PhD Project 2009
Ecole Doctorale I-MEP2
LEGI UMR 5519 GRENOBLE

PhD Title

Numerical simulation of turbulent flows and analysis of passive and reactive scalars for stable atmospheric boundary layer along a slope model, application to air quality modeling in valleys.

PhD Coordination

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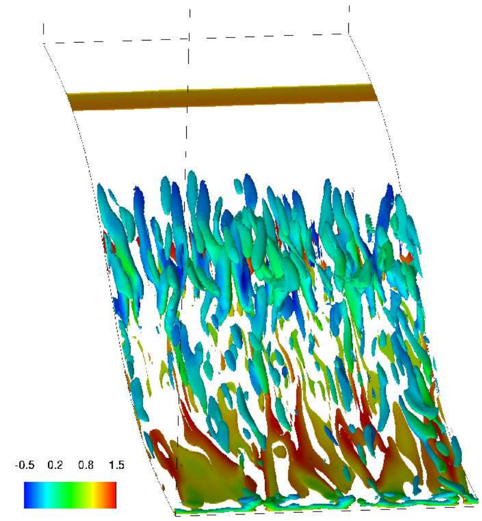

Q-criterion isovalues (colored by velocity) for turbulent structure detection in a stable atmospheric boundary layer along a slope.

Project description

Turbulence modeling for Atmospheric Boundary Layers (ABL) is still an open issue for complex terrains and during thermodynamics transients. A precise description of the flow dynamics is necessary when studying contaminants transport, including passive and reactive scalars [1]. Convective and neutral ABL in term of temperature stratification have been numerically studied since long. Stable ABL involve much smaller energy containing scales. In the frame of modern numerical methods for turbulence modeling, such as LES (Large-Eddy Simulation), numerical resolution needs to be increased. Such configuration is now being affordable [2, 3].
The present project deals with modeling and numerical simulation for atmospheric flows along slopes. Situations involving complex terrains and night-day thermodynamics cycles are concerned. At night, the ABL is stably stratified and the radiative cooling of the surface yields the development of a katabatic flow. This flow consists of a downslope wall-jet which has the structure of both wall turbulence in the inner-layer zone and shear layer turbulence in the outer-layer zone and enhances a relative mixing even though stable stratification is considered.
The numerical code used, Meso-NH, has been developed in CNRM/Météo-France and Laboratoire d'Aérologie Toulouse, and consists of a non-hydrostatic model solving the pseudo-incompressible Navier-Stokes equations with an anelastic approximation. The numerical code accounts for the whole scales involved in the atmospheric dynamics, includes models for the surface canopy and is coupled to a tool solving chemical transport and reactions. The code is parallelised (MPI) on Nec-SX8 (IDRIS France) for high performance computing and high resolutions. Preliminary computations for a 3D turbulent ABL have been performed on a slope model with 5 million grid points on 4 to 8 processors (fig. page 1). Numerical simulations involving about 100 million grid points will be performed on the new Blue Gene/P computer at IDRIS France and will allow for a precise description of the stable ABL.
Sensitivity of the model to boundary conditions will be determined to describe the effects of thermodynamic night/day cycle, surface roughness impact, space/time scalar sources. First, pollutants will be considered as passive scalars. Second, reactive mechanisms will be considered through the use of simple chemical reactions. LES of reactive scalar involve an extra subgrid-scale (SGS) term, the segregation coefficient [1, 4]. A part of the study will be dedicated to improve SGS modeling for such stable ABL configuration [5].

Numerical simulations on real complex terrains with valleys will be considered as well and configurations involving winter and/or night situations with stable ABL inducing high level of pollution will be particularly of interest [6]. Such study will be linked with similar realistic practical situations already tackled in the past [7, 8]. A systematic comparison of the transport and mixing mechanisms will be performed between the realistic and the model configuration. Results will be compared as well with experimental measurements for pollutants and used for model validation.

References

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[4] J.F. Vinuesa, F. Porté-Agel, S. Basu, and R. Stoll. SGS modeling of reacting scalar fluxes in LES of atmospheric boundary layers. *Environmental Fluid Mechanics.*, 6:115–131, 2006.

[5] C. Brun, G. Balarac, da Silva, C.B., and O. Métais. Effects of molecular diffusion on the subgrid-scale modelling of passive scalars. *Physics of Fluids*, 20(2):025102, 2008.

[6] E. Chaxel and Chollet. Ozone production from grenoble city during the august 2003 heat wave. *Atmos. Environment*, 2008. in press.

[7] C. Chemel. Simulations numériques du transport de traceurs passifs dans une atmosphère de vallée. In *Thèse de l'Université Joseph Fourier -Grenoble 1*, 2005.

[8] E. Chaxel. Photochimie et aérosols en région alpine : mélange et transport. In *Thèse de l'Université Joseph Fourier -Grenoble 1*, 2006.

Required background

- Numerical tools for turbulence modeling
- Numerical programming with fortran90
- Fluid mechanics and turbulence
- Passive and reactive scalars, chemical reactions
- Atmospheric flows