MATHEMATICAL MODELING OF POLLUTANT DISPERSION AROUND AN ISOLATED OBSTACLE UNDER DIFFERENT ATMOSPHERIC STABILITY CONDITIONS

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Abstract. In the present work, numerical simulations were carried out using CFD to study gaseous pollutants dispersion behavior around an isolated building, under different atmospheric conditions. The mathematical modeling was based on the solution of conservative equations (mass, momentum, energy and chemical species) using the standard κ-ε turbulence model. The numerical results were validated wind tunnel data available in literature. The unstable atmospheric condition presented the highest levels of turbulence in the stagnation zone as well as higher TKE generation near the ground. The dispersion plumes for the tested atmospheric stability scenarios showed no significant differences in the concentration profile. The most significant concentration values were found in the center line of the pollutant plume, presenting the largest concentration differences in the simulated stability conditions. Numerical simulation has proved to be a powerful tool in the analysis of the concentration field and a feasible alternative in environmental impacts evaluation of new sources in urban environment.

Keywords: Atmospheric dispersion, turbulence, thermal stratification, computational fluid dynamics.

1. INTRODUCTION

The study of the dispersion behavior of pollutants around buildings is important mainly for evaluation of building design (Blocken *et al*., 2013), internal and external air quality (Liu *et al*., 2010; Tominaga and Stathopoulos, 2016), and population health (Romero-Lankao *et al*., 2013; Chen *et al*., 2013).

There is a considerable amount of work in the literature that has evaluated the behavior of flow and dispersion around buildings from field measurements, wind tunnel laboratory tests and numerical simulations (Zhang *et al.*, 2015; Perry *et al.,* 2016; Mavroidis *et al*., 2012; Tominaga and Stathopoulos, 2017). One of the main advantages of numerical simulation is the possibity to provide variable information throughout the entire computational domain, while observational measurements allow only a limited number of discrete points in space (Tominaga; Stathopoulos, 2016).

Mavroidis *et al.* (2012), Santos *et al.* (2009) and Yassin (2013a, b) studied the effects of atmospheric stability variation on the flow and dispersion of pollutants around built environments. They concluded that atmospheric stability is an important parameter to be evaluated in studies of dispersion behavior of pollutants near buildings in urban areas, due the fact of causing variations in turbulent kinetic energy (TKE) levels, incident wind speed and, consequently, the concentration field.

In this context, the main objective of the present work is to investigate the behavior of dispersion of gaseous pollutants around an isolated building in an urban environment in order to evaluate the effects of thermal stratification on the flow and concentration field. In addition, the formation of the plume and dispersion of different pollutants around an idealized building in neutral atmosphere conditions is also studied in order to evaluate the use of computational fluid dynamics applied to environmental engineering.

2. METHODOLOGY

The computational domain simulated was based on the wind tunnel experiment carried out by Yassin (2013b), performed on a small scale model. The commercial software ANSYS FLUENT 17.0 was used to solve the conservation equations in each element of the discretized computational domain. The dimensions of the simulated domain has 20H x 6H x 5H, where H is the height of the isolated cubic obstacle. For computational cost reduction, only half of the domain was constructed, due the symmetric nature of the flow. An unstructured mesh with approximately 3.2 million elements was used, whose smallest element has 5×10^{-3} m in size. Figure 1 shows the computational domain scheme.
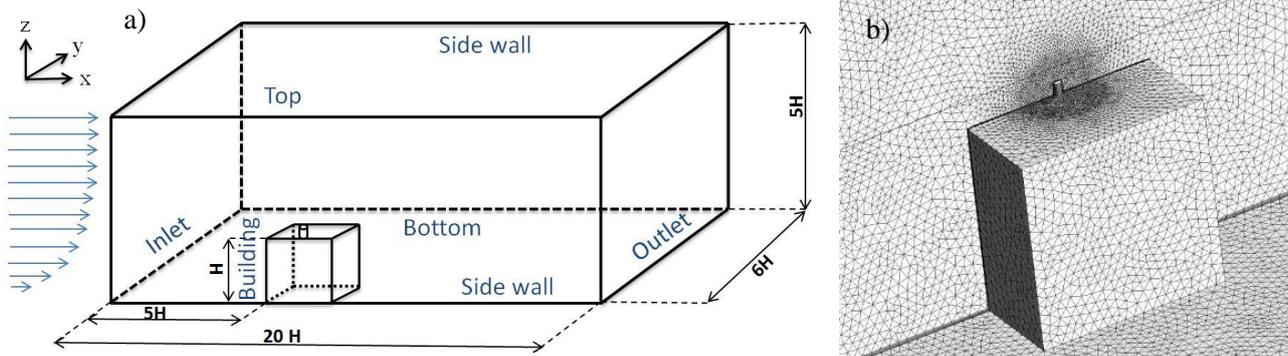

Figure 1. Domain scheme and computational mesh

The conservation equations of mass, momentum, energy, and chemical species were modeled based on the decomposition of Reynolds averages. The steady state condition, incompressible flow, Newtonian fluid, constant viscosity and inert gas were adopted in order to simplify the equations.

The transport equations were solved by the finite volume method (FVM). For the pressure-velocity coupling the SIMPLE algorithm was used, first order Upwind was chosen to discretize turbulent kinetic energy and dissipation TKE were used, and second order Upwind method was used for conservation equations of momentum, energy and chemical species.

The boundary conditions were: (I) Inlet: imposition of vertical profiles of longitudinal velocity, turbulent kinetic energy and turbulent kinetic energy dissipation, based on the data of Yassin (2013b); (II) Top: symmetry; (III) Sidewalls: symmetry; (IV) Bottom: no-slip and (V) Outlet: zero static pressure.

The atmosphere stratification was simulated based on the temperature profiles obtained in the wind tunnel experiment conducted by Yassin (2013b). The temperature profiles were imposed as inlet conditions of the computational domain in order to simulate stable and unstable stratification conditions. Richardson bulk (Ri_{bulk}) is a stability parameter that describes the relationship between forces related to the effects of thermal thrust and mechanical turbulence. Reynolds number (Re_b) is the ratio between surface and viscous forces. The parameters values with the corresponding atmospheric stability are listed in Table 1.

Table 1. Details of atmospheric stability conditions.

Atmospheric stability	U_H (m/s)	Ri_{bulk}	Re_b
Stable	0.76	1.15×10^{-2}	5.17×10^3
Neutral	0.86	0	5.93×10^3
Unstable	1.00	-7.64×10^{-3}	6.90×10^3

The emission rate was determined based on 50% of building height velocity (U_H), according to the stability class. Ethylene (C_2H_4) was the tracer gas used in the comparison of the concentration range under different stability conditions. Furthermore, the dispersion analysis of different pollutants (ethylene and methane) was performed in a neutral atmosphere condition in order to evaluate the effect of different Schmidt numbers.

3. RESULTS AND DISCUSSION

3.1 Mesh sensibility and validation

The mesh sensibility test was performed for three meshes containing 1.8, 3.2 and 5.2 million of elements. The vertical and horizontal profiles of velocity and turbulent kinetic energy were compared in mesh test. No significant modifications were observed from coarse to finest mesh, and the choice was based on refinement near the source, for better detailing of concentration field.

Different κ-ε models (Standard, RNG and Realizable) were used in order to identify the more accurate model to reproduce the atmospheric transport mechanisms associated with low computational cost. The numerical results were compared with the experimental work developed by Yassin (2013b). In spite of overestimating the turbulent kinetic energy and not having predicted the exact velocity field, the standard κ-ε model proved to be able to simulate the atmospheric conditions with a good agreement with the experimental results. Therefore, standard κ-ε was the chosen model for the present work.

3.2 Turbulent Kinetic Energy

The vertical temperature profile generates variation in the levels of atmospheric turbulence that can be observed in the production of TKE, as shown in Figure 2. TKE is one of the main variables studied in the flow field since its distribution can affect the velocity and concentration field (Santos et al., 2009).

The highest TKE values were found in the corners of the side walls and near the top of the building in the incident wind region. The effect of the atmospheric stability on the TKE was relatively greater in furthest regions within the turbulent wake.
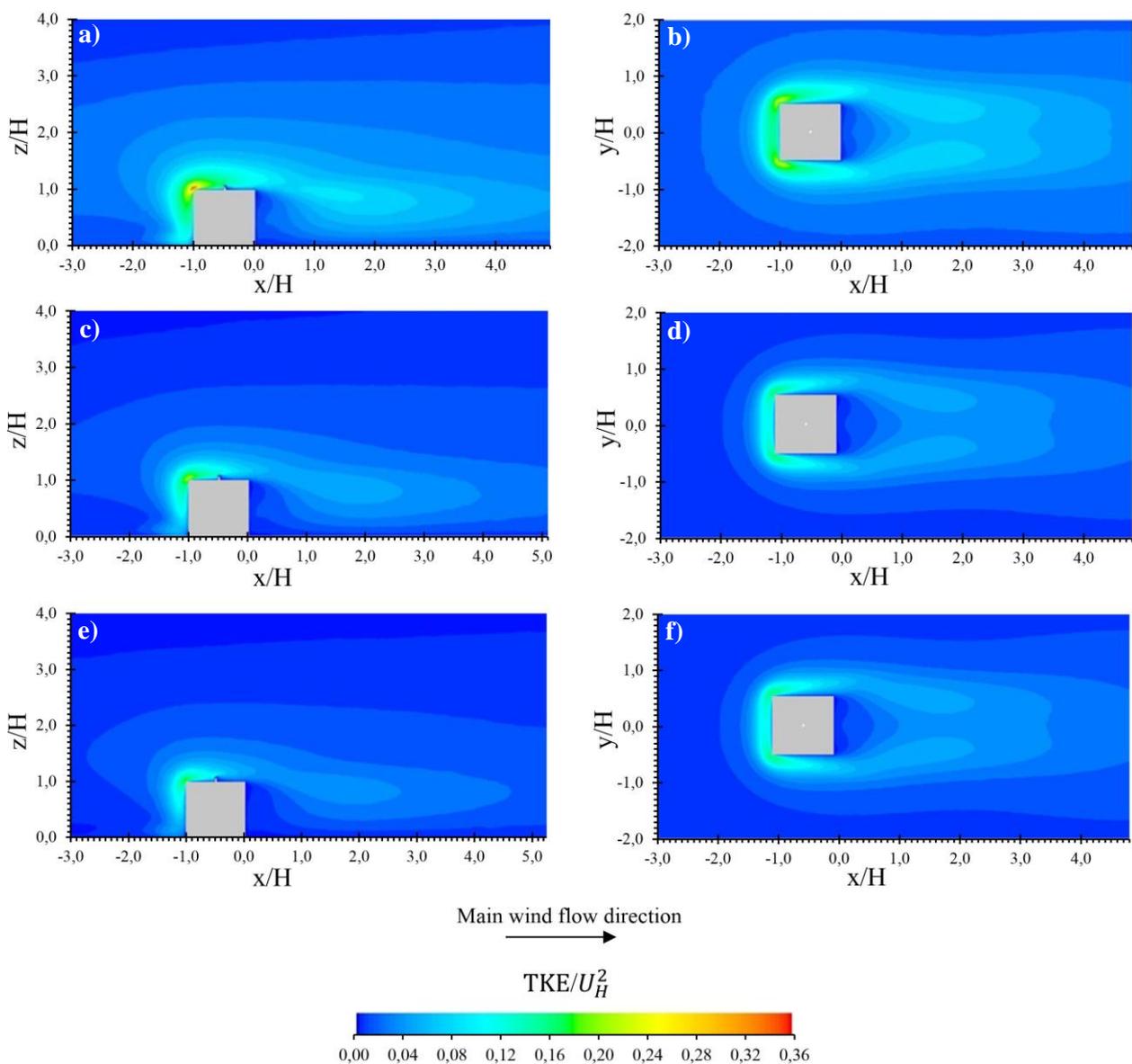

Figure 2. Distribution of Turbulent Kinetic Energy in the planes (xz) at y/H = 0 e (xy) at z / H = 0.05 around an obstacle under stability conditions: unstable (a) and (b), neutral (c) and (d), stable (e) and (f).

In unstable atmosphere condition (Figure 2a, b) were found the highest levels of turbulence in incident flow as well as the greatest generation of TKE near the ground. This behavior is mainly related to the intense temperature gradients

in this region, responsible to create a strong buoyancy effect (Santos et al., 2009). As a result, the approaching flow has higher TKE levels than those observed in neutral (Figure 2c, d) and stable conditions (Figure 2e, f).

3.3 Concentration

The concentration was normalized by reference concentration C_0, calculated as $C_0 = Q/U_H H^2$, where Q is the emission rate (m^3/s), U_H is the building height velocity (m/s) and H is the building height (m).

In vertical plane (y/H = 0), a high concentration gradient was observed near the source and in upper region. The highest concentrations remained until x/H = 1 within the turbulent wake at the building height. Downstream the obstacle, the concentration plume moves to ground direction, increasing the concentration in that region. The concentration values at building height was evidently higher than the ground region, due the localization of the source far from recirculation zone.

As shown in Figure 3, the change in stability class resulted in subtle modifications in the concentration range and behavior of the pollutant plume.
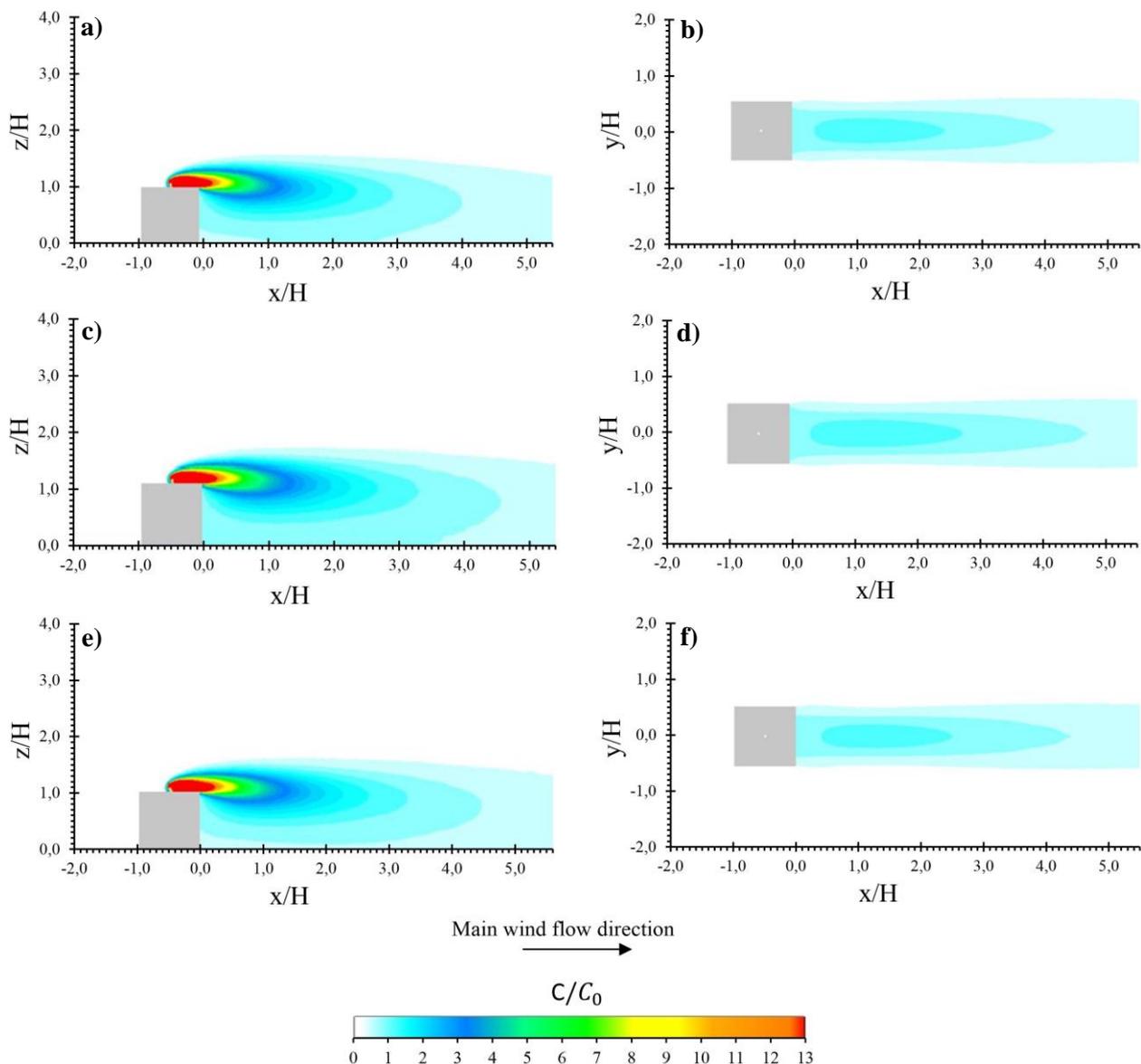

Figure 3. Concentration distribution in the planes (xz) at y/H = 0 e (xy) at z / H = 0.05 around an obstacle under conditions of stability: unstable (a) and (b), neutral (c) and (d), stable (e) and (f).

Neutral atmosphere condition (Figure 3c, d) presented the highest concentration values and a larger coverage area. In unstable condition (Figure 3a, b), the pollutant released is quickly transported away from the building, resulting in

lower concentrations of contaminants near the building. On the other hand, stable condition (Figure 3e, f) show the lowest concentration near the ground since the plume does not reach it at any point downstream of the building.

In the horizontal plane (z = 0.05H), the plume behavior was quite similar in all three cases. A little lateral spread and highest concentration levels in the centerline were observed. The greatest difference was observed in the pollutant propagation in space, with a variation of 4.5% between neutral and stable, and 9% between neutral and unstable. Neutral atmosphere presented the highest concentration values and the largest propagation distance.

3.4 Dispersion behavior of pollutants in neutral stability condition

The behavior of the pollutant plume was similar for the two simulated gases regarding some aspects such as the highest concentration gradient in the building roof, near the source. However, significant differences can be pointed out. The high concentration area was much lower for methane gas. Ethylene plume has a greater trend to descend in ground direction, while methane remains more buoyant.

As shown in Figure 4, the concentration field presented very different results among the evaluated pollutants. The methane plume presented lower concentrations near the ground and lower amplitude of propagation in horizontal and lateral directions. This result can be explained by the Schmidt number (Sc) analysis since flow rate and geometry characteristics were maintained unaltered in both cases. The calculated values of Sc were 0.21 and 0.73 for ethylene and methane, respectively. Since the Schmidt number is the ratio of the kinematic viscosity and diffusivity of the compound, lower Schmidt number provides greater diffusivity to the compound. Therefore, Ethylene has the greatest mass transfer rate and, consequently, an increased range of dispersion.
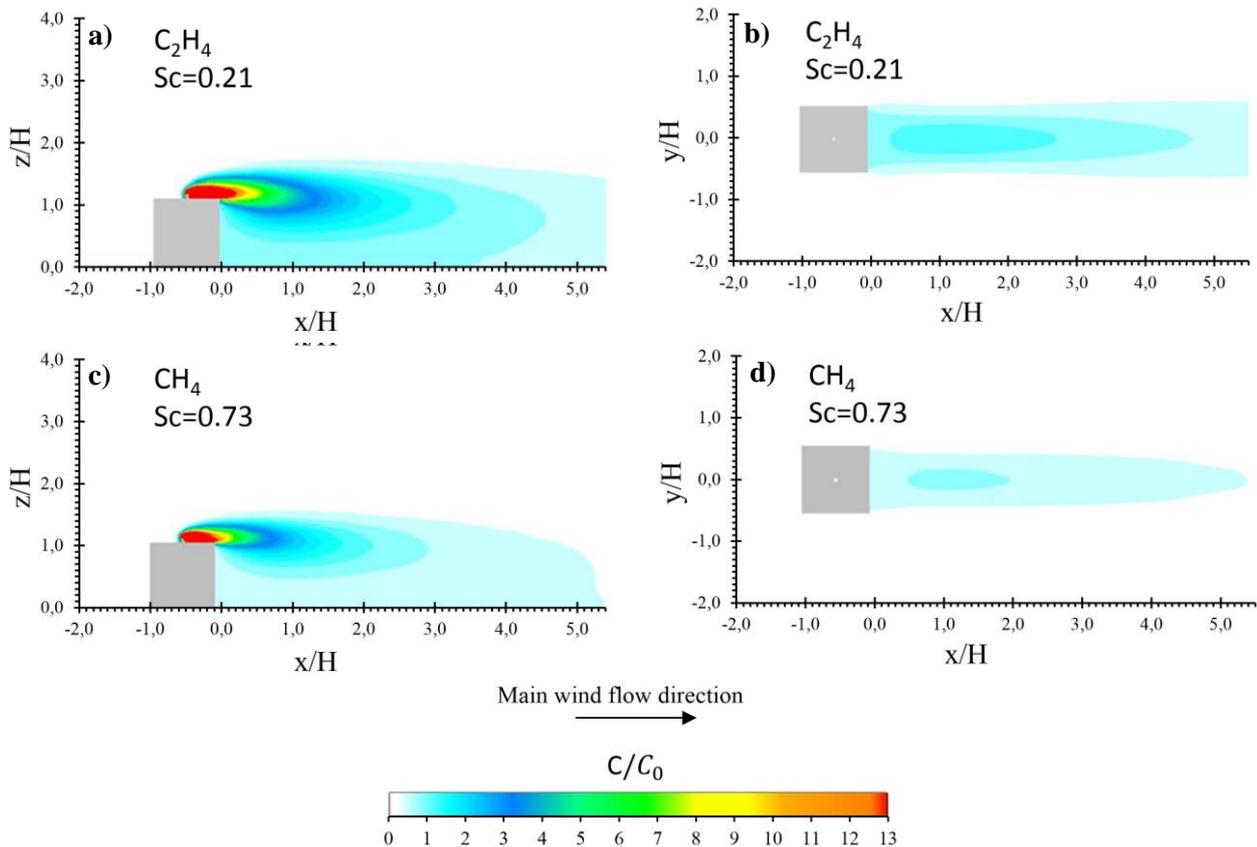

Figure 4. Mean concentration in side and plan view for (a, b) ethylene and (c, d) methane.

Numerical simulation results of the concentration field of a real pollutant and the application of turbulence models in the modeling of mechanisms associated with dispersion in the atmosphere have shown that a numerical simulation is an important tool that can be used in the studies of environmental impact assessment.

4. CONCLUSIONS

In present work, the dispersion behavior of gaseous pollutants around an isolated building in an urban environment under unstable, neutral and stable atmospheric stability was studied.

The atmospheric stratification by the action of the thermal buoyancy forces generated important contribution in the levels of turbulence of the flow, resulting in the variation of the turbulent kinetic energy field around the obstacle.

Pollutants spread and plume behavior were similar in all three stability classes studied, indicating that changes in stability conditions are not capable of causing significant variation in the concentration distribution of pollutants around obstacles.

The dispersion analysis of different pollutants showed that the properties of the pollutants are important and alter the behavior of the plume and, consequently, interfere and modify the concentration field.

Turbulent kinetic energy distribution simulated with the standard κ-ε model had satisfactory agreement when compared to the experimental results of Yassin (2013b). Moreover, for the purposes of previous environmental impact assessment studies, the model was also efficient simulating atmospheric conditions. The performance of the applied methodology showed that numerical simulation is an important tool which can be used in environmental engineering studies.

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6. RESPONSIBILITY NOTICE

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