difficult to obtain precise inventories and to keep them up-to-date. The possibility of modifying existing inventories seems therefore promising for a better understanding of photo-oxidant pollution.

Inverse modeling is one of the possible approaches. This kind of methodology was successfully used at global scale for climate studies. Unfortunately, a new approach has to be developped over urbanized areas because of the different spatial and time scales (with several order of magnitudes in term of emissions, meteorology with turbulence and pollutant reaction rates).

The aim of this presentation is to describe the choices made to compute correction factors for the available (called first-guess) inventory so that the optimized fluxes of NO_x and VOCs minimize the difference between simulated and measured ozone and/or concentrations. Two main issues are dealt with:
(i) The elaboration of a method for the spatial aggregation of emission fluxes to take into account the a priori correlations of fluxes. The correlations are built upon the kind of sources (location and intensity) together with the sensitivity of the concentrations to the fluxes.
(ii) The use of a kriging method to obtain analyzed maps of ozone concentrations, which are a continuous field. The analyzed values with their (co)variances are then used as constraints in the inverse.

This information is integrated in an inversion code based on CHIMERE chemistry-transport model and its adjoint, performing 4D-integration. Academic cases are run in order to validate the inverse code and quantify the limitations of the new methodology that is particularly suited to local pollution. The way to take into account other relevant parameters such as the turbulent mixing intensity, boundary layer height and temperature is discussed.