EVALUATION OF CFD SIMULATIONS PREDICTING DIFFUSE SOURCES EMISSION DISPERSION: COMPARISON BETWEEN LARGE EDDY SIMULATIONS (LES) AND REGULATORY MODELS

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Abstract: Several studies have already been carried out concerning diffuse dust emissions quantification by applying empirical models and CFD simulations. The methodology proposed by the United States Environmental Protection Agency (USEPA) is the most widely used to that aim. Based on emission factors, this model allows the estimation of the emission rate of particles from an agglomeration of granular materials of a wide range of particle sizes on open storage yards. The use of these emission rate data in the analysis of atmospheric dispersion from diffuse sources (oblong storage piles of granular materials) is original and similar studies were not found in literature. For that aim, Large Eddy Simulations (LES) and a RANS model (k-ω SST) were performed using the CFD commercial package Ansys Fluent for the prediction of the flow field surrounding the pile and particle dispersion surrounding and downstream the diffuse source by using a model of particle tracking. The tested cases are oblong coal stockpiles normally found on steel plants. Precedent emission studies concerning piles of granular materials found out that these sources emit a large amount of particles to the atmosphere.
Key words: *Diffuse sources, Dust emission, LES, Particle model, Dispersion.*

CONTEXT AND OBJECTIVES

Urban populations directly exposed to air pollution suffer serious damage due to their impacts. Aiming the evaluation of the impacts of air pollution on health and the environment there is a need to determine the concentration of a pollutant in the air. Studies of atmospheric dispersion arise accordingly. Previous works performed by the present authors and others references, have already investigated the dust emission quantification from diffuse sources. The quantification of dust emitted and emission rate were already carried out with the USEPA model (Furieri et al., 2012; Turpin and Harion, 2009; Badr and Harion, 2005, 2007; Cong et al., 2012). The main results obtained with this methodology (USEPA, 2006) has shown that the velocity pattern on a stockpile being eroded is significantly modified presenting high wind velocities and shear stress values near and on the surface, respectively. This condition implicates on a strong erosion potential which is confirmed by the amount of emitted particles. The turbulence plays an important role in the atmospheric dispersion and the common regulatory dispersion models may not have the accuracy to predict this phenomenon. The fact is that, instead of the mean wind velocity, the instantaneous wind velocity may exceed the threshold velocity and particles detach from the surface of the source. It suggests that turbulence near the source wall decreases the threshold friction velocity of an agglomeration of particles (Xuan, 2004).

The evaluation of atmospheric dispersion of granular material emitted from stockpiles was not performed in the published literature. The USEPA model data may be used as input value in atmospheric dispersion studies of dust emitted from diffuse sources. The context evaluated in this paper is related to the use of numerical simulations with a CFD software. Turbulence modelling is applied to predict the turbulent structures in the flow field downstream and upstream the sources, as well as, the particle tracking of those detached from the diffuse source surface by applying a particle model available in the software. The first numerical approach focused in this paper is the LES (Large Eddy Simulation) of the turbulent flow impinging the diffuse source being analysed. The LES intends to answer several questions concerning the effects of turbulent structures on the stockpile surface (impacting on the amount of dust emitted) and on the pile's downstream zone of fluid flow. The velocity flow field issue of a transient simulation (instantaneous and mean) is useful to better understand the physics behind the RANS technique results, fastidiously published. Some tests using an Euler-Lagrangian approach of particles dispersion in the atmosphere (performing a steady Reynolds Averaged Navier-Stokes (RANS) modelling) was also an objective. The preliminary results will then show a test case (isolated perpendicular oblong stockpile) carried out in the commercial software Ansys Fluent.

TURBULENCE MODELLING

In the present work, numerical simulations were carried out solving the main governing equations by the means of two classes of turbulence models: a steady RANS model (k-ω SST) useful in the present work to test the particle tracking model available in the commercial CFD package and Large Eddy Simulation (LES), at this point, exclusively to predict the instantaneous and mean turbulent flow field.

The pollutant dispersion studies are governed by conservation equations of mass, momentum and chemical species. The wind flow in the presence of particles is considered as Newtonian and isothermal.

$$\frac{\partial \rho}{\partial t} + \frac{\partial \rho u_i}{\partial x_i} = 0 \tag{1}$$

$$\frac{\partial \rho u_i}{\partial t} + \frac{\partial \rho u_i u_j}{\partial x_i} = \frac{\partial}{\partial x_i}\left(\mu\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right)\right) - \frac{\partial p}{\partial x_i} + \rho g_i \tag{2}$$

where, Equation (1 is called continuity, ρ represents the specific mass of the fluid, while u_i and x_i, present respectively the vector components of velocity and coordinates. Equation (2, presented above, is called momentum conservation. μ is the fluid viscosity, p is the pressure and ρg_i is the term representing the body force from the gravitational field.

The effects of turbulent fluctuations are usually included by setting a coefficient of turbulent diffusion. An important alternative for modeling turbulence is the LES. The large scales of turbulent flow are directly simulated and small scales are modeled using a sub-grid model. In the simulation of large scales the idea of averages in time as held in RANS models are abandoned (Sagaut, 2002). Instead, a filter is applied to the space conservation equations and the computational solution is obtained transiently.

The LES methodology consists on a filter in the equations of momentum and the decomposition of the flow variables in large and small scales. Therefore, the large scales may be defined as:

$$\bar{f}(x_i,t) = \int_{vol} G(x_i - x_i') f(x_i',t) dx_i' \tag{3}$$

where $G(x_i - x_i')$ is the filter function.

Essentially, equations used to simulate large scales are the Navier-Stokes equations written for the variables filtered with an additional term for modeling the effects of unresolved scales. After applying the filter to the Navier-Stokes equations we obtain (Sagaut, 2002):

$$\frac{\partial(\rho \bar{u}_i)}{\partial t} + \frac{\partial(\rho \bar{u}_i \bar{u}_j)}{\partial x_i} = \frac{\partial}{\partial x_i}\left(\mu\left(\frac{\partial \bar{u}_i}{\partial x_j} + \frac{\partial \bar{u}_j}{\partial x_i}\right)\right) - \frac{\partial p}{\partial x_i} + \rho g_i - \frac{\partial\left(\tau_{ij}^S\right)}{\partial x_j} \tag{4}$$

where, τ_{ij}^S is the term referring to the sub-grid scales, or the effects of turbulence or small scale (scale modeled). There are several mathematical models to treat the sub-grid stress tensor. The sub-grid scale model chosen, the Wall Adapted Local Eddy-Viscosity (WALE), is given by the following Equations (5 and(6:

$$\mu_t = \rho L_S^2 \frac{(S_{ij}^d S_{ij}^d)^{3/2}}{(S_{ij}^d S_{ij}^d)^{5/2} + (S_{ij}^d S_{ij}^d)^{5/4}} \tag{5}$$

$$L_S = \min(\kappa d, C_w V^{1/3}), S_{ij}^d = \frac{1}{2}\left(\bar{g}_{ij}^2 + \bar{g}_{ji}^2\right) - \frac{1}{3}\delta_{ij}\bar{g}_{kk}^2, \; \bar{g}_{ij} = \frac{\partial \bar{u}_i}{\partial x_j} \tag{6}$$

where, C_w is a constant, which by default is 0.325 and has been found to yield satisfactory results for a wide range of flow.

The steady RANS calculations performed in the present study are justified by the fact that it has already been validated with experimental works for similar geometries. The intending tests with the particle model were observed to be easily available by performing steady RANS simulations. Two models are well used and validated for this class of problem. As described in the contexts we will take into consideration the model k-ω developed by Wilcox (1980) rather than the k-ε model. It corresponds to the resolution of two transport equations, one for turbulent kinetic energy (k), as in the model k-ε, and the other for the dissipation (ε) per unit of turbulent kinetic energy, called ω.

$$\frac{\partial(\rho k)}{\partial t}+\frac{\partial(\rho k u_i)}{\partial x_i}=\frac{\partial}{\partial x_j}\left(\Gamma_k\frac{\partial k}{\partial x_j}\right)+G_k+Y_k,\ \frac{\partial(\rho\omega)}{\partial t}+\frac{\partial(\rho\omega u_i)}{\partial x_i}=\frac{\partial}{\partial x_j}\left(\Gamma_\omega\frac{\partial \omega}{\partial x_j}\right)+G_\omega+Y_\omega \tag{7}$$

where, G_k and G_ω represent the production of k and ω, Γ_k and Γ_ω represent respectively the effective diffusivity of k and ω and Y_k and Y_ω represent respectively the dissipation of k and ω. The term ω was then redefined by Kolmogorov as the rate of dissipation of energy by volume and time. In this model, the turbulent viscosity may be presented by the left equation below.

$$\omega=\frac{Ck^{1/2}}{l},\ \mu_t=\alpha^*\rho\frac{k}{\omega} \tag{8}$$

where C is a constant and l is a characteristic length of turbulence. The term ω may be defined, approximately as the ratio between ε and ω inserting a coefficient determined empirically. α^* is calculated in a function of the Reynolds number. For a high Reynolds number problem this coefficient is the unit. The model used in this problem is a variant of the original k-ω, called k-ω SST. This model used the formulation of the original model near the wall and that of the k-ε in the exterior region. The main modifications found in this model are: a modification in the turbulent viscosity modified to well represent the effects of the shear stress and the addition of a diffusion term in the ω transport equation and a function that ensure that the model equations are acceptable in both regions, exterior and near wall.

Figure 1 presents the computational domain used in the calculations performed in the present study. Dimensions, stockpile location and boundary conditions are the main features shown. For each numerical simulation may be set a different boundary condition. Lateral and upper boundaries are free slip walls. The ground and stockpile walls are no-slip walls. The outlet is an outflow condition. However, the inlet condition differs between the two simulations presented. In the k-ω SST simulation, the inlet data of velocities, turbulent kinetic energy and its specific dissipation were obtained from a precursor calculation. In LES, the inlet condition is a definition of a mean velocity and its fluctuations. The velocity profile is built every time step due to the called Spectral Synthesizer method. The unsteady simulations were set to have a time step size equals to 0.00001 s and 42000 time steps were calculated.

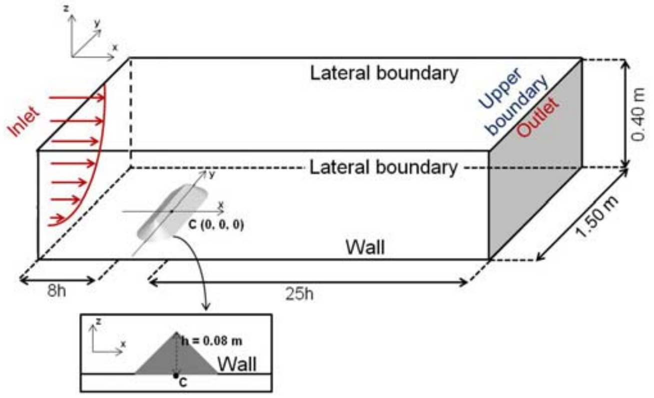

Figure 1. Computational domain.

The particle tracking in Ansys Fluent is possible due to a model that takes into account a force balance in each particle injected in the domain from the stockpile surface. The fluid flow and particles treated in this paper follow the Euler-Lagrange approach. The fluid phase is treated as a continuum by solving the Navier-Stokes equations, while the dispersed phase is solved by tracking a large number of particles through the flow field.

PRELIMINARY RESULTS AND DISCUSSIONS

The numerical simulation tool used in the present work is being tested to be representative among the best techniques to predict the atmospheric dispersion of contaminant particles. The paper is devoted to expose the preliminary results concerning the coupling of several models aiming the most possible accurate result of particle dispersion from a diffuse source. The diffuse source analysed in the present paper is a granular material storage pile. The coupling of models cited above takes into consideration: USEPA model for dust emission quantification, particle model for its tracking and LES for a more accurate turbulence prediction.

Firstly, we intend to show the preliminary turbulent flow field predicted by LES. Due to a lack of simulation time, the results presented herein are not yet in its aimed convergence. However, it is already possible to discuss some features observed in the mean and instantaneous field associated to emission and dispersion. Figure 2 show an initial (and partial) validation of LES results by comparing some vertical velocity profiles with PIV experiments carried out in wind-tunnel by Turpin (2010). The plots (Figure 2) indicate a good similarity between the three approaches represented. Even if we are not in the final convergence level, the results are very interesting and the profiles are developing to reach the experimental profiles.

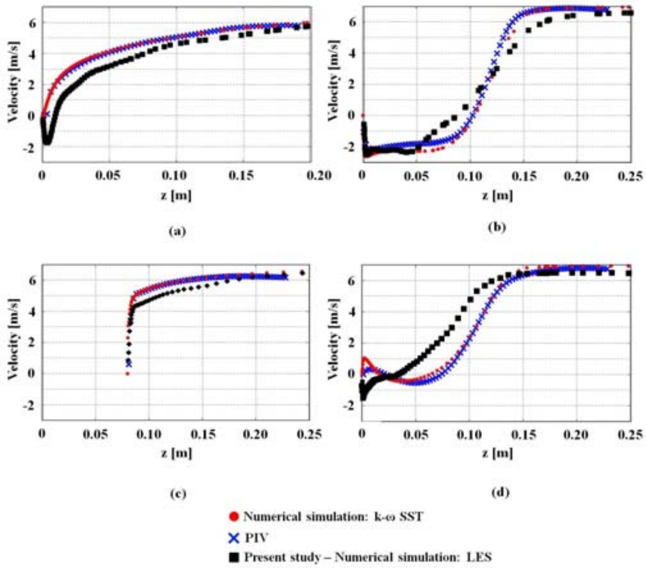

Figure 2 - Comparisons between four vertical profiles along the domain upstream and downstream the pile: (a)

Figure 3(a) and Figure 3(b) present mean and instantaneous results of velocity magnitude in two locations in the domain. Figure 3(a) plot the velocity magnitude in a longitudinal plan (*y=0*) and Figure 3(b) over the surface near the stockpile wall (the velocity undertaken over this surface is an input data of the USEPA model for dust emission quantification). Figure 3(a-1) and (b-1) show the mean field while the others show the instantaneous field for four time instants. Hence, the contours show the complex and three-dimensional features in the flow. The instantaneous velocity field indicates a highly perturbed zone downstream the pile and the recirculation region.

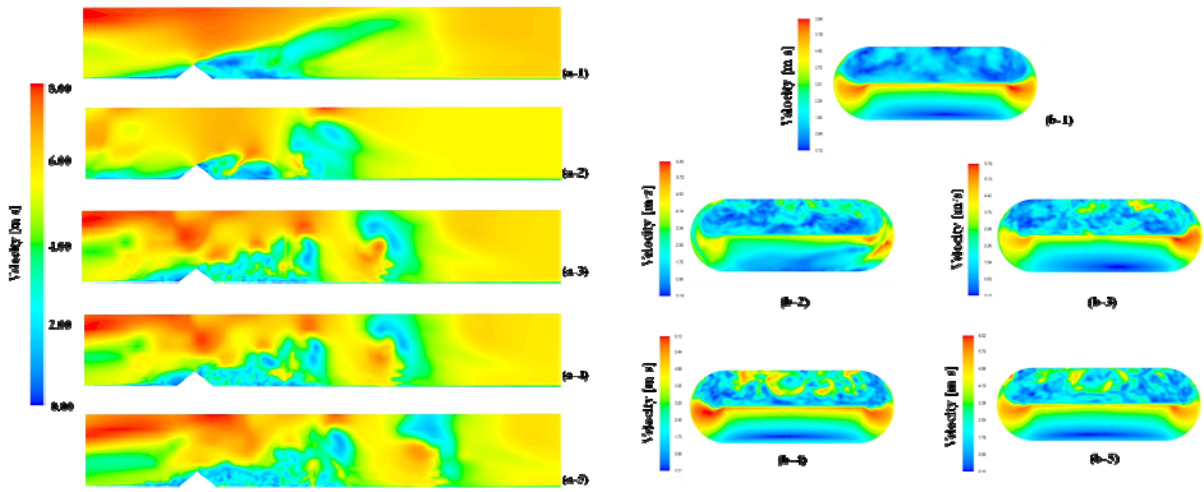

Figure 3 - (a) mean (a-1) and instantaneous (a-2 to a-5) magnitude velocity flow field on the domain middle plan; (b) mean (b-1) and instantaneous (b-2 to b-5) magnitude velocity on a surface near the stockpile wall.

The same condition is noticed in Figure 3(b) where, on the leeward wall, peaks of velocity magnitude indicate that the instantaneous field may result in increased dust emission. In the dispersion, the middle plan velocity magnitude field presents this very complex and turbulent pattern which may characterize an increase of diffusion and consequently in turbulence.

Figure 4 shows the distribution of particles as a result of a steady RANS simulation in which particles are injected from a surface. The surface considered in the software to be the source is the stockpile. The particles are uniformly distributed, it means that all of them has the same diameter. The diameter of each carbon particle is 10^{-4} m. The sequence of frames (Figure 4 (a)-(f)) is a very good description of particles trajectory. The contours show the longitudinal velocity on the plan ($y=0$) and the carbon particles are coloured by their identification number. The first frame (a) is the initial distribution of particles on the surface (it is worth noting that not all the injected particles are represented here). Only the right part of the pile is represented in the frames. The second frame (b) illustrates the initial particle take-off mainly on the windward wall. In the others frames it is interesting to note the large amount of particles being eroded and following the detachment flow along the crest line. In the fourth frame (d) some particles remains over the surface and others may be seen on the ground surrounding the source. The deposition of some particles indicates that the weight has over passed the other forces (lift, for example) that would sustain the particle in the air flow.

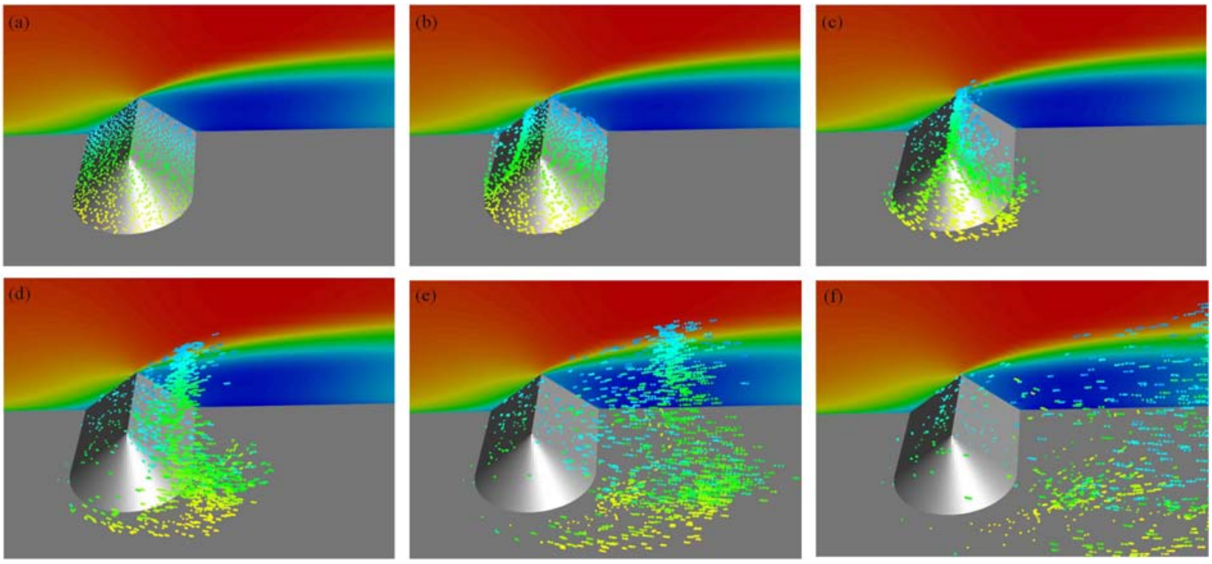

Figure 4 - Frames of particle dispersion pulse: plan is coloured by the longitudinal velocity and particles are coloured by the particle identification number.

Some preliminary conclusions may be obtained in this study. The LES being performed for the flow surrounding stockpiles are in the correct way of the final solution as show the preliminary results in the paper. Indeed, the contours of instantaneous velocity illustrate the presence of high unsteadiness levels which is essential to produce turbulence. The influence of turbulence on the atmospheric dispersion field can be obtained by means of numerical simulation. The most widely used regulatory dispersion models may not have the enough representation of turbulence as well as CFD does. Their results are very representative of the reality, however it can be enhanced by the information acquired when using CFD. It has shown to be a very good approach in predicting the dispersion and our results tend to give very interesting discussions. The fact that we used data from the USEPA model for dust emission estimation has never been published to study dispersion.

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