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# NUMERICAL SIMULATION OF POLLUTANT DISPERSION IN THE ATMOSPHERE

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**Abstract.** Air pollution can cause both environmental and human health damage, so it is necessary to study the best way these pollutants can be emitted, predicting how their effects will be. For this, a scenario involving a pollution source is modeled and tests are carried out on how the emission of pollutants in this area would behave, using different heights for the pollution source. In this sense, this work proposes a way of modeling complex two-dimensional meshes with the use of elliptic equations for generating meshes in the curvilinear coordinate system, in which the computational grid coincides with problem geometry, which makes computational processing more suitable. For a better representation of the domain, the multiblock technique will be used too. Similarly, curvilinear coordinates will be used for the discretization of the Navier-Stokes and transport of pollutants equations, using first order upwind scheme in the convective term. To test the proposed method, three test cases were performed varying the relation between the height of chimney and obstacle that made up their geometries. Through the performed tests, it was verified that the results obtained are satisfactory.

**Keywords:** pollutant dispersion, atmospheric pollution, numerical simulation, multiblock technique

## 1. INTRODUCTION

The emission of pollutants into the atmosphere interferes with air chemical composition and can cause both environmental and human health damage. Several sources are responsible for emitting such pollutants, and can be classified as natural, such as natural fires and volcanic emissions, or anthropogenic, such as burning fossil fuels in factories and automobiles. Studying how emissions occur from these sources, especially the anthropogenics, it is fundamental to try to reduce such damages (Cavalcanti, 2010).

One way of conduct this study is through the simulation of how pollutants dispersion would occur in a given situation. This can be done through mathematical modeling, where, initially, the computational mesh representing the physical domain of the scenario is modeled, followed by the numerical simulation of Navier-Stokes and transport equations.

The precision of solutions obtained by the simulations of fluid dispersions depends on how well computational mesh represents the studied geometry. For problems with complex geometries, it is convenient to use the curvilinear coordinate system instead of Cartesian coordinates, due to the fact that the Cartesian coordinates lead to a poor boundary fit, since the physical domain doesn't always coincide with mesh domain. Other reasons that lead to the use of curvilinear coordinate system in the discretization of the computational mesh refer to less difficulty in programming computational codes to solve complex problems and the ease in developing generic methodologies.

Despite the advantages of using curvilinear coordinates for mesh construction, it is still possible to obtain elements of poor quality. A way to circumvent the quality of mesh elements, not necessarily improving refinement, because it would increase the number of nodes in the mesh, and consequently, the computational costs with memory and execution time, is the use of multiblock technique, in which the domain is divided into parts, called blocks or sub-grids, and equations are solved independently in each one. With independent block separation, it is possible to increase mesh refinement at important areas or decrease it in less relevant areas, allowing the generation of structured grids keeping simulation costs balanced. A comparison between computational meshes generated using a single block, Figure 1a, and multiblocks, Figure 1b, is shown. For such comparison be made, the meshes were generated with the same amount of partitions, being possible to perceive improvement in elements quality.

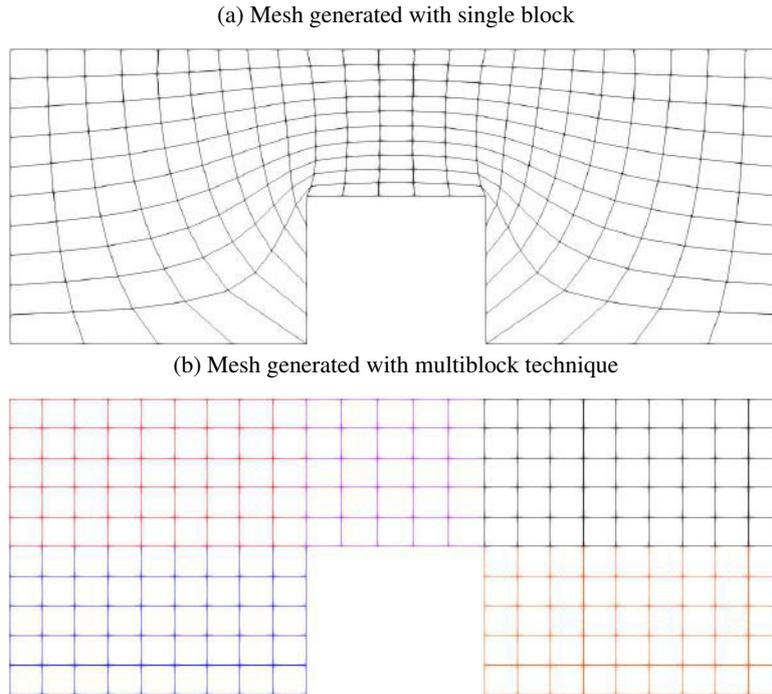


Figure 1. Comparison between meshes generated with a single block and multiblock techniques, both with the same number of elements

Thus, this work proposes the use of multiblock technique for mesh generation, resolution of Navier-Stokes equations, to obtain simulation velocity vectors modules, and resolution of the transport equation, to model pollutant dispersion, whose discretizations will be obtained by the finite difference method using curvilinear coordinates and using first order upwind scheme in the convective term.

## 2. METHODOLOGY

To generate the meshes, the blocks were represented as shown in Figure 2, where W side represents west direction, E, east, N, north and S, south direction. Then, to generate the blocks, parameters with the number of elements in  $\xi$  and  $\eta$  directions and their points coordinates to each side were passed.

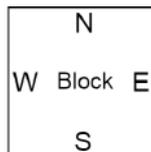


Figure 2. Blocks representations

The boundary conditions are important for a fluid dispersion numerical solution, since they define the simulation limits and help to guarantee method stability and convergence. Thus, correctly define the blocks boundaries is extremely important. The implemented algorithm recognizes boundary conditions type of the four sides of each mesh block.

For solution of Navier-Stokes equations, the used types of boundary condition were:

- CNEI: non-slip and impermeability condition of the fluid, indicates that there is no flow through this wall, which means the fluid velocity in relation to the surface is zero;
- CIPR: prescribed fluid injection condition, used at boundaries where fluid is injected into the system;
- CECO: continuous fluid flow condition, indicates fluid output from the system;
- ADJA: indicates adjacency between blocks, there will be data transfer between these boundaries.

The used types of boundary condition to solve the transport equation were:

- CIPRCONC: prescribed concentration injection condition, indicates concentration entry into the system across this boundary;

- CCONCCONC: continuous concentration condition, indicates concentration continuous dispersion, there may be concentration output from the system;
- ADJA: used to indicate adjacency between blocks.

A concern when using multiblocks technique is to maintain simulation consistency, and for this, a treatment occurs in the boundaries that indicate adjacency between blocks. The two bands of previous/posterior elements of neighboring blocks serve as transfer area, with no solution calculation in them. To guarantee simulation continuity, it is required that the adjacent boundaries points have the same coordinate in both neighboring blocks. Figure 3 shows an example of adjacency.

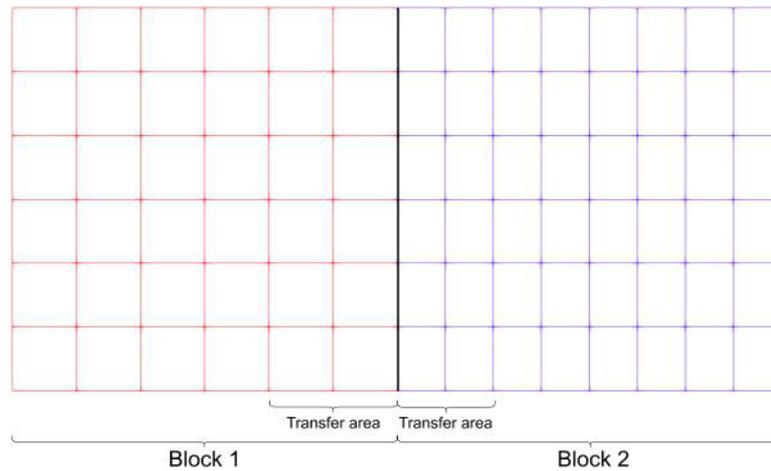


Figure 3. Adjacency treatment between blocks. Data is transferred in the two bands near the border in each block.

### 3. RESULTS AND DISCUSSION

Tests were carried out on three meshes composed of a chimney and an obstacle. In the first case, chimney height is smaller than obstacle height, in the second case, chimney height is greater than obstacle height, and in the third case, chimney and obstacle have the same height.

The meshes were divided into 8 blocks, the division form and parameters for their generation are presented next to each case. The boundaries conditions were kept the same in three cases. Table 1 shows the conditions to solve dispersion velocity field and Table 2 presents the conditions to solve the concentration of pollutants in the system.

Table 1. Boundary conditions to solve Navier-Stokes equations

Block	Boundary			
	W	E	N	S
1	CIPR	CNEI	ADJA	CNEI
2	CIPR	ADJA	CNEI	ADJA
3	ADJA	ADJA	CNEI	CIPR
4	CNEI	CNEI	ADJA	CNEI
5	ADJA	ADJA	CNEI	ADJA
6	ADJA	ADJA	CNEI	CNEI
7	CNEI	CECO	ADJA	CNEI
8	ADJA	CECO	CNEI	ADJA

The required parameters to solve the Navier-Stokes equations, final time, time lapse ( $\Delta t$ ), specific mass  $\rho$ , dynamic viscosity  $\mu$  and velocity injection  $v_i$ , were maintained the same for the three cases and are shown in Table 3. According to Table 1 information, velocity injections were made on the left boundary of the geometry and at the chimney output, trying to simulate ambient conditions and chimney operation.

Air specific mass  $\rho$  value was based on the normal conditions of temperature and pression, equivalent to 0 °C and 101325 Pa, respectively (Taylor, 2013). The dynamic viscosity  $\mu$  value was calculated by equation(Reynolds, 1883):

$$\mu = \frac{\rho L v_i}{Re} \quad (1)$$

Table 2. Boudary conditions to solve transport equation

Block	Boundary			
	W	E	N	S
1	CCONCONC	CCONCONC	ADJA	CCONCONC
2	CCONCONC	ADJA	CCONCONC	ADJA
3	ADJA	ADJA	CCONCONC	CIPRCONC
4	CCONCONC	CCONCONC	ADJA	CCONCONC
5	ADJA	ADJA	CCONCONC	CCONCONC
6	ADJA	ADJA	CCONCONC	CCONCONC
7	CCONCONC	CCONCONC	ADJA	CCONCONC
8	ADJA	CCONCONC	CCONCONC	ADJA

Table 3. Parameters to solve Navier-Stokes equations

Parameters	Values
Final time	100 s
Time lapse ( $\Delta t$ )	0.001 s
Specific mass $\rho$	1.293 kg/m <sup>3</sup>
Dynamic viscosity $\mu$	0.07758 N.s/m <sup>2</sup>
Velocity injection $v_i$	Boundary 0.2 m/s Chimney output 0.2 m/s

where  $Re$  corresponds to Reynolds number and  $L$ , to the mesh height.  $L = 3$  was used in all three cases and, in order to reach a laminar flow, a small Reynolds number equal to  $Re = 10$  was used.

Table 4 shows the parameters to transport equation, final time, time lapse ( $\Delta t$ ), species diffusion coefficient, species decay coefficient and concentration injection. These parameters were also kept the same for all three cases. The concentration injection occurs only at the chimney output, as shown in Table 2.

Table 4. Parameters to solve transport equation

Parameters	Values
Final time	100 s
Time lapse	0.001 s
Diffusion coefficient	0.3 m <sup>2</sup> /s
Decay coefficient	0.01 s <sup>-1</sup>
Concentration injection	1 kg/m <sup>3</sup>

**First case: chimney height smaller than obstacle height**

The mesh used for the first case is shown in Figure 4, where it is possible to notice that chimney height is smaller than obstacle height. Its division into 8 blocks is also shown in the Figure 4. The parameters required for its generation, the number of partitions in  $\xi$  and  $\eta$  directions, are reported in Table 5.

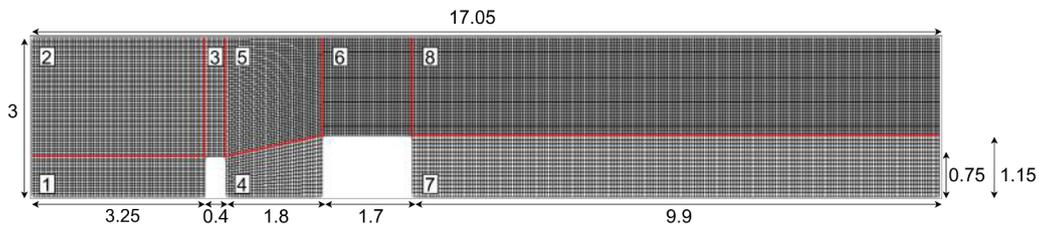


Figure 4. Mesh of the first case, where the chimney height is smaller than the obstacle height.

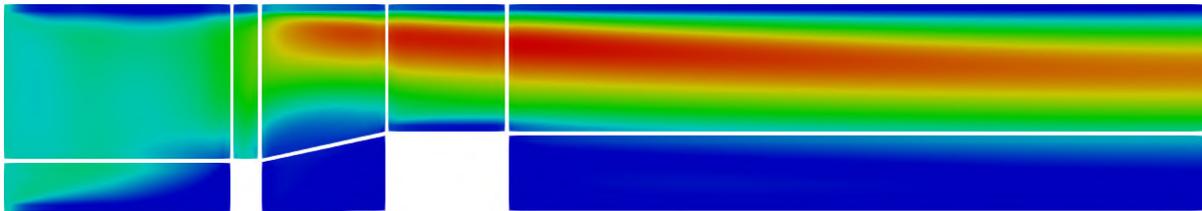
The obtained wind flow is presented in Figure 5. It is noticed that higher velocities are concentrated near the obstacle and decrease as the dispersion area increases, as seen in 5a. In 5b, orientation of the velocity field is shown over the entire mesh extension. Vortices formations are observed at left of the chimney, between chimney and obstacle and at right of the obstacle. A more detailed view of these formations is illustrated in 5c.

The final concentration field, resulting from the transport equation, is shown in Figure 6a. It is possible to notice accumulation of pollutants in the vortex located between chimney and obstacle, and this concentration decreases as it distances from the source. In Figure 6b, contours of this situation are presented.

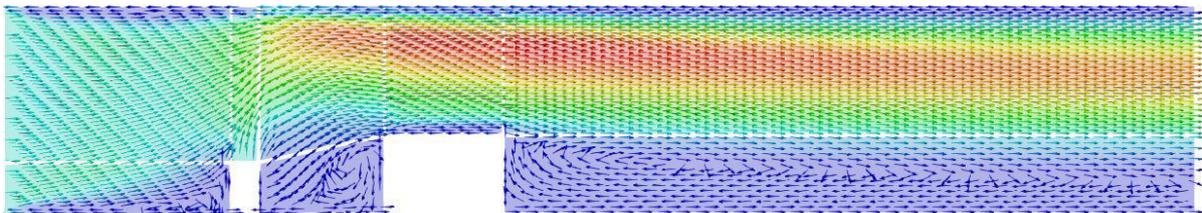
Table 5. Parameters for generating the mesh of the first case

Block	Partitions in $\xi$	Partitions in $\eta$
1	67	15
2	67	45
3	8	45
4	40	15
5	40	45
6	38	45
7	219	15
8	219	45

(a) Velocity field module



(b) Orientation of velocity vectors



(c) Velocity field vortices

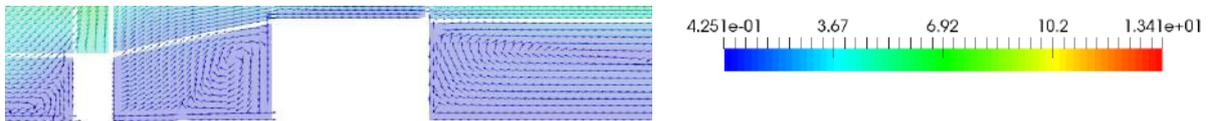
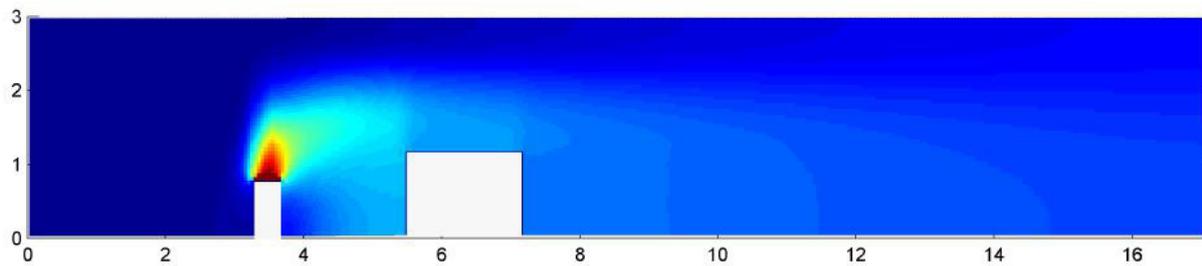


Figure 5. Velocity field for the first case

(a) Concentration module



(b) Concentration contour

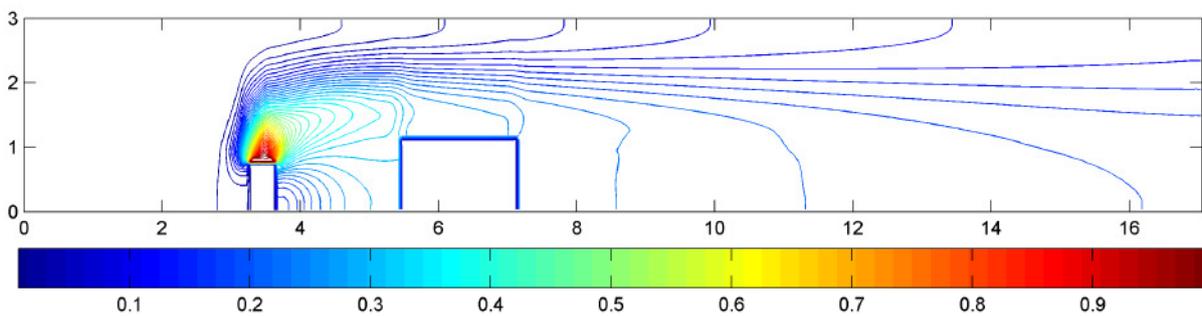


Figure 6. Concentration of pollutants for the first case

**Second case: chimney height greater than obstacle height**

Mesh configuration for second case is shown in Figure 7, where chimney height is greater than obstacle height. Its block division and identification of this blocks is also shown in Figure 7. The number of partitions in  $\xi$  and  $\eta$  directions for each block is presented in Table 6.

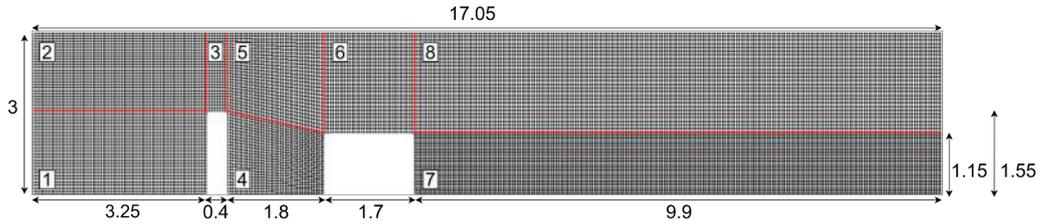


Figure 7. Mesh of the second case, where the chimney height is greater than the obstacle height.

Table 6. Parameters for generating the mesh of the second case

Block	Partitions in $\xi$	Partitions in $\eta$
1	67	27
2	67	27
3	8	27
4	40	27
5	40	27
6	38	27
7	219	27
8	219	27

The velocity vector module for this scenario, obtained as result from simulating the Navier-Stokes equations, is presented in Figure 8a. In 8b, the orientation of velocity vectors over the entire mesh is shown. In 8c, a view focused on the vortices is made. In this case, vortices were formed at left of the chimney and at right of the obstacle.

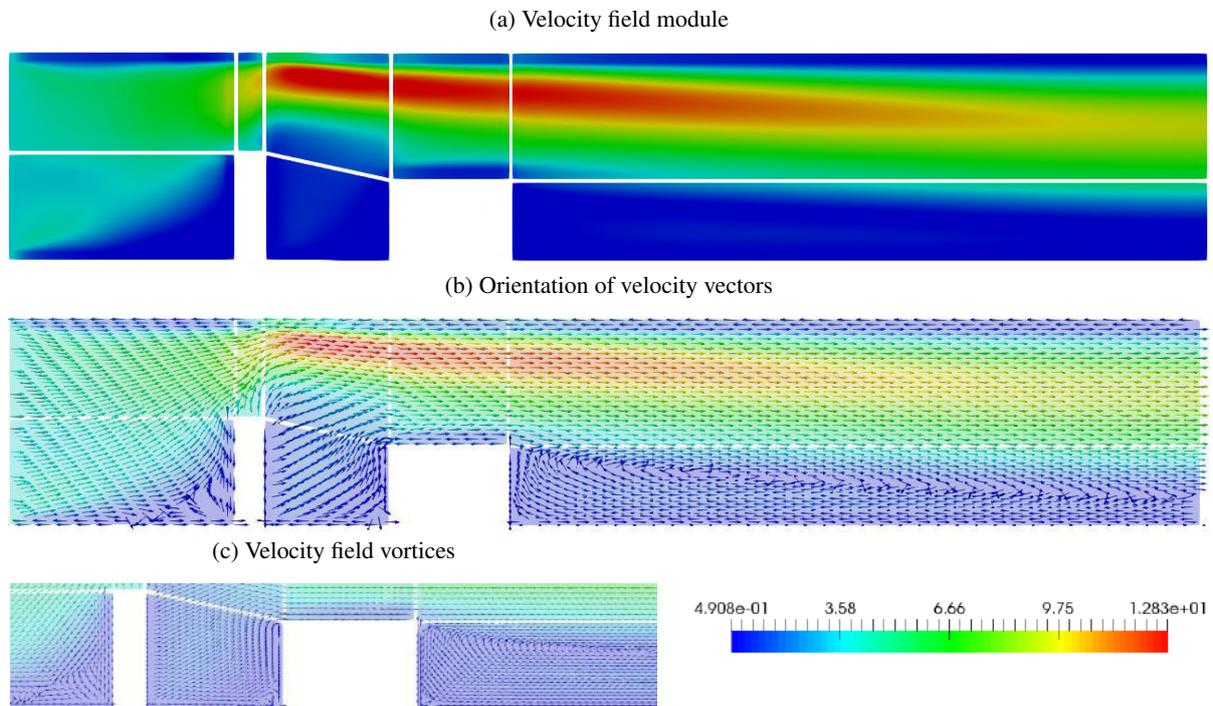


Figure 8. Velocity field for the second case

In Figures 9a and 9b, module and contour of the final result of the transport equation simulation are presented, respectively. It is possible to notice that pollutants are dispersed throughout the geometry. However, since there is no vortex in the velocity field between chimney and obstacle, there is almost no concentration of pollutants.

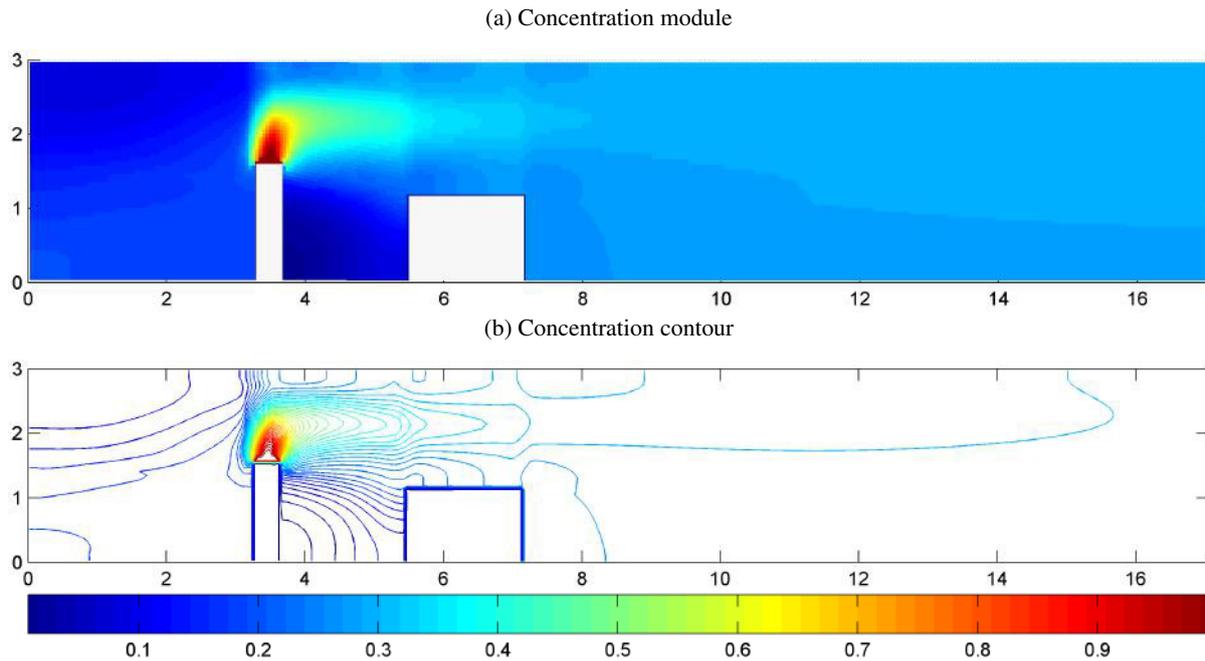


Figure 9. Concentration of pollutants for the second case

### Third case: chimney and obstacle with the same heights

Dimensions and blocks identification of the third mesh, which presents chimney and obstacle with the same height, are presented in Figure 10. Parameters to generate this mesh, partitions in  $\xi$  and  $\eta$  directions for each block, are presented in Table 7.

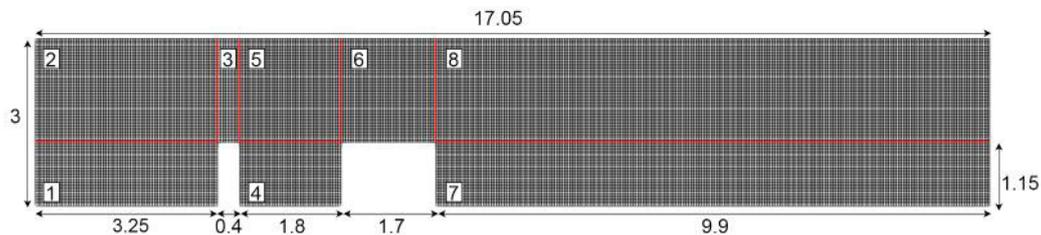


Figure 10. Mesh of the third case, where the chimney and obstacle have the same heights.

Table 7. Parameters for generating the mesh of the third case

Block	Partitions in $\xi$	Partitions in $\eta$
1	67	27
2	67	45
3	8	45
4	40	27
5	40	45
6	38	45
7	219	27
8	219	45

Velocity field module obtained for the dispersion flow is presented in Figure 11a, the orientation of its vectors is shown in 11b, and a more detailed view of vortices formed at left of the chimney, above and at right of the obstacle is made in 11c. In this case, two more vortices were formed, one between the 7th and 8th blocks and other in the top right of the 8th block, which can not be completely seen because of limitations in the geometry size.

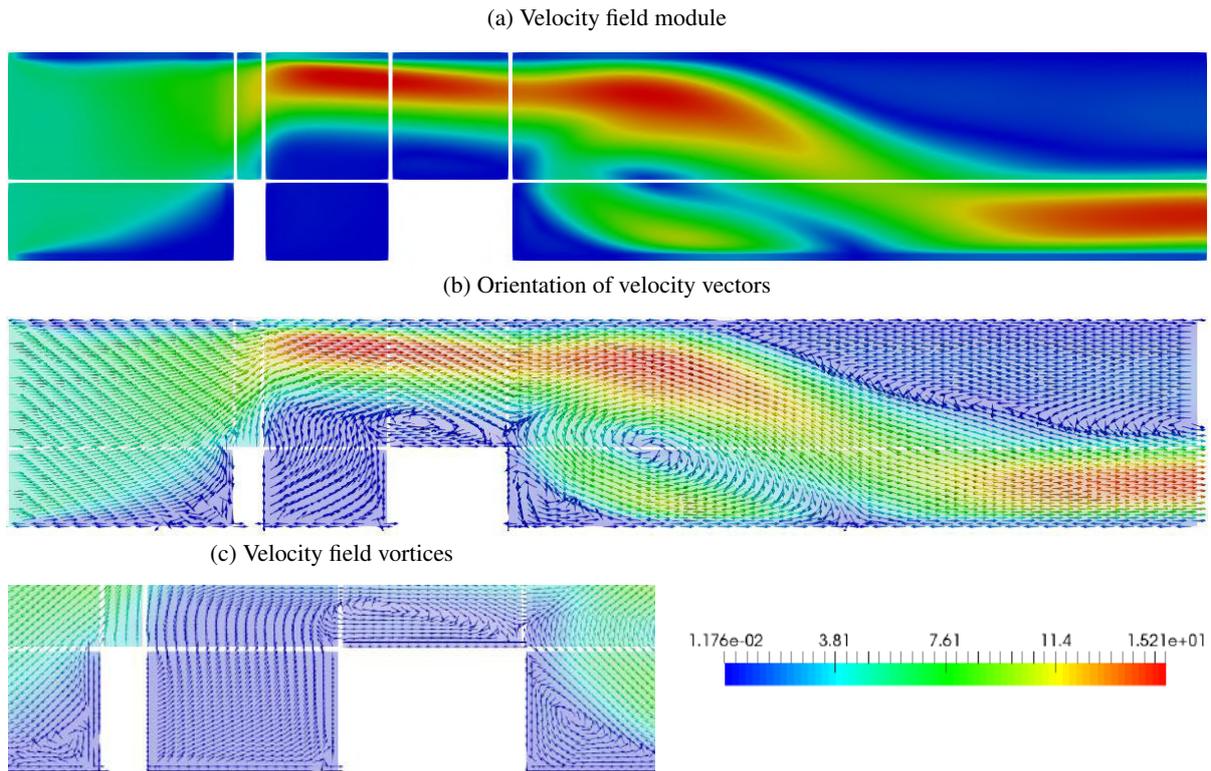


Figure 11. Velocity field for the third case

Final concentration module, obtained at the end of transport equation simulation, is show in Figure 12a where it is possible to notice accumulation of pollutants around the obstacle and after it, reaching the right boundary of the geometry. The contours of this situation are seen in 12b, in which vortex center between the 7th and 8th blocks is noted.

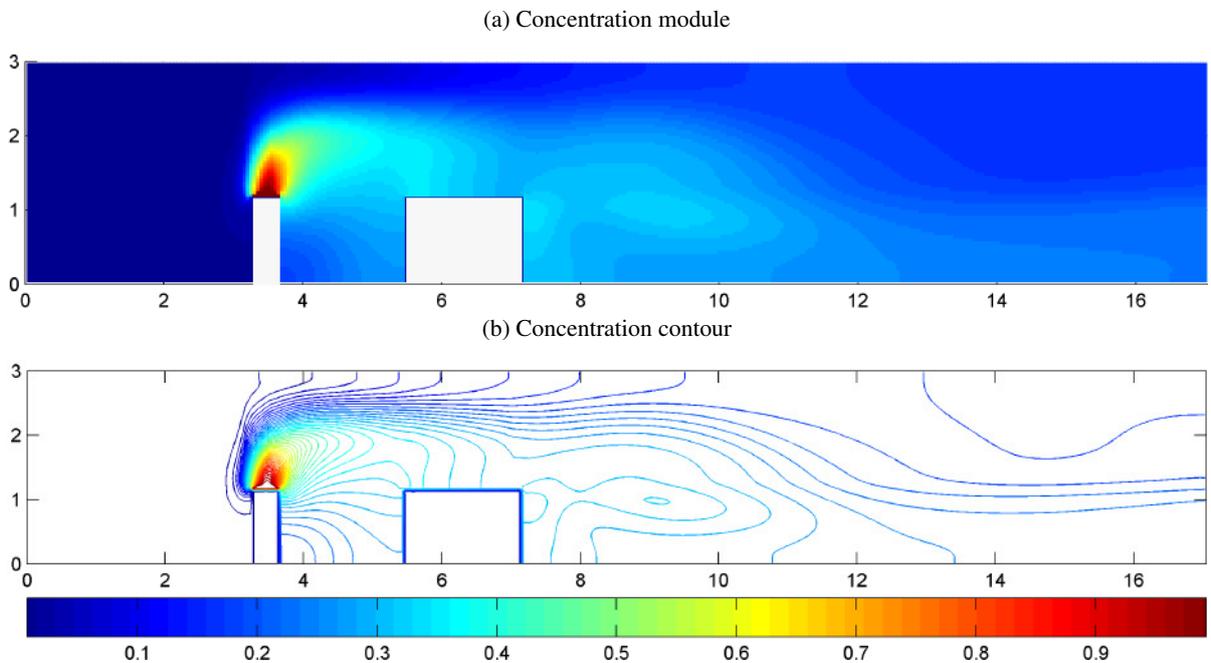


Figure 12. Concentration of pollutants for the third case

#### 4. CONCLUSION

This paper presented a way of simulating, in two dimensions, the dispersion of pollutants in a complex domain. For computer mesh generation, it was proposed to use the curvilinear coordinate systems and the multiblock technique, which allowed to obtain a mesh coincident to the physical domain, with good quality elements and without big increases in

computational costs. Continuity of the fluid dispersion simulation in meshes partitioned in blocks was guaranteed through the treatment of adjacent boundaries, in which a data transfer area has been selected in each block, there being no solution calculation in these elements.

Velocity field vectors simulating winds in the physical domain were obtained by simulating Navier-Stokes equations and pollutants concentration, obtained through the simulation of the transport equation, both discretizations were achieved using finite difference method with curvilinear coordinates and first order upwind scheme in the convective term.

To test the proposed method, three test cases were made varying chimney height in relation to obstacle height. Comparing the results obtained, it is possible to notice that case 2 leads to a lower pollutant concentration in the region between chimney and obstacle, but the pollutants end up spreading throughout the mesh, leading to a small accumulation in the region after the obstacle. From case 1 transport equation solution, a great pollutant concentration in the region after the pollution source is perceived, but in the region after the obstacle, there is almost no polluting reaching the ground, the same not occur in case 3, where there is pollutant concentration in the region between chimney and obstacle, above the obstacle, and just after the obstacle there is more pollutants accumulation, caused by vortex formation in the velocity field, leading to pollution of both areas.

Thus, analyzing the solutions obtained we conclude that they are as expected, considering the characteristics of each mesh, with vortices formations at predicted locations of velocity field, and pollutants concentration following velocity vectors. Therefore, the results obtained were satisfactory in the sense of theoretical proof, showing the feasibility of the proposed method.

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