Modelling diabatic atmospheric boundary layer using a RANS-CFD code with a k-ε turbulence closure

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Introduction

Context

- Modelling of pollutant dispersion over industrial areas implies the description of the stratified surface layer flow and its interaction with buildings or complex obstacles
- Better computers performances make it possible today to simulate this flow using CFD models and RANS equations (Fluent, Phoenics, StarCD…)
- But, generally standard parameterization implemented in these commercial models are not really adapted so as to represent the atmosphere

So the question is : how to parameterize the atmospheric processes, particularly thermal stratification in a RANS-CFD code?

Introduction

CFD modelling of the SBL in the literature

- **Application of CFD models in neutral stability conditions**
  - Richards P.J. and Hoxey R.P., 1993
  - Blocken B. and al., 2007
  - Hargreaves D.M. and Wright N.G., 2007
- **Application in stable or unstable stability conditions (less studied)**
  - Duynkerke P.G., 1988 : modification of the k-ε model constants to match the physical characteristic of atmospheric surface layer in neutral and stable conditions
  - Huser A. and al., 1997 : inlet turbulence profiles does not maintain with distance (turbulence increase in stable stratification)
  - Pontiggia M. and al., 2009 : add a source term in turbulent dissipation rate ε equation

Introduction

Main points to model

- To model a surface boundary layer with RANS-CFD codes, we focus on two main points :

Top boundary conditions

Inlet boundary conditions

Equations solved :

•Momentum equations

•Energy equation

•Turbulence closure

Outflow boundary conditions

Ground boundary conditions

Introduction

Some questions unsolved

- Equations solved :
  - Which set of equations models properly the flow and the turbulence for a diabatic surface layer ?
  - How to treat the inconsistency between the k and ε profiles (stable/unstable conditions) and the conservation equations ?
- Boundary conditions :
  - How to describe the pressure profile in order to define appropriate downwind boundary conditions for stable and unstable cases ?
  - How to describe the inlet profiles to represent diabatic surface layer ?
  - How to impose a constant flux of momentum and energy with the altitude (surface boundary layer assumption) ?

Summary

1. Reference model of the surface boundary layer
2. Consistency with k and ε equations
3. Parameterization of a diabatic surface layer in a RANS CFD simulation

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1. – Reference model of the surface boundary layer

Surface boundary layer assumptions

- The flow is oriented along the x direction and the mean vertical velocity is equal to zero : $\bar{v} = \bar{w} = 0$ (1)

- The vertical turbulent fluxes (Reynolds stresses and heat flux) are constant with respect to altitude *(Garratt J.R., 1992)* :

$$\begin{cases} \overline{u'w'} = cste = -u_*^2 \\ \overline{w'\theta'} = cste = \dfrac{H_0}{\rho_0 C_p} = -u_* \theta_* \end{cases} \qquad (2)$$

- The Monin-Obukhov similarity theory predicts that the dimensionless gradient of velocity and potential temperature only depends on z/L_{MO} *(Garratt J.R., 1992)* :

$$\begin{cases} \dfrac{\kappa z}{u_*} \dfrac{\partial \bar{u}}{\partial z} = \phi_m(\zeta) \\ \dfrac{\kappa z}{\theta_*} \dfrac{\partial \bar{\theta}}{\partial z} = \phi_h(\zeta) \end{cases} \quad \text{where} \quad \zeta = \frac{z}{L_{MO}} \quad \text{and} \quad L_{MO} = -\frac{\rho_0 C_p \theta_0 u_*^3}{\kappa g H_0} \qquad (3)$$

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1. – Reference model of the surface boundary layer

Surface boundary layer assumptions

- The turbulence satisfies a local equilibrium within the surface layer *(Tennekes, H. and Lumley, J. L., 1972)* :

$$P + B = \varepsilon \quad \text{with} \quad \begin{cases} P = -\overline{u'w'}\dfrac{\partial \overline{u}}{\partial z} = shear\ TKE\ production \\ B = \dfrac{g}{\theta_0}\overline{w'\theta'} = thermal\ TKE\ production / destruction \\ \varepsilon = turbulent\ dissipation\ rate \end{cases} \qquad (4)$$

- Influence of buoyancy effects in the momentum equation can be taken into account using Boussinesq approximation (the density is constant except in the buoyancy term of the momentum equation) :

$$\rho \approx \rho_0 = cste \qquad (5)$$

$$(\rho - \rho_0)g \approx -\rho_0 \beta (\theta - \theta_0) g \quad \text{with} \quad \beta \approx \frac{1}{\theta_0} \quad \text{for an ideal gas} \qquad (6)$$

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1. – Reference model of the surface boundary layer

Conservation equations

- When using the precedent assumptions, the Reynolds Averaged Navier-Stokes (RANS) conservation equations for the mass, horizontal momentum and energy are verified and the vertical momentum equation reduces to :

$$\frac{\partial \overline{P}}{\partial z} = -\rho_0 \beta (\theta - \theta_0) g \qquad \text{with} \qquad \overline{P_{abs}} = \overline{P} + P_0 - \rho_0 g z \qquad (7)$$

Where $\overline{P}$ is defined as difference between absolute and hydrostatic pressure.

- Integration of this equation will give the vertical profile of $\overline{P}$ in a stable boundary layer.

- $\overline{P}$ is constant for the neutral case, where $\theta(z) = \theta_0$

1. – Reference model of the surface boundary layer

k-ε turbulence closure

- In order to model the turbulence fluxes, we use in this work a k-ε turbulent closure :

$$\begin{cases} \overline{u'w'} = -K_m \dfrac{\partial \overline{u}}{\partial z} \\ \overline{w'\theta'} = -K_h \dfrac{\partial \overline{\theta}}{\partial z} \end{cases} \quad \text{with} \quad K_m = C_\mu \frac{k^2}{\varepsilon} \quad \text{and} \quad K_h = \frac{K_m}{\mathrm{Pr}_t} \tag{8}$$

Where k is the turbulent kinetic energy, ε the turbulent dissipation rate and K_m and K_h are the turbulent diffusivity of momentum and heat.

- k and ε are given by two conservation equations (steady surface layer) :

$$\underbrace{\frac{\partial}{\partial z}\left(\frac{K_m}{\sigma_k}\frac{\partial k}{\partial z}\right)}_{D} + P + B - \varepsilon = 0 \tag{9}$$

Where D is the diffusion term

$$\frac{\partial}{\partial z}\left(\frac{K_m}{\sigma_\varepsilon}\frac{\partial \varepsilon}{\partial z}\right) + C_{\varepsilon 1}\frac{\varepsilon P}{k} - C_{\varepsilon 2}\frac{\varepsilon^2}{k} = 0 \tag{10}$$

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1. – Reference model of the surface boundary layer

k-ε turbulence closure

- Focus on the turbulent dissipation rate equation :

$$\frac{\partial}{\partial z}\left(\frac{K_m}{\sigma_\varepsilon}\frac{\partial \varepsilon}{\partial z}\right)+C_{\varepsilon 1}\frac{\varepsilon P}{k}-C_{\varepsilon 2}\frac{\varepsilon^2}{k}=0$$

- No term for the buoyancy effects *(Duynkerke P.G., 1988)*
- The use of k-ε model requires values for the parameters C_μ, σ_k, σ_ε, $C_{\varepsilon 1}$, $C_{\varepsilon 2}$
- For simulating realistic atmospheric values of the TKE in the surface layer ($k = 1/2\left(\sigma_u^2+\sigma_v^2+\sigma_w^2\right)\approx 5.5u_*^2$ *Garratt J. R., 1992*), we use the modified constant set proposed by *Duynkerke P. G., 1998*.

c_μ	σ_k	σ_ε	$c_{\varepsilon 1}$	$c_{\varepsilon 2}$
0.033	1.0	2.38	1.46	1.83

Table 1. Duynkerke constants for the k-ε model

$$\begin{cases} \overline{u'w'} = cste = -u_*^2 \\ \overline{w'\theta'} = cste = -u_*\theta_* \end{cases} \quad (2)$$

$$\begin{cases} \frac{\kappa z}{u_*}\frac{\partial \overline{u}}{\partial z} = \phi_m(\zeta) \\ \frac{\kappa z}{\theta_*}\frac{\partial \overline{\theta}}{\partial z} = \phi_h(\zeta) \end{cases} \quad (3)$$

$$P + B = \varepsilon$$

with

$$\begin{cases} P = -\overline{u'w'}\frac{\partial \overline{u}}{\partial z} \\ B = \frac{g}{\theta_0}\overline{w'\theta'} \end{cases} \quad (4)$$

$$\frac{\partial \overline{P}}{\partial z} = -\rho_0\beta(\theta-\theta_0)g \quad (7)$$

$$\begin{cases} \overline{u'w'} = -K_m\frac{\partial \overline{u}}{\partial z} \\ \overline{w'\theta'} = -K_h\frac{\partial \overline{\theta}}{\partial z} \end{cases}$$

with

$$K_m = C_\mu\frac{k^2}{\varepsilon}$$

and

$$K_h = \frac{K_m}{\Pr_t} \quad (8)$$

1. – Reference model of the surface boundary layer

Set of equations for the vertical profiles

- Integration of (3) gives classical logarithmic velocity and temperature profiles :

$$\begin{cases} \overline{u}(z) = \frac{u_*}{\kappa}\left[\ln\left(z/z_0\right) - \psi_m(\zeta)\right] \\ \overline{\theta}(z) = \theta_0 + \frac{\theta_*}{\kappa}\left[\ln\left(z/z_t\right) - \psi_h(\zeta)\right] \end{cases} \quad (11)$$

Where ψ_m et ψ_h are the integrated universal functions of the Monin-Obukhov theory

- Integrations of (7) using the precedent relations (11) provides :

$$\overline{P}(z) = -\frac{\rho_0 g\theta_*}{\kappa\theta_0}\int_0^z\left[\ln\left(z/z_t\right) - \psi_h(\zeta)\right]dz \quad (12)$$

- With equation (2), (3), (4), one can derive the profile of ε:

$$\varepsilon(z) = \frac{u_*^3}{\kappa z}\phi_m(\zeta)\left[1 - \frac{\zeta}{\phi_m(\zeta)}\right] \quad (13)$$

- Combining equations (2), (8), (13) gives the profile of k :

$$k(z) = \frac{u_*^2}{\sqrt{C_\mu}}\sqrt{1 - \frac{\zeta}{\phi_m(\zeta)}} \quad (14)$$

- Equations (8), (13), (14) provide the profile K_m: $K_m(z) = \frac{u_*\kappa z}{\phi_m(\zeta)}$ (15)

$$\underbrace{\frac{\partial}{\partial z}\left(\frac{K_m}{\sigma_k}\frac{\partial k}{\partial z}\right)}_{D}+P+B-\varepsilon=0 \quad (9)$$

$$\frac{\partial}{\partial z}\left(\frac{K_m}{\sigma_\varepsilon}\frac{\partial \varepsilon}{\partial z}\right)+C_{\varepsilon 1}\frac{\varepsilon P}{k}-C_{\varepsilon 2}\frac{\varepsilon^2}{k}=0 \quad (10)$$

$$P+B=\varepsilon \quad (4)$$

1. – Reference model of the surface boundary layer

Conclusion

- This set of solution has been used by several authors to define the upwind boundary conditions for a RANS-CFD calculation of a diabatic surface layer *(Huser A. and al., 1997; Pontiggia M. and al., 2009)*

- The main problem is that the conservation equation for k (9) and the conservation equation for ε (10) have not been used to derive this set of solution
  - In neutral condition k is constant, so D is equal to zero and the equation (9) becomes (4). In order to satisfy (10), the next relation must be verified :

$$\sigma_\varepsilon=\frac{\kappa^2}{(C_{\varepsilon 2}-C_{\varepsilon 1})\sqrt{C_\mu}}$$

  - In stable/unstable conditions we have seen that k depends of z, so D is not null :

So for a diabatic surface layer these conservations equations have no reason to be satisfied by the two turbulent profiles described before

$$P + B = \varepsilon$$

with

$$\begin{cases} P = -\overline{u'w'}\dfrac{\partial \overline{u}}{\partial z} \\ B = \dfrac{g}{\theta_0}\overline{w'\theta'} \end{cases} \quad (4)$$

$$\underbrace{\frac{\partial}{\partial z}\left(\frac{K_m}{\sigma_k}\frac{\partial k}{\partial z}\right)}_{D} + P + B - \varepsilon = 0 \quad (9)$$

2. – Consistency with the *k* and *ε* conservation equations

Equation of *k*

- The consistency between equations (4) and (9) implies that the diffusion term D should be equal to 0. If σ_k is a constant, one can show that D cannot be null, except for the neutral case.
  - *Freedman F.R. and Jacobson M.Z. (2003)* suggest that the value of D does not exceed 10^{-3}.(P+B)
  - We propose to evaluate the ratio between D and the TKE k, which can be interpreted as the inverse of a characteristic time t_k for k to vary significantly from the "pseudo" equilibrium value. Near the ground :

$$t_k = \left|\frac{k}{D}\right| \approx \left|\frac{2L_{MO}\sigma_k}{u_*\kappa}\right| \quad \text{for} \quad \zeta = \frac{z}{L_{MO}} << 1 \qquad (15)$$

$$k(z)=\frac{u_*^2}{\sqrt{C_\mu}}\sqrt{1-\frac{\zeta}{\phi_m(\zeta)}} \qquad (14)$$

2. – Consistency with the k and ε conservation equations

Interpretation

- For example, with L_{MO}=50 m and u_*=0.25 m.s^{-1}, the characteristic time t_k for k to vary significantly from (14) is about 1000 s
- More generally, one can predict that for studying an atmospheric SBL in a short domain (<1 km), an inflow boundary condition based on equation (14) for k will remain almost constant when using k-ε turbulence model with a constant σ_k
- For larger domains, we suggest to introduce a non-constant parameterization of σ_k, in order to ensure the local equilibrium

$$\frac{\partial}{\partial z}\left(\frac{K_m}{\sigma_\varepsilon}\frac{\partial \varepsilon}{\partial z}\right)+C_{\varepsilon 1}\frac{\varepsilon P}{k}-C_{\varepsilon 2}\frac{\varepsilon^2}{k}=0 \quad (10)$$

$$\varepsilon(z)=\frac{u_*^3}{\kappa z}\phi_m(\zeta)\left[1-\frac{\zeta}{\phi_m(\zeta)}\right] \quad (13)$$

2. – Consistency with the *k* and *ε* conservation equations

Equation of *ε*

- In the assumption of an homogeneous and steady SL, it is required that the profile of ε will be solution of the conservation equation. But introducing (13) in (10) gives :

$$T=\frac{\partial}{\partial z}\left(-\frac{R_i'}{\sigma_\varepsilon R_i}\right)+\frac{1}{L_{MO}^2}\frac{\sqrt{1-R_i}}{R_i^2}\left(\frac{C_{\varepsilon 2}\sqrt{C_\mu}}{\kappa^2}R_i-\frac{1}{\sigma_{\varepsilon,N}}\right)=0 \quad (17)$$

with $R_i=\frac{\zeta}{\phi_m(\zeta)}$, $R_i'=\frac{dR_i}{d\zeta}$ and $\sigma_{\varepsilon,N}=\frac{\kappa^2}{(C_{\varepsilon 2}-C_{\varepsilon 1})\sqrt{C_\mu}}$

- In the neutral case, this equation is satisfied by “adjusting” the value of the constant σ_ε, but in the diabatic case, it is no more possible to satisfy equation (17) with a constant value of σ_ε
- In the same way we estimate the ratio ε/T. It can be derived near the ground :

$$t_\varepsilon=\left|\frac{\varepsilon}{T}\right|\approx\left|\frac{\kappa L_{MO}\sigma_k}{C_{\varepsilon 2}\sqrt{C_\mu}u_*}\right| \quad \text{for} \quad \zeta=\frac{\zeta}{L_{MO}}<<1 \quad (18)$$

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2. – Consistency with the *k* and *ε* conservation equations

Interpretation

- For example, with L_{MO}=50 m and u_*=0.25 m.s^{-1}, the characteristic time t_ε for ε to vary significantly from the equilibrium is about 240 s
- More generally, one can predict that for studying an atmospheric SBL even on a relatively short distance (>100 m), solution (13) for turbulent dissipation rate will not maintain with distance when using a k-ε turbulence model with a constant σ_ε
- Therefore we suggest introducing a non constant parameterization of σ_ε :

$$\sigma_\varepsilon = \frac{1}{\frac{\sqrt{C_\mu} C_{\varepsilon 2}}{\kappa^2 L_{MO}} \cdot z \cdot \ln(z + z_0) + \frac{1}{\sigma_{\varepsilon,N}}} \quad \text{for} \quad \zeta = \frac{\zeta}{L_{MO}} << 1$$

$$\begin{cases} \bar{u}(z) = \frac{u_*}{\kappa}\left[\ln\left(z/z_0\right) - \psi_m(\zeta)\right] \\ \bar{\theta}(z) = \theta_0 + \frac{\theta_*}{\kappa}\left[\ln\left(z/z_t\right) - \psi_h(\zeta)\right] \end{cases} \quad (11)$$

$$\bar{P}(z) = -\frac{\rho_0 g \theta_*}{\kappa\theta_0}\int_0^z \left[\ln\left(z/z_t\right) - \psi_h(\zeta)\right] dz \quad (12)$$

$$\varepsilon(z) = \frac{u_*^3}{\kappa z}\phi_m(\zeta)\left[1 - \frac{\zeta}{\phi_m(\zeta)}\right] \quad (13)$$

$$k(z) = \frac{u_*^2}{\sqrt{C_\mu}}\sqrt{1 - \frac{\zeta}{\phi_m(\zeta)}} \quad (14)$$

3. – Parameterization in a RANS-CFD simulation

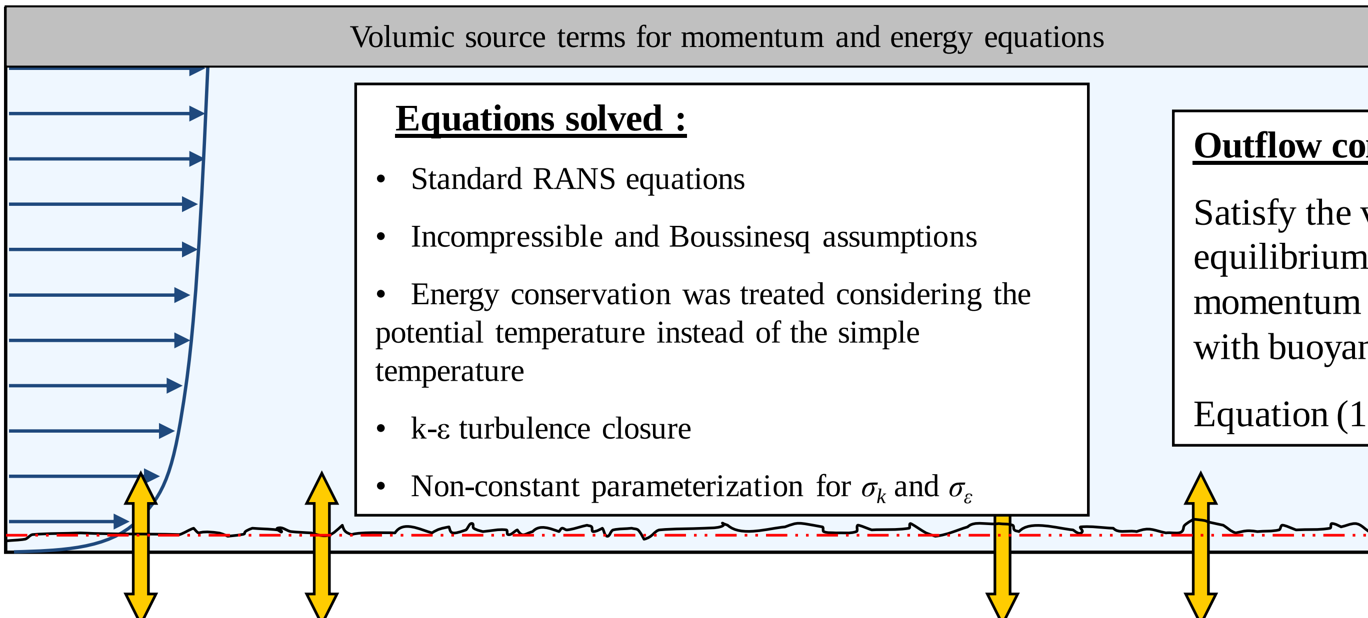
Settings used in the CFD code Fluent to simulate a diabatic surface layer

Top boundary conditions :

Shallow numerical layer (20 m) for preserving the momentum and heat fluxes through the thickness of the domain

Inlet Dirichlet condition

Equations (11), (13), (14)



Equations solved :

- Standard RANS equations
- Incompressible and Boussinesq assumptions
- Energy conservation was treated considering the potential temperature instead of the simple temperature
- k-ε turbulence closure
- Non-constant parameterization for σ_k and σ_ε

Outflow condition :

Satisfy the vertical equilibrium of the momentum equation with buoyancy effects

Equation (12)

Ground boundary conditions :

Wall function based on the rough logarithmic law for the velocity *(see Blocken B. and al., 2007)*

Sensible heat flux H_0 (positive or negative)

3. – Parameterization in a RANS-CFD simulation

Results

- The parameterization based on the different conditions was implemented and tested with commercial CFD software Fluent 6.3.
- The simulation domain used is 2D domain of 20 km long
- Simulation for different stability conditions (stable, neutral and unstable) were performed in order to evaluate the conservation of the upwind boundary condition along a such domain.
- We illustrate the results for a stable condition :
  - H_0 = -15 W.m^{-2}, u_* = 0.4 m.s^{-1} and L_{MO} = 392 m
- We can observe that the vertical inlet profiles remain perfectly preserved along the 20 km of the domain

3. – Parameterization in a RANS-CFD simulation

Results

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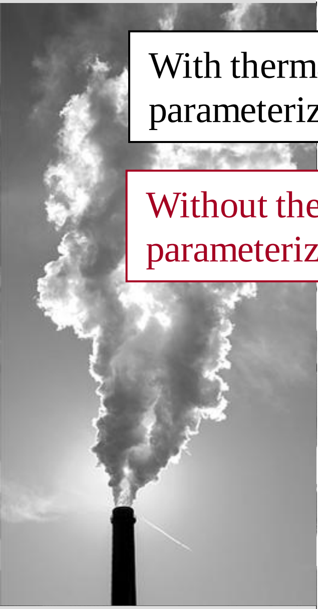
- A simulation without any specific treatment of the atmospheric thermal stratification effect was performed. We compare the results with our parameterization



With thermal stratification parameterization

Without thermal stratification parameterization

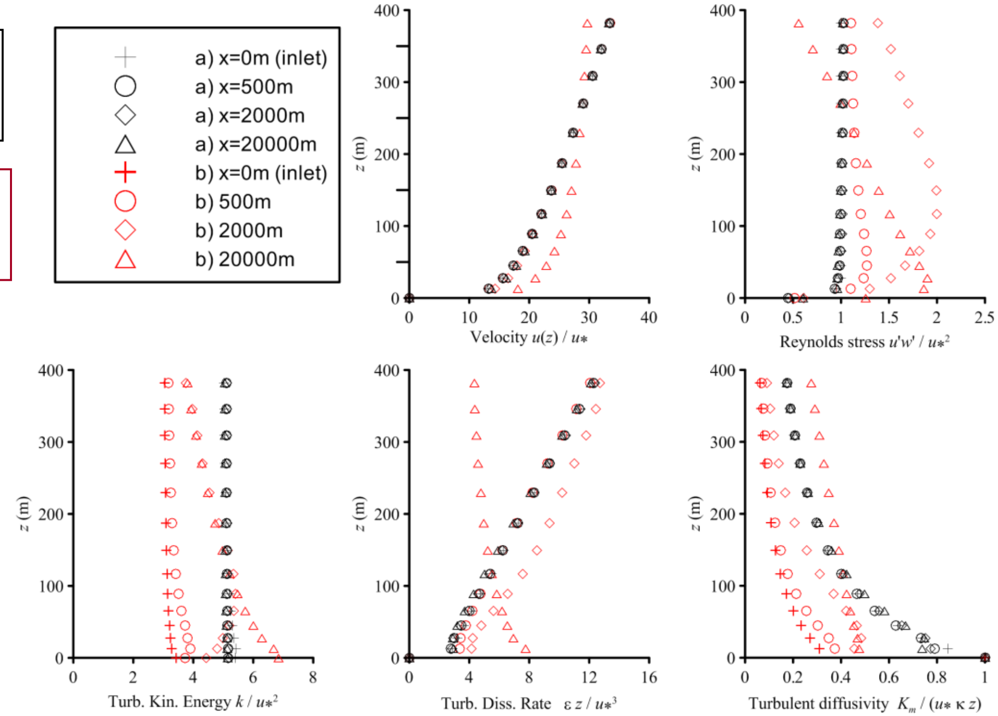


Figure 1. Vertical profiles of pressure, velocity, Reynolds stress, *k* and ε for different position in the simulation domain. a) Black profiles correspond to our methodology. b) Red profiles correspond to a RANS / *k*-ε simulation without thermal stratification parameterization.

Conclusions

- In this work, we have proposed an analysis of the application of a RANS-CFD approach with a k-ε closure to the simulation of a diabatic atmospheric surface layer
- We have discussed the consistency of the upwind turbulence profiles with conservation equations for *k* and *ε*
- We have proposed an approach to modify the outlet pressure condition and to include a top flux condition so as to satisfy the main physical patterns of the surface layer
- The results illustrate the ability of our approach to maintain the inlet profiles and the problems encountered if no parameterization is used for the stratification effects

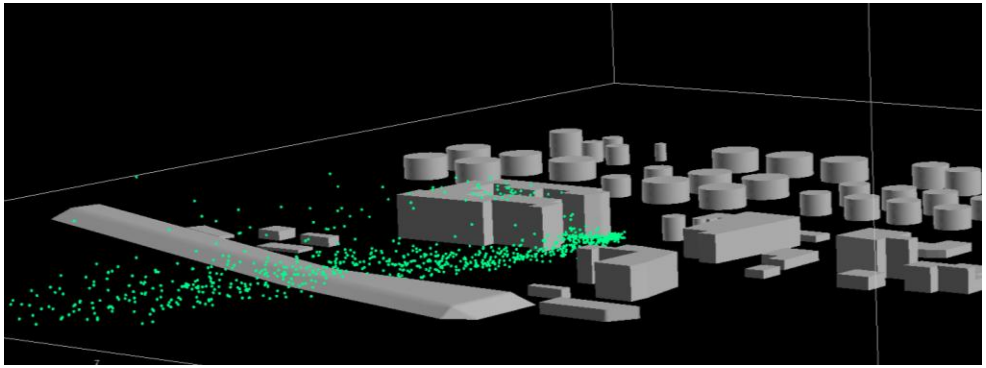
Limitations and future works

- **<u>Limitations :</u>**
  - Approach limited to the surface boundary layer
  - This approach needs a correction of the k-ε constants
    - Ideal solution : parameterization of the « constants » depending on the distance with obstacles
    - Today : need to choose between Duynkerke and standard parameterizations according to the importance of building effects vs. stratification effects
- **<u>Future works :</u>**
  - Instable case
  - Make the analysis for more complex turbulence models (Reynolds stress model)

Applications

See Poster 6 or H13-124

- Develop 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
- Precise CFD calculations are made thanks to the presented methodology and take into account the diabatic surface layer to create the database before the operational use
- During the operational use of our model, a wind field is interpolated from the data base and coupled with a lagrangian dispersion model, so as to provide short computational time and study dispersion on a complex industrial areas



Lagrangian dispersion on the refinery of Feyzin

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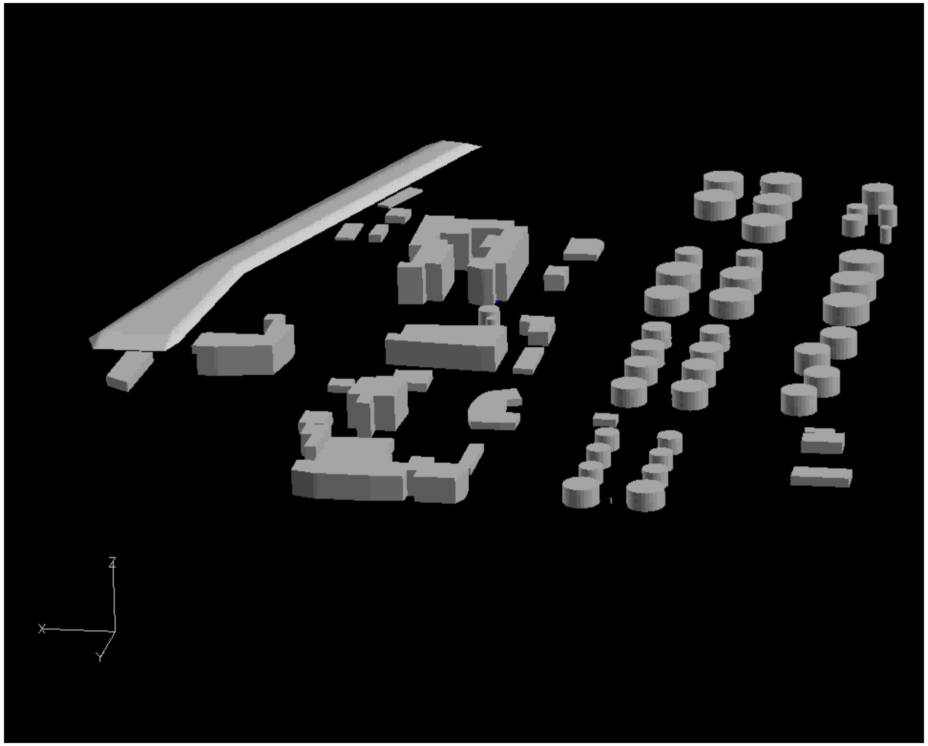
Thanks for your attention



Lagrangian dispersion on the refinery of Feyzin