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Computational aspects of scalar dispersion modeling and simulation in complex flows

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Summary. — We present an overview of nowadays modeling capabilities and numerical challanges in the simulation of scalar dispersion phenomena in complex flows. Results from the simulation of a passive plume emitted from a line source downstream of a square obstacle are summarized to provide an example of a basic test case where the reliability of computational techniques can be carefully established.

PACS 47.27.E- – Turbulence simulation and modeling.
PACS 47.27.ek – Direct numerical simulations.
PACS 47.27.em – Eddy-viscosity closures; Reynolds stress modeling.
PACS 47.27.T- – Turbulent transport processes.

1. – Introduction

The theoretical understanding and modeling of scalar transport phenomena play a key role in several research fields, including basic fluid mechanics, heat and mass transfer and meteorology [1]. In the framework of atmospheric dispersion, the analysis of scalar transport is typically connected with the problem of predicting the dispersal of pollutants emitted from localized sources. Despite simplified models are available to predict dispersion phenomena with reasonable accuracy at the level of the regional scale, which is of the order of hundred kilometers, the analysis of scalar transport in urban areas is noticeably complicated by the geometrical details arising at the street scale, which is of the order of hundred meters [2]. An example of this scenario is presented in fig. 1, where large-scale computations in the city of Chicago are presented. The picture shows the effect of displacing the scalar source from the original position (left panel) to a location closer to the Chicago river (right panel). It is clear from the iso-surface of scalar concentration how the predicted scalar field is significantly affected by the different interaction of the plume with the underlying flow field.

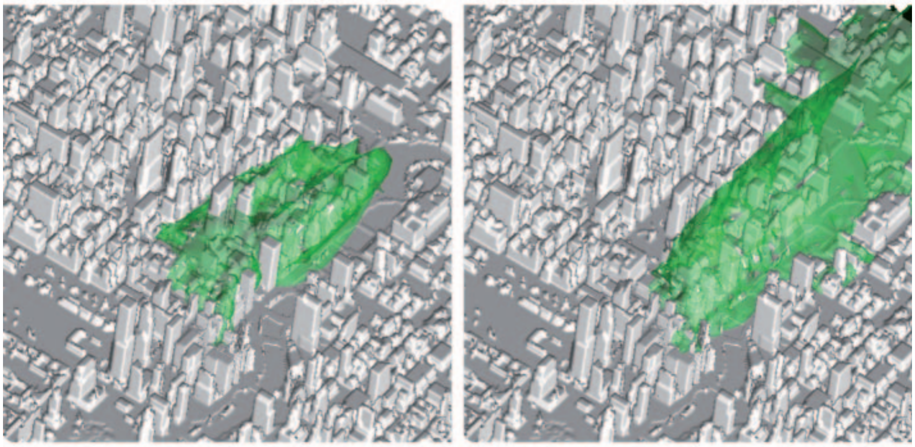

Fig. 1. – Effect of scalar source displacement in large-scale computations of urban environments.

Although experimental testing of urban dispersion has been pursued since more than three decades, Computational Fluid Dynamics (CFD) has also become a valuable and reliable tool to predict scalar transport phenomena. In this short paper, we present some results from the numerical simulation of scalar dispersion in complex flows, with the aim to provide an example of nowadays modeling capabilities as well as the numerical challanges that we still need to face in the upcoming future.

2. – Mathematical and numerical models

In this paper we restrict our attention to the dynamics and modeling of non-reacting and non-buoyant scalars. In such conditions, the scalar advection can be approximated to a *passive* mechanism, and the scalar field is governed by the following non-dimensional advection-diffusion equation:

(1) $$\frac{\partial C}{\partial t} + \frac{\partial}{\partial x_j}(U_j C) = \frac{1}{ReSc}\frac{\partial^2 C}{\partial x_j x_j}\,,$$

where Re is the flow Reynolds number and the Schmidt number $Sc = \nu/D$ gives the ratio between the momentum diffusivity of the fluid and the mass diffusivity of the scalar. From the numerical point view, the most reliable prediction of turbulent scalar transport is obtained using Direct Numerical Simulations (DNS), that is, by solving eq. (1) directly and thus without introducing further approximations into the mathematical model. As is well known in the fluid mechanics community, the scaling arguments introduced by the Kolmogorov theory of turbulence [3] show that DNS is affordable only at relative low Re numbers. In the case of atmospheric dispersion, direct simulations become even more proihibitive because of the wider range of turbulent scales occurring at large Schmidt numbers. This is shown by the following estimate of the wave number characterizing the dissipative range of the scalar field, originally introduced by the work of Batchelor [4]:

(2) $$k_{\eta c} = (\epsilon/\nu D^2)^{1/4},$$

TABLE I. – *Computational cost of numerical tools.*

Tool	No. EQs	DIMs	Grid size	Time steps	NCPUs	Total time
DNS	5	3D	586.000	100.000	64	48 h
RANS	7–10	2D	63.000	200	2	0.5 h

where ϵ denotes the dissipation of the kinetic energy associated with the momentum turbulence. Therefore, although has been proven that reliable DNS of turbulent scalar transport can be performed using numerical schemes suitable for complex geometries [5], this numerical tool can be only used to improve the basic understanding of the physical phenomenon or to establish very accurate numerical database.

Since large-scale computations of the type shown in fig. 1 cannot be afforded by direct simulations, we are forced to introduce some level of modeling in order to ameliorate the requested computational effort. The most common and less demanding approach is given by taking an ensamble average of eq. (1), which leads to the RANS (Reynolds-Averaged Navier-Stokes) formulation of the scalar transport equation

$$\frac{\partial \overline{C}}{\partial t} + \frac{\partial}{\partial x_j}(\overline{U}_j \overline{C}) = \frac{1}{ReSc}\frac{\partial^2 \overline{C}}{\partial x_j x_j} - \frac{\partial}{\partial x_j}(\overline{u_j c}), \tag{3}$$

where the overline denotes averaged quantities and lowercase letters represent fluctuating values of primitive variables. The new unknown $\overline{u_j c}$ at the right hand side of eq. (3) is usually termed the vector of *turbulent scalar fluxes*. It originates from the averaging operation and represents the effect of turbulent motions on the mean scalar field. Most of empirical models developed in the past to provide an approximation to $\overline{u_j c}$ relied on the analogy with molecular transport phenomena. This leads to the so-called *gradient-transport* type closures

$$\overline{u_i c} = -D^t_{ij}\frac{\partial \overline{C}}{\partial x_j}\,, \tag{4}$$

where D^t_{ij} represents the *turbulent-diffusivity* tensor. Despite the simplicity of such type of models, recent studies have shown that they can be applied successfully to scalar dispersion in complex flows when a suitable estimate of velocity fluctuations u_j is available and retaining the anisotropic character of the diffusivity tensor D^t_{ij} [6]. In the next section, we present briefly some results from the numerical simulation of scalar dispersion downstream of a square obstacle fully immersed in a turbulent boundary layer. The computations are performed using DNS as well as RANS models, while numerical discretization is carried out using unstructured finite-volume schemes. Table I provides a summary of the computational effort required by the different simulation techniques.

3. – Results

The turbulent dispersion of a passive plume emitted from a line source downstream a square obstacle provides a basic test case to establish the reliability of computational techniques. The obstacle is fully immersed in a turbulent boundary layer and flow separation occurs behind it. The flow Reynolds number is 700, based on the free-stream velocity and the obstacle height H.

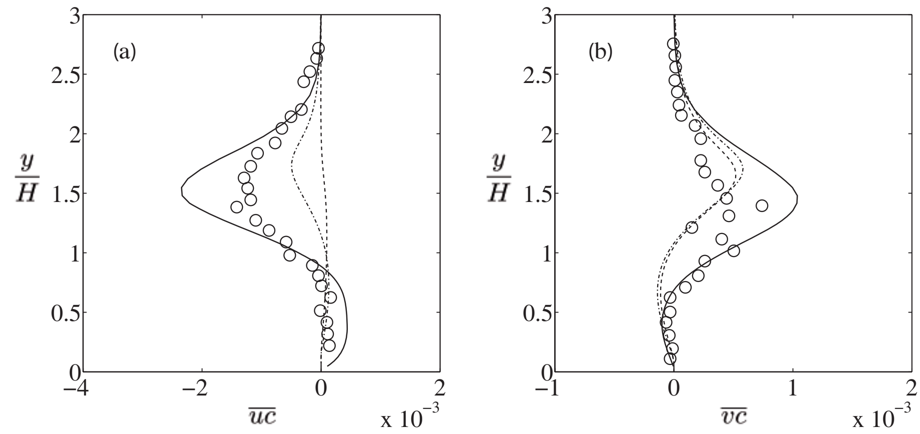

Fig. 2. – Profiles of turbulent scalar fluxes in a passive plume emitted downstream of a square obstacle: (a) streamwise flux, (b) vertical flux; —— DNS, –·– anisotropic scalar flux model, – – – isotropic scalar flux model, ∘ measurements [7].

Since accurate predictions of mean scalar concentration require reliable estimations of turbulent scalar fluxes, the computed profiles of $\overline{u_j c}$ using DNS and scalar flux models of the type (4) are compared in fig. 2 to experimental measurements [7]. The results given by DNS show that unstructured finite-volume schemes can be applied successfully to scalar dispersion in complex flows. However, the analysis of several inflow conditions, not reported here for the sake of brevity, has shown that the generation of realistic velocity fluctuations in the approaching flow is mandatory in order to get satisfactory results [8].

Although the modeling of momentum turbulence is always of prime concern in the framework of RANS modeling, fig. 2 also shows that isotropic models, which are customary in the CFD community, are not consistent with experimental and DNS results. Therefore, a significant effort should be also directed toward the improvement of scalar flux modeling.

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