H13-123

A NEW OPERATIONAL MODELLING APPROACH FOR ATMOSPHERIC DISPERSION IN INDUSTRIAL COMPLEX AREAS

Florian Vendel[1], Guillevic Lamaison[1], Lionel Soulhac[1], Ludovic Donnat[2], Olivier Duclaux[2], and Cécile Puel[2]

[1]Laboratoire de Mécanique des Fluides et d'Acoustique, Université de Lyon CNRS, Ecole Centrale de Lyon, INSA Lyon, Université Claude Bernard Lyon I, 36 avenue Guy de Collongue, 69134 Ecully, France
[2]TOTAL, Centre de Recherche de Solaize, France

Abstract: In this paper, we present an operational modelling approach for atmospheric dispersion in industrial complex area. This approach is based on the idea that the flow, in the surface boundary layer and in the vicinity of the obstacles, depends on the geometry of the surface, which is given, and on a few meteorological parameters: the velocity scale u_*, the wind direction φ and a stability parameter $1/L_{MO}$. We showed by a dimensional analysis that it is possible to eliminate the velocity scale so that the normalized wind and turbulence fields are only functions of two parameters. Then we create, by CFD numerical simulations, a wind field database for a finite number of discrete values of these two parameters. Once the database is completed, one can calculate the wind field for any meteorological situation by interpolation between the wind fields in the database. A sensitivity analysis of the sampling intervals for the wind direction φ and the stability parameter $1/L_{MO}$ was done in order to limit the interpolation error. Finally, for use in operational conditions, a lagrangian dispersion model was developed and coupled with the interpolated wind field to simulate rapidly the concentration impact.

Key words: *CFD simulations, wind field database, operational tools, lagrangian dispersion model*

INTRODUCTION

Monitoring the emission of air pollutants, either canalized or fugitive ones, is a key issue for industrials to quantify and reduce their environmental impact. In the near field of sources located close to the ground, it becomes important to take into account the effects of the complex topography (buildings, obstacles) on the flow field and on the turbulent dispersion of pollutants. But the modelling of flow and dispersion over complex terrain is a difficult task which requires generally expensive CFD numerical simulations which are rarely compatible with operational needs such as pollution monitoring and emergency response. Therefore it is necessary to develop simplified modelling approaches to describe the atmospheric dispersion over complex industrial areas.

Simplified empirical or analytical approaches exist for modelling obstacles (such as parameterization of isolated obstacles or "street-canyon" models) but they do not fit with the complexity of industrial areas. The "mass consistent wind field model" approaches (Rockle, 1990) is an interesting solution regarding calculation time, but it is generally too simplified concerning the modelled physical processes since only the mass conservation equation is satisfied. In this paper, we propose a new modelling approach, based on the use of precise and detailed CFD calculations, which are stored in a database and then coupled with a real time lagrangian particle dispersion model.

In the first part, we present the modelling approach. In the second part, we discuss the discretization of the wind field database and in the last part we describe briefly the coupling with a lagrangian dispersion model for the operational applications.

DESCRIPTION OF THE MODELLING APPROACH

Physical analysis

In this paper, we are interested to describe the atmospheric flow in the surface boundary layer (about one tenth of the atmospheric boundary layer height) and in the building canopy, for horizontal areas smaller than 2 km. At this scale, one can assume that the wind field depends on three parameters groups:

- **Geometrical parameters**, which describe all the complexity of the ground surface, including buildings, obstacles, micro relief, etc. For a given industrial area, we will consider that these parameters are fixed, so that it will not be possible to change a geometrical characteristic during the operational use of our modelling tool.
- **Meteorological parameters**: at the selected scale, one can assume that the only three meteorological parameters needed to describe the surface layer are the friction velocity u_*, the wind direction φ and the Monin-Obukhov length L_{MO} which represents the stratification effects.
- **Source release conditions**: the momentum and thermal characteristics of the releases influence the flow in the vicinity of the sources. In this work, we make the important assumption that the interaction between the sources dynamical effects and the complex buildings are small so that it will be possible to model these effects through a parameterization in the dispersion model (integral jet and plume rise model).

Assuming that the geometrical parameters are fixed and that the source effects will be parameterized in the dispersion model, one can conclude that the wind field over a complex area depends only on u_*, φ and L_{MO}.

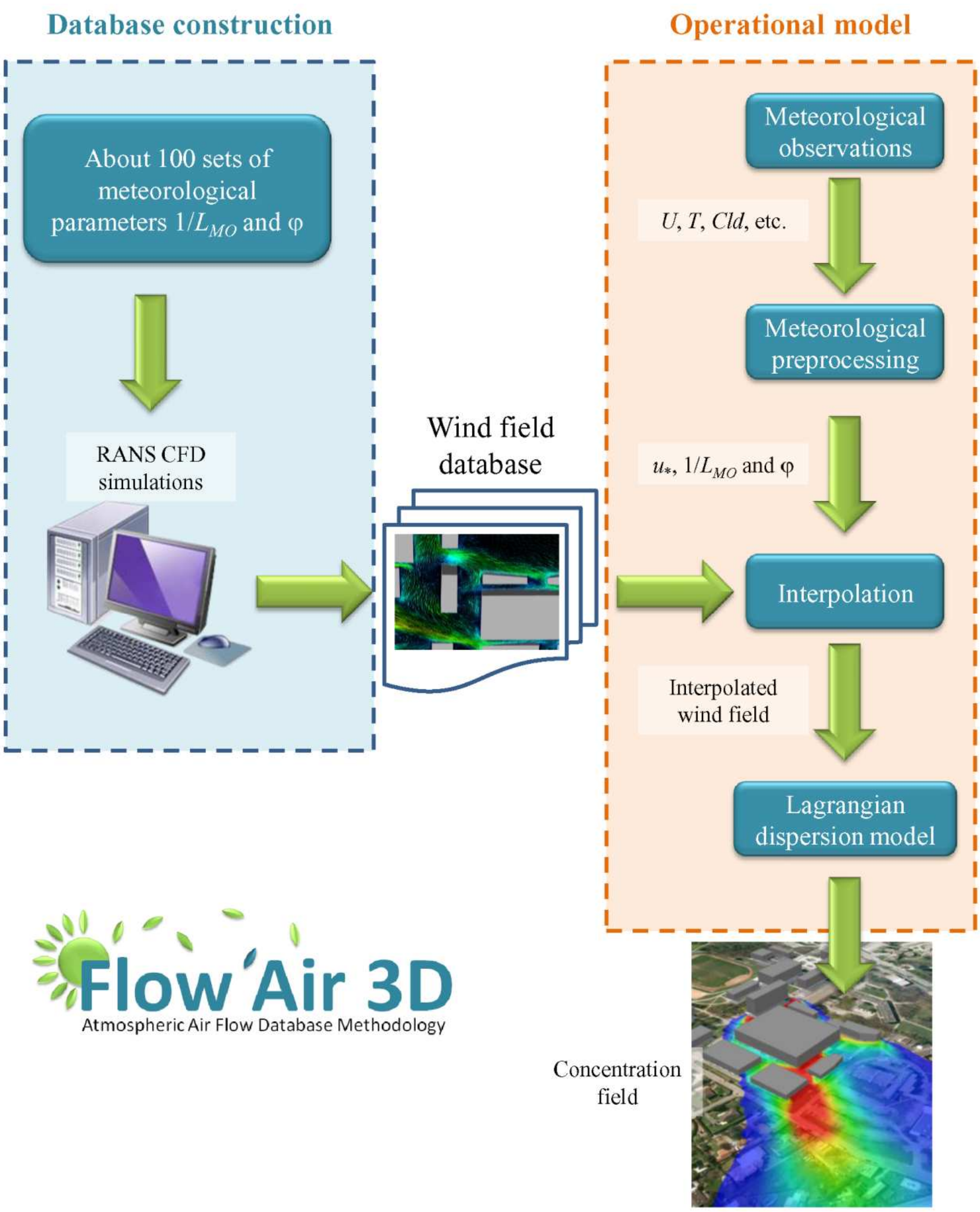


Figure 1. Principles of the atmospheric air flow database methodology.

The Monin-Obukhov length L_{MO} is a non continuous variable because it tends to infinity near the neutral stratification. In order to avoid mathematical discontinuity near the neutral case, in our analysis we will use the parameter $1/L_{MO}$. By dimensional analysis, it is easy to show that the dependence on the parameter u_* is linear so that the velocity field can be expressed as:

$$\vec{u} = u_* \vec{f}_u \left(1/L_{MO}, \varphi\right) \tag{1}$$

where $\vec{f}_u$ is a normalised velocity field. For the same reason, we can derive such expressions for the turbulent kinetic energy k and for the turbulent dissipation rate ε:

$$k = u_*^2 f_k \left(1/L_{MO}, \varphi\right) \tag{2}$$

$$\varepsilon = \frac{u_*^3}{\kappa z} f_\varepsilon \left(1/L_{MO}, \varphi\right) \tag{3}$$

The function f_u, f_k and f_ε are obviously 3D fields which depends on the space coordinates (x,y,z) but this dependence will not be explicitly written in the equations for more readability. To calculate these functions, we use CFD calculations, based on the solution of the full conservation equations for mass, momentum and energy. As detailed in another Harmo13 paper (Vendel F. *et al.*, 2010 – H13-124), these equations are solved with the Reynolds Averaged Navier-Stokes (RANS) formulation, with the turbulence modeled by a k-ε closure.

Wind field database approach

Then, the main idea of our approach (see figure 1) is to perform many CFD calculations to represent the flow in the surface layer and around buildings for various meteorological conditions (direction and stability). All the velocity and turbulence fields are collected to create a large wind field database. This database is created before the operational use so that it allows detailed calculations without the limitation of computational time. The number of meteorological conditions studied is about 100 in order that the duration of the database construction does not exceed one month.

During the operational use, the wind field is selected from the database according to the meteorological conditions recorded on the site. To do that, a meteorological pre-processor, based on the works review of Fischer B.E.A. *et al.* (1998), is used to estimate the friction velocity u_* and the stability parameter $1/L_{MO}$. The wind field is then interpolated for these parameters, from the nearest wind fields in the database. We apply a bi-dimensional linear interpolation procedure, as expressed in the equation:

$$\tilde{\vec{u}} = u_* \left[a_1 \vec{f}\left(1/L_{MO,\inf}, \varphi_{\inf}\right) + a_2 \vec{f}\left(1/L_{MO,\inf}, \varphi_{\sup}\right) + a_3 \vec{f}\left(1/L_{MO,\sup}, \varphi_{\inf}\right) + a_4 \vec{f}\left(1/L_{MO,\sup}, \varphi_{\sup}\right)\right] \quad (4)$$

where $L_{MO,\inf}$, $L_{MO,\sup}$, $\varphi_{\inf}$ and $\varphi_{\sup}$ are the parameters defining the four nearest wind fields in the database and a_1, a_2, a_3 and a_4 are the corresponding interpolation coefficients. Finally, given the sources characteristics and the interpolated wind field, a lagrangian dispersion model is used to make the calculation of the pollutants concentrations.

Validity and limitations

The construction of the final wind field by interpolation is certainly the main approximation of this methodology because there is no evidence that the interpolated field will be solution of the conservation equation for momentum, energy and turbulence. The only equation that is rigorously satisfied is the mass conservation equation. Indeed, the linearity of the interpolation procedure of equation (4) implies that the interpolated wind field is solution of the continuity equation since each database field is solution of the same equation. Consequently, one can say that our methodology is "at least" a mass consistent approach.

In order to verify that the interpolated wind field is a good approximation of the "exact" wind field, we have done a sensitivity analysis on the discretization of the wind field database. This discussion is presented in the next part.

DISCRETIZATION OF THE WIND FIELD DATABASE

The aim of this section is to evaluate and quantify the differences between the interpolated and the exact wind fields, for different values of the interpolation interval for φ and $1/L_{MO}$. This analysis is described firstly for the wind direction φ and then for the stratification parameter $1/L_{MO}$.

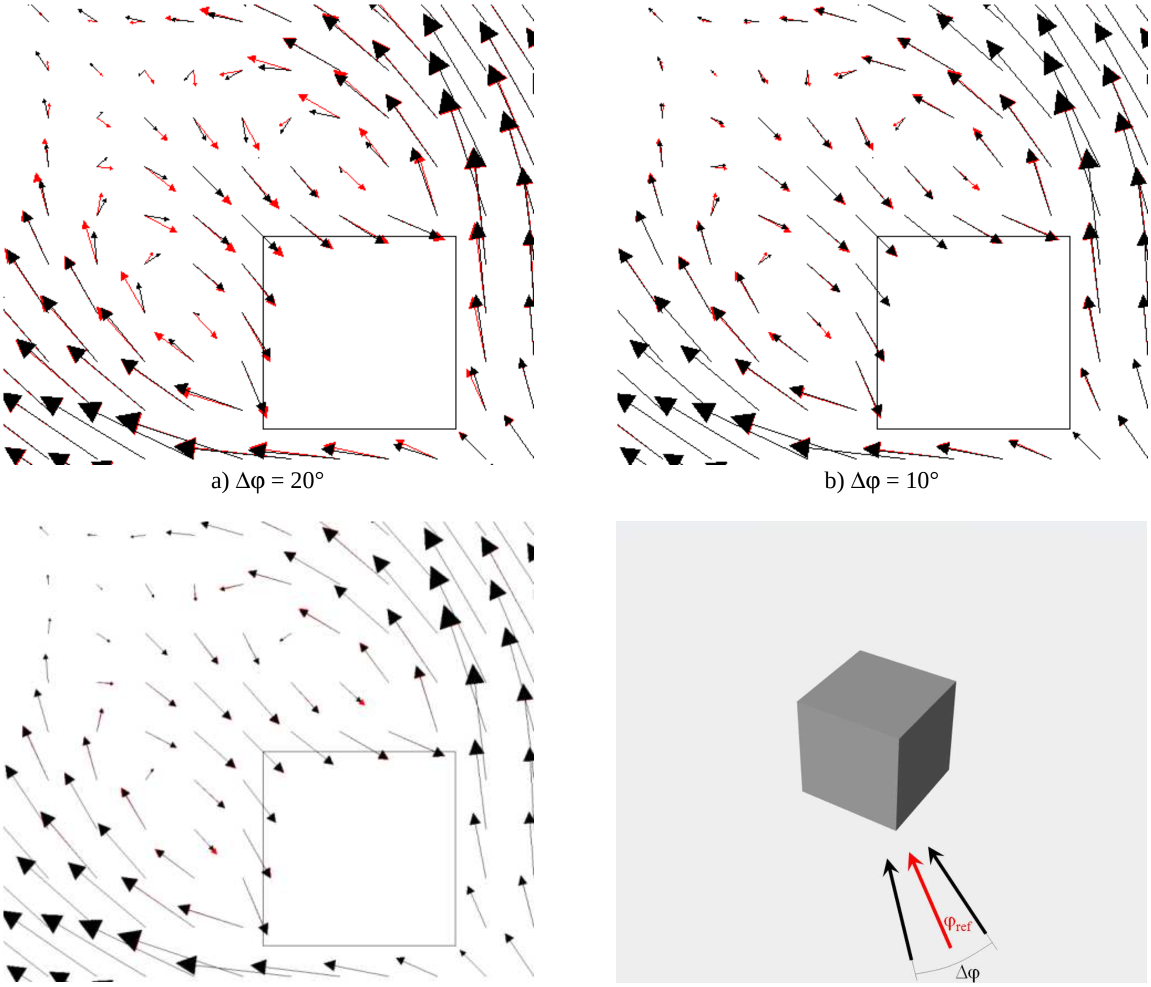
Discretization of the wind direction

The main difficulty of the discretization analysis is that it is not possible to find a general argumentation to demonstrate that a certain value of the discretization interval Δφ will make sure that the interpolation error will be bounded, whatever the flow considered. In this work, our methodology was to choose a geometrical setup sufficiently complex and representative of real cases to be studied, in order to test the interpolation process efficiently.

We present on figure 2 the case of the flow around a cubical obstacle. The methodology consists in a comparison between the "exact" wind field (in red) simulated for a wind direction φ_{ref} = 135° and the wind field linearly interpolated (in black) between two wind fields calculated for $\varphi = \varphi_{ref} \pm \frac{1}{2}\Delta\varphi$. Figure 2 illustrates the results for Δφ = 20°, Δφ = 10° and Δφ = 4°. One can observe that the interpolation error increases with Δφ but also that the differences are mainly located in the near wake of the obstacle. A quantitative analysis over the entire wind field shows that for Δφ = 20°, the error is larger than 2% for less than 2% of the volume of fluid. These error zones are mainly located in the recirculation zones where the mean velocity is close to zero. Different sensitivity tests allow us to conclude that a discretization interval of 20° gives relatively good results for the interpolation between two wind fields.

Discretization of the stratification parameter $1/L_{MO}$

In order to evaluate the interpolation procedure for the stratification parameters, we consider the case of a diabatic surface layer on a flat ground. One can assume that the presence of obstacles would limit the influence of the thermal stratification and that the case of the flat ground can be seen as a "worse case test" for stratification. In order to compare the interpolated wind field with a reference case, we have used the reference solution for u, k and ε derived from the Monin-Obukhov similarity theory and given by equation (5), (6) and (7) (see Vendel F. *et al.*, 2010 – H13-124 for details):



a) Δφ = 20° b) Δφ = 10°

c) Δφ = 4° d) Geometrical settings

Figure 2. Comparison between the “exact” wind field (in red) and the interpolated wind field (in black) for different interpolation intervals for the wind direction Δφ.

- Mean velocity:

$$u(z) = \frac{u_*}{\kappa}\left[\ln(z/z_0) - \psi_m(\zeta)\right] \tag{5}$$

where $\zeta = z/L_{MO}$, ψ_m and ψ_h are the integrated universal functions of the Monin-Obukhov theory for which one can find analytical expressions in Garratt J.R. (1992).

- Turbulent kinetic energy:

$$k(z) = \frac{u_*^2}{\sqrt{c_\mu}}\sqrt{1 - \frac{\zeta}{\phi_m(\zeta)}} \tag{6}$$

where c_μ is a constant of the k-ε turbulence model (given equal to 0.033 by Duynkerke P.G., 1988) and ϕ_m is the universal functions of the Monin-Obukhov theory (Garratt J.R., 1992).

- Turbulent dissipation rate:

$$\varepsilon(z) = \frac{u_*^3}{\kappa z}\phi_m(\zeta)\left[1 - \frac{\zeta}{\phi_m(\zeta)}\right] \tag{7}$$

The k-ε turbulence model provides also an equation for the momentum turbulent diffusivity:

$$K_m = c_\mu \frac{k^2}{\varepsilon} \tag{8}$$

Comparisons between “exact” and interpolated profiles for u, k, ε, and K_m are plotted as a function of $1/L_{MO}$ on figure 3. Seven discrete values for $1/L_{MO}$ are chosen not regularly spaced: –0.2, – 0.05, – 0.002, 0, 0.002, 0.05, 0.2. With this discretization, one can observe that the error does not exceed 7% for u, 5% for k, 12% for ε and 15% for K_m. One can conclude that such errors are acceptable for an operational model.

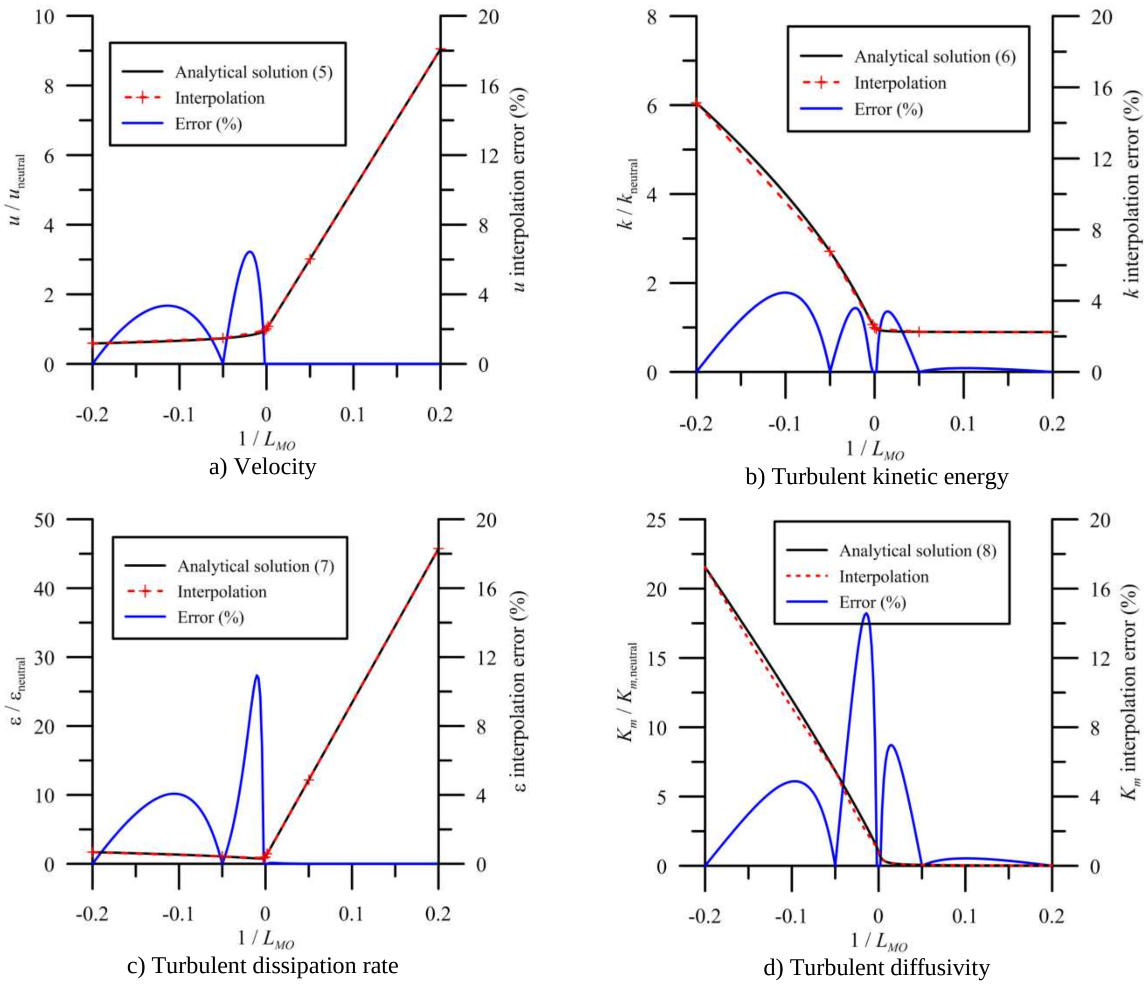


Figure 3. Comparison between the "exact" profiles (in black) and the interpolated profiles (in red) for u, k, ε, and K_m plotted as a function of the stability parameter $1/L_{MO}$. The red cross represents the discrete values of $1/L_{MO}$.

COUPLING WITH A LAGRANGIAN DISPERSION MODEL

Once an interpolated wind field is calculated, we use a lagrangian particle dispersion model based on a Langevin equation to simulate the dispersion of non-reactive species. Such modelling approach is well adapted to the complexity of the wind and turbulence fields around obstacles and requires low computational cost. The velocity fluctuations and the lagrangian time scale needed by the dispersion model are calculated from the turbulent variables k and ε. An integral jet and plume rise model has been added to take into account the near source effects that have not been treated in the wind field calculation.

CONCLUSION

In this work, we have proposed a new modelling approach based on the application of RANS CFD simulations to build a wind field database. During the operational use of our model, a wind field is interpolated from the database and coupled with a lagrangian dispersion model. In this paper, we have discussed the validity of the interpolation approach and we have presented a sensitivity analysis in order to evaluate the interpolation error for different sampling intervals in the database. The good validity and the short computational time needed by this operational modelling methodology make it well adapted to study dispersion over complex industrial areas.

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