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Paper 101

Finite Element Simulation of Chimney Emissions: A Proposal for Near Field Impact Assessment in Highly Complex Terrains

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This work presents a strategy for three-dimensional finite element simulation of pollution evolution in highly complex terrains. The strategy is useful for the impact assessment of punctual emissions in the near field, up to few tens of kilometres. This scale is appropriate to be linked with the standard meshes used in most advanced air quality photochemical models, where the minimum grid size is about 2 to 4 km. These mesoscale models are specially designed for simulations up to hundreds of kilometres and are properly linked to meteorological prognostic models. Remarkably, most advanced mesoscale models include in-grid parcel evolution (puff) models for the near field impact of punctual emissions. The proposal of this work is to show that the finite element simulation is an appropriated alternative to this hybrid approach.

The simulation of the pollution evolution is driven by the wind field, which is computed with a mass consistent model for wind field adjustment [1,2]. The transport and reaction model is given by a convection, diffusion, reaction system of equations. The reaction term includes the photochemical modelling of pollutants. Two simple reaction models are considered here: First, a linear reaction model between two components, and second, the RIVAD acid rain model, which involves four components and a highly nonlinear coupled relationship [3].

Finite element problems involving highly complex terrains and detailed discretization of punctual emission sources can easily involve hundreds of thousands of tetrahedral elements and tens of thousands of grid nodes. Remarkably, they include element sizes ranging to four orders of magnitude (from a few meters close to the source to few kilometers faraway). Meshes are appropriate from the point of view of wind simulation. However, corresponding transport reaction problems present strong numerical requirements due to different scales involved. The linear case (constant rate transformation between species) is solved using a *Least Square* approach with the Crank-Nicolson scheme for time integration [4]. The discretized problems are a sequence of symmetric linear systems with common system matrix, which are solved with an incomplete Cholesky factorization as a preconditioner of the conjugate gradient iteration technique [5]. The nonlinear problem is solved using splitting schemes between reaction and convection-diffusion operators, following the work of [6]. The approach for linear models is used for transport steps and an uncoupled node by node second order Rosenbrock time integration scheme is used for the reaction ones [7].

The strategy is applied to successfully solve the problem in windy and extremely windy situations. Further work is being developed to efficiently compute the nonlinear evolution problem. Some mesh adjustments for transport reaction problem in extremely windy situations are still needed, as well as further work to couple efficiently the proposal with standard mesoscale photochemical simulation models.

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