NUMERICAL PREDICTION OF POLLUTANT DISPERSION AND TRANSPORT IN AN ATMOSPHERIC BOUNDARY LAYER

S. Zeoli, L. Bricteux, Faculté Polytechnique

Introduction

The ability to accurately predict concentration levels of air pollutant release from point sources is required in order to determine their environmental impact.

Industrial pollution over Moscow city (photo credit A. Petrenko)

A wall modeled large-eddy simulation (WMLES) of the atmospheric boundary layer (ABL) is performed using the OpenFoam based solver SOWFA (Churchfield and Lee, NREL). WMLES are usually performed using a standard Smagorinsky model or its dynamic version. It is proposed here to investigate a subgrid scale (SGS) model with a better spectral behavior.

Governing equations

The equations are the standard incompressible Navier-Stokes equations projected on a LES grid.

\[ \frac{\partial \tilde{u}_i}{\partial t} + \frac{\partial (\tilde{u}_i \tilde{u}_j)}{\partial x_j} = -\frac{\partial P}{\partial x_i} + \frac{\partial}{\partial x_j} \left[ \alpha \left( \frac{\tilde{u}_i \tilde{u}_j}{\tilde{S}_{ij}} \right) \right] + F_i \]

\( \tilde{P} = P/\rho \) is the reduced pressure, \( \frac{\partial \tilde{u}_j}{\partial x_i} \) is the driving pressure gradient (used for ABL modeling), \( \tilde{S}_{ij} \) is the sub grid scale stress model and \( F_i = -2 \epsilon_{ij} \dot{\Omega} \dot{u}_i \) is the Coriolis force (used for ABL modeling).

Subgrid scale modeling

The subgrid scale model implemented here, is based on the Regularized Variational Multiscale model (RVMs, Hughes et al. 2001). Any field is decomposed into a low pass filtered and a high pass filtered part (\( f = \tilde{f} + f' \)). The subgrid scale viscosity \( \nu_{sgs} \) is evaluated only on the high pass filtered part of the field so that the SGS model only triggers when small scales are produced in the flow.

\[ \nu_{sgs} = C \Delta \left( 2 \hat{S}_{ij} \hat{S}_{ij} \right)^{1/2} \frac{1}{2} \left( \frac{\partial \tilde{u}_i}{\partial x_j} + \frac{\partial \tilde{u}_j}{\partial x_i} \right) \]

The model only acts on the small scale part of the fields, ensuring its spectral selectivity.

\[ \frac{\epsilon_{ij}}{\nu_{sgs}} = 2 \hat{S}_{ij} \]

High pass filtering is performed using a standard Laplacian (easy to implement in a finite volume code) with \( \alpha = 1/12 \) and \( n = 1.2 \),

\[ \tilde{u} = (-1)^n \alpha \Delta^2 V^3 \tilde{u} \]

OpenFoam - SOWFA

SOWFA is an open source ABL solver developed on the OpenFoam platform. It uses second order cell centered finite volume method and a Piso algorithm to enforce mass conservation. This standard numerical method offers moderate performance (compared to high order codes) but allows great geometrical flexibility. The wall modeling is performed using a standard Schuman\&Grotzbach model. The computation presented here ran several weeks on 128 processors of CECI ("Consortium des Equipements de Calcul Intensif") infrastructure.

Atmospheric boundary layer

A Neutral boundary layer with a height \( H = 1000 \text{m} \) is considered. The box computed is periodic in the streamwise and the spanwise direction. We use a geostrophic wind forcing, imposed using a constant driving pressure gradient computed from Coriolis force.

Passive scalar transport

The pollutant transport is modeled using a passive scalar (concentration field \( C \)) transport equation with a source term \( S \) and \( \alpha_{C_1} = \nu_{sgs}/\alpha_{sgs} = 0.7 \).

\[ \frac{\partial C}{\partial t} + \frac{\partial \tilde{C} u_i}{\partial x_i} = \frac{\partial}{\partial x_j} \left( \kappa \frac{\partial C}{\partial x_j} \right) + S. \]

Spherical pollutant source is located at \( z/H = 0.2 \), corresponding to a realistic release height \( (h + \Delta h) \), where \( h \) is the chimney height and \( \Delta h \), the plume rise due to a combination of the gases momentum and buoyancy effects.

Statistics

The proposed model (dash line) is compared with a Lagrangian-averaged scale-independent (Meneveau et al., 1996) dynamic Smagorinsky model (solid line). The wind velocity statistics are space and time averaged. For the scalar statistics, the scalar concentration field is mapped in a cross-plane \( (z/H = 0.25) \) onto a polar grid and azimuthal averages are performed to obtain radial profiles.

Wind velocity profiles.

Scalar radial profiles.

The results obtained for mean velocity profile and for the predicted pollutant concentration are similar. The performances of the proposed model used with basic filtering and wall modeling approaches are comparable to those of advanced model at much less cost.

Snapshot of the wind velocity magnitude in a turbulent boundary layer.

The grid size is 256x256x128 = 8.4 \times 10^6 \text{ cells.}