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NUMERICAL SIMULATION OF FLOW AND DISPERSION AROUND AN ISOLATED CUBICAL BUILDING UNDER NEUTRAL STABILITY: STUDY OF THE SENSITIVITY OF THE k-ω SST TURBULENCE MODEL TO ITS EMPIRICAL CONSTANTS

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Abstract: The main objective of the present study was to evaluate the performance of the Shear Stress Transport (SST) model by means of numerical simulations based on the solution of conservation equations (mass, momentum and chemical species). The flow and dispersion of a gaseous compound around isolated cubic obstacle was investigated under the condition of neutral atmospheric stability (energy equation is not solved). Numerical simulations were performed using the Ansys Fluent Computational Fluid Dynamics software. The turbulence model k-ω SST was evaluated by comparisons with experimental results from previous measurements in wind tunnel performed by Murakami et al. (1990) with Reynolds number approximately 70000 (based on velocity at the height of the building and the building height). This analysis carried out was done to test the sensitivity of empirical constants of the turbulence model – a_1 (influences on eddy viscosity) and C_{lim} (influences on the limitation of turbulent kinetic energy production). The results of the sensitivity analysis showed a significant influence on the length of the recirculation zone behind the building and the production of turbulent kinetic energy in the stagnation zones when comparing with wind tunnel results and other previous works performing LES and different turbulence models. The numerical modeling showed that the adjustment of the empirical constant a_1 to values greater than the standard condition of the model got better results for the recirculation zone length. On the other hand, the results of turbulent kinetic energy (TKE), did not have good agreement with the experimental data when C_{lim} was set to the standard value. However, the adjustment of C_{lim} improved the agreement between TKE values of numerical simulation and experiment in the stagnation zones, in contrast, a greater length of the recirculation zone behind the building was observed for the cases tested. The study also evaluated the effect of the dispersion of a gaseous compound to this configuration, in order to evaluate the influence of the empirical constants in the dispersion.

Key words: *Pollutant dispersion, CFD Models, isolated building*

1. INTRODUCTION

Pollutants in the atmosphere can be emitted in the form of particles or gases, and their impact in the receptores (human been, flora, fauna and material) results from the emission process of source, dispersion and deposition. In urban regions, those process are alter by the edification presence that are obstacle to the flow, that can intensifies the levels of concentration near to surface (TOMINAGA; BLOCKER, 2016; JADIDI et al., 2016).

The prediction of the flow and dispersion of pollutants in urban regions faces great challenges. Since experimental analysis of wind tunnel or field can be costly, execution is difficult, and applications are limited, the mathematical modeling is presented as an alternative to experimental analysis, especially the RANS model, which presents low computational cost.

This study seeks to verify the performance of the model in the standard condition and calibrate the model to reproduce the flow and dispersion of pollutants under the same conditions used in experiments. The main objective of the present study was to evaluate the performance of the Shear Stress Transport (SST) model by means of numerical simulations based on the solution of conservation equations (mass, momentum and chemical species). The flow and dispersion of a gaseous compound around isolated cubic obstacle was investigated under the condition of neutral atmospheric stability (energy equation is not solved). Numerical simulations were performed using the Ansys Fluent Computational Fluid Dynamics software. The turbulence model k-ω SST was evaluated by comparisons with experimental results from previous measurements in wind tunnel performed by Murakami et al. (1990) with Reynolds number approximately 70000 (based on velocity at the height of the building and the building height).

The equation to determine turbulent viscosity and the expression used to determine the energy kinetic production in the model k-ω SST present empirical constants that aim, respectively, to improve the next prevision of the solid surface (without of law of the wall) and to avoid the overestimation of production of turbulent kinetic energy in regions of stagnation. Otherwise, the values of those empirical constants were determined to some kinds of flow and still need the verification in its generality to the use, new parameter to those empirical constants were tested in this study, in the flow and dispersion field were evaluated.

2. METHODOLOGY

2.1 Wind tunnel experiment

A cube-shaped model, 200 mm in height, was placed in the turbulent boundary layer. The Reynolds number of the experiment, based on height of the building, was about $7x10^4$. The wind velocity was measured by a tandem-type hot wire anemometer which could monitor each component of an instantaneous velocity vector.

The experiment performed by Murakami et al. (1990) measured the flow field. This study included a point source upstream of the building with the purpose of evaluating the sensitivity of the model to the modifications of the empirical constants a_1 and C_{lim}, according to the configuration established in the experiment Mavroidis et al. (1999) presented in the following figure.

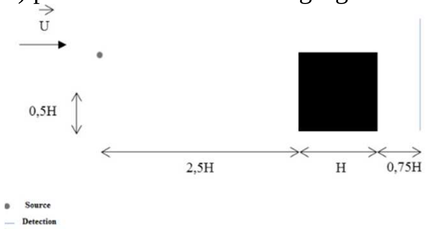

Figure 2. Disposição da fonte e dos detectores do experimento Mavroidis et al., (1999).

2.2 Modelling tool

2.2.1 Computational tool

The Reynolds-Averaged equations for mass, momentum and species transport were solved with ANSYS FLUENT 15.0, a CFD code which solves the transport equations numerically using the finite volume method for structured and non-structured meshes. Turbulence clousured was obtained thought the eddy viscosity concept. The simulations employed the k-ω SST turbulence model. This model combine different elements of existing models and is considered superior to their RANS alternatives and leads to major improvements in the prediction of adverse pressure flows (Menter, 1994).

2.2.2 Grid and domain characteristics

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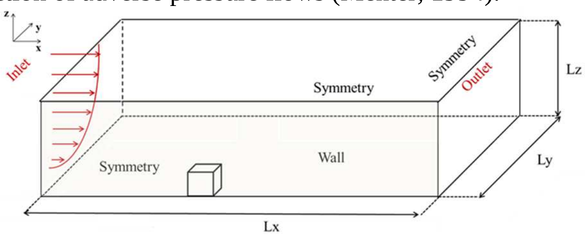

Figure 1. Schematic representation of the computational domain and boundary conditions

The boundary conditions used in this study (Figure 1) are now described. Inlet: wind velocity, k and ω profiles; upper and side walls: symmetry; floor: no slip condition; outlet: Outflow condition.

The unstructured mesh (Figure 2a) was generated using ANSYS MESHING 15.0 and consisted of 3 million tetrahedral elements; the mesh was refined near the obstacle.

In order to verify the independence of the results of the computational mesh used, the size of the smallest element of the sphere of influence for the generation of three computational meshes (gross, average and fine) was modified. At the end of the mesh test, for presenting lower computational cost.

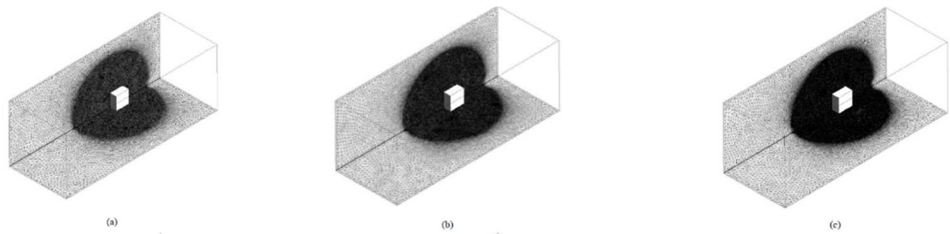

Figure 2. Computational meshes tested: (a) gross, (b) average and (c) fine

3. RESULTS AND DISCUSSION

3.1 Flow field

This section has the aim to show the sensitivity test to the model empirical constant variation k-ω SST, in the average results of longitudinal velocity and turbulent kinetic energy (TKE). Besides, the average results of sensibility test that could best represent the longitudinal velocity of the field and turbulent kinetic energy are compered with studies resultes before done to flow field of validation. The empirical constant a_1 is presented in the turbulent viscosity formulation of developed model for Menter (1994):

$$\nu_T = \frac{a_1 k}{\max(a_1 \omega, SF_2)} \quad (1)$$

The modification of a_1 in the equation of viscosity have aimed to minimize the length of zone of recirculation behind the building. This effect in the flow can improve significantly the average results in the field of velocity to the experiment representation.

As bigger the value the empirical constant a_1 assumes, less will be the lenght of re-circulation of zone behind of the building, otherwise, in the zones of stagnation occurs modification in the turbulent kinetic energy. To improve this prediction, some modifications are proposed in the empirical constant C_{lim} that compounds the function "Production Limiter", this function has the finality to do some restriction in the terms of turbulent kinetic energy of production and with that improves the capacity of prediction in the separation zone in accordance with studies done by Valger et al., (2015).

$$P_k = \min(P_k, C_{lim}.\rho.\varepsilon) \quad (2)$$

With the adjustment of empirical constant, C_{lim}, to improve the performance of model to represent kinetic energy of production in the stagnation zones, because the test already done to this empirical constant until this present studies happened in the standard condition of model. Next are presented the results of eight sensitivity tests (**TS-1** to **TS-8**) of model of turbulence to the flow field.

Figures 3 (**TS-1**) – (**TS-8**) present velocity contours in the longitudinal direction in the xz plan at y= (0,0), dimension by velocity in the direction x of the high of the building, to differents empirical constants that were tested. The subtitle of colors presented showed us lower values of longitudinal velocity in the blue color. It can be observed that in the **TS-1**, standard conditon of the model, the region of lower velocity is bigger than all other situation that were tested, so, the length of the recirculation zone (ZR) diminishes when we increase the value of a_1, when you observe the equation (1), turbulent viscosity to the model used in this present study.

Increasing the empirical constant a_1 means to increase turbulent viscosity of the fluid of the flow, making the flow more viscous, then it presents less recirculation behind of the building. In the **TS-1**, it can be notice that the recirculation in the top of the building is bigger and indicates that there are no reattachment in the top of the building. The length of the dimensionless ZR in a wind tunnel study by Murakami et al. (1990) is equal to 1.2H (where H is defined as building height).

Figures 4 (**TS-1**) - (**TS-8**) presents contours turbulent kinetic energy (TKE) in the *xz* plan at (y = 0,0), dimensioned by the square of the velocity in the direction x at the height of the building, for different constants empirical studies that have been tested. The color shown shows the lowest TKE values in blue colour. It can be observed that in **TS-1**, the standard condition of the model, the region with the highest TKE occurs in the roof of the building, very similar to the results of the wind tunnel experiment performed by Murakami et al., (1990). The proposed **TS-4** improved the length of the ZR as can be observed in Figure 4 (**TS-4**) and consequent worsening of the TKE representation in the zones of stagnation. Table 1 presents a comparison of the length of the ZR between the sensitivity tests performed, it can be observed that the **TS-4** represented the smallest dimensionless length of the ZR.

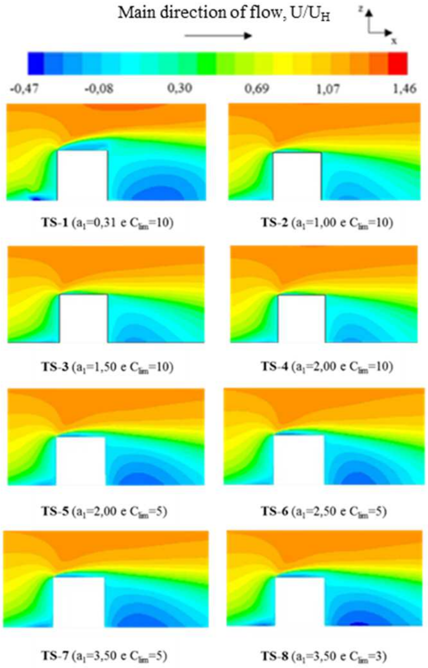

Figure 3. longitudinal velocity contour in vertical plane xz at y=(0.0).

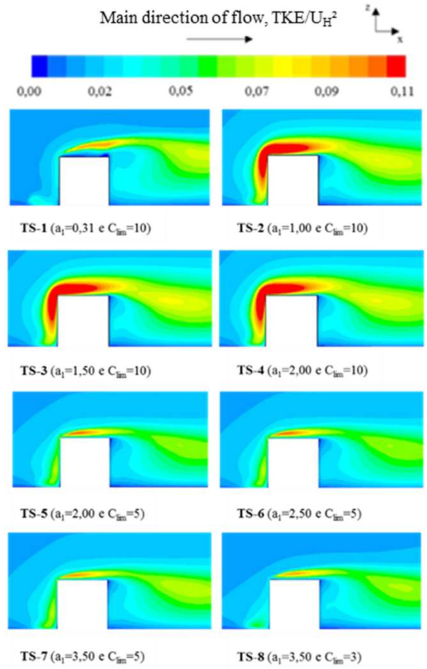

Figure 4. Turbulent kinetic energy contour in vertical plane xz at y=(0.0).

Figures 5 and 6 compare results from previous studies with **TS-4** and **TS-6**. Figure 5 shows avarege velocity field in the central plan of the cubic building obtained in the wind tunnel experiment, LES and k-ε Standard conducted by Murakami et al. (1990), of k-ε Modified by Santos (2000). It also shows the result of the ω and ω-BSL model obtained in the study by Cezana (2007). It can be observed that **TS-4** presents less recirculation behind the building than **TS-6**. It is also noted that the vectors reattachment on the roof of the building, as the experimental results. Figure 6 shows the distribution of turbulent kinetic energy in the *xz* plan at (y = 0,0), there are some discrepancies of the turbulence model of the present study, when compared with the experimental data. The **TS-4**, although presented a relatively good result for the length of the ZR, is discrepant in the TKE distribution with performance similar to the model k-ε Standard. **TS-6** and LES reproduce with good precision the TKE distribution, being considerably better than the other models used. Table 2 shows the calculation of the length of the recirculation zone behind the building for the experiment and the different models used to represent Murakami et al. (1990). This length is dimensionless with the height of the obstacle. It can be observed that the result found for **TS-4** is closer to the experimental result: the length of the ZR is bigger only than the LES modeling. Considering the higher computational cost of the LES model in relation to the RANS models used in the present study, this data is positive. The length of the ZR for TS-6 presents an increase over **TS-4**, however it is compatible with the results of the other models tested.

Table 1. Length of the recirculation zone behind the building.

Description	X_R
TS-1 (a_1 = 0,31 e c_{lim} = 10)	2,70H
TS-2 (a_1 = 1,00 e c_{lim} = 10)	2,12H
TS-3 (a_1 = 1,50 e c_{lim} = 10)	2,00H
TS-4 (a_1 = 2,00 e c_{lim} = 10)	1,63H
TS-5 (a_1 = 2,00 e c_{lim} = 5)	2,25H
TS-6 (a_1 = 2,50 e c_{lim} = 5)	2,20H
TS-7 (a_1 = 3,50 e c_{lim} = 5)	2,38H
TS-8 (a_1 = 3,50 e c_{lim} = 3)	2,50H

Table 2. length of recirculation zone behind the building.

Description	X_R
Wind tunnel (Murakami et al., 1990)	1,2H
LES (Murakami et al. 1990)	1,4H
k-ε Standard (Murakami et al., 1990)	-
k-ε Modified (Santos, 2000)	2,17H
ω-BSL (Cezana, 2007)	2,1H
ω (Cezana, 2007)	2,1H
k-ω SST (TS-4)	1,63H
k-ω SST (TS-6)	2,2H

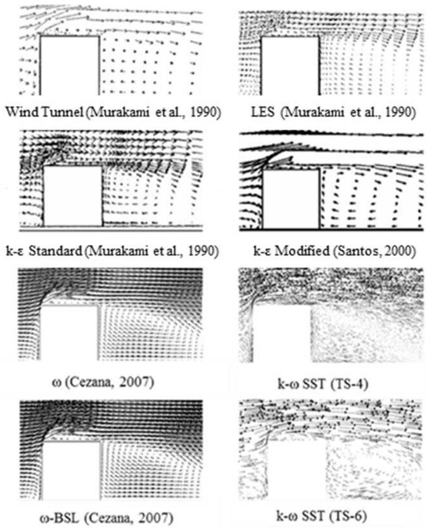

Figure 5. Vector field in plane of symmetry.

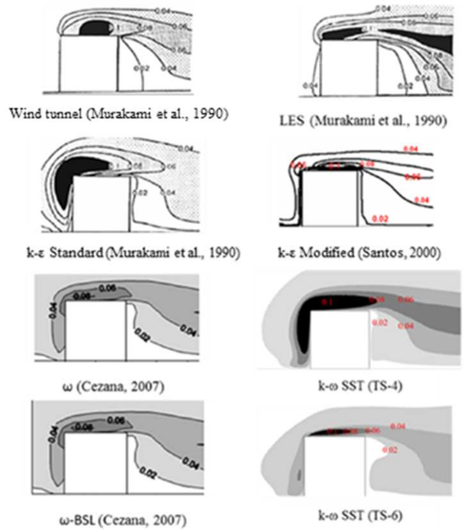

Figure 6. Turbulent kinetic energy contour in vertical plane xz at y=(0.0).

3.2 Dispersion field

This section had the aim to evaluate the effect of the sensitivity tests carried out in the field of dispersion of the propylene gas compound in the air, the arrangement for the source and detection is used according to Figure 2. The dimensionless concentration (K_{adim}) presented in this section corresponds to the following relation:

$$K_{adim}=\frac{C}{C_0} \tag{3}$$

$$C_0=\frac{Q}{U_H H^2} \tag{4}$$

where,

Q - Source flow; C_0 - velocity in the height of the building; C - Molar fraction of the gaseous compound; C_0 - Reference concentration of the gaseous compound.

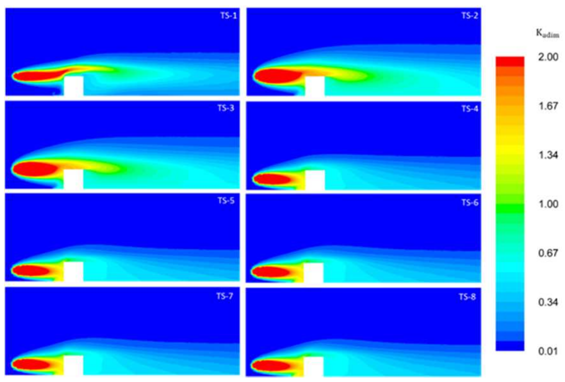

Figure 7. Contour of dispersion field, K_{adim}, view of the simmetry plan of the building for the sensitivity tests (TS-1) – (TS-8)

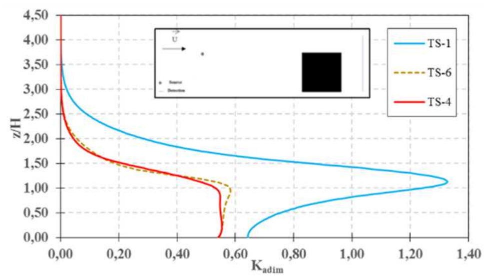

Figure 8. Dispersion profiles downstream of the building.

Figures 7 (**TS-1**) - (**TS-8**) show the view of the xz plan at y = (0.0) for dimensionless concentration. It can be observed in **TS-1** that RANS computational model used in the present study, in the standard condition, presents the lowest dilution of the pollutant among all the cases tested, as it can be visualized. It is possible to verify when analyzing the other sensitivity tests from the modification of the empirical constants a_1 and C_{lim} that the increase of the dilution of the gaseous compound.

Figure 8 presents results of vertical profiles that are obtained in the *xz* plan at (y= 0.0), these vertical profiles are located at x = 0.75H downstream of the building. The graph shows that the results **TS-4** and **TS-6**, which have a lower recirculation zone length and better prediction of turbulent kinetic energy (when compared with experimental results), respectively, influence the dilution of the boom. In this way, both the turbulent kinetic energy and the length of the recirculation zone behind the building modified the behavior of the pollutant boom by increasing the dilution of the gaseous compound when compare with standard condition (**TS-1**).

4. SUMMARY AND CONCLUSIONS

The present work investigated the flow and dispersion around an isolated cubic obstacle with neutral condition through numerical simulations using the RANS based k-ω SST turbulence model. Results were compared to experimental wind tunnel data. The following aspects were revealed:

- In general, the results of the sensitivity tests of the k-ω SST model met expectations regarding the adjustment of the ZR length behind the building by increasing the empirical constant a_1.
- In general, the results of the sensitivity tests of the k-ω SST model met expectations regarding the TKE adjustment in the stagnation zones and were visualized in the results of the flow field a as a function of the modification of the standard value of the empirical constant C_{lim}. On the other hand, there was no result among the tests performed in which at the same time the adjustment of ZR and TKE was verified simultaneously when compared to the experimental results.
- Analysis of the dispersion field showed that both the length of the recirculation zone and the turbulent kinetic energy in the stagnation zones appear to influence the dispersion of the compound since the **TS-4** and **TS-6** sensitivity tests showed higher dilution of pollutant plume than the standard condition of the RANS model used in the present study.

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