WIT CONFERENCES This paper is part of the Proceedings of the 24th International Conference on Modelling, Monitoring and Management of Air Pollution (AIR 2016)
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Simulation with the finite element method of air pollution with carbon monoxide in the City of Arequipa (Peru)

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Abstract

Many Latin American cities present issues with air pollution, especially with carbon monoxide (CO). In the specific case of the city of Arequipa (Peru) where the population of vehicles tend to be old and deteriorated, monitoring the values of CO in all the points of a large city is impractical. The objective of this investigation is to mathematically simulate this problem, solving the differential equations in a two-dimensional transient state of pollutant transport, considering the following terms: diffusion, convection, source and reaction. The procedure was to discretize the city in more than three thousand triangular elements, then we transformed these differential equations into integral equations. For that we use the Petrov–Galerkin method, later we transformed these integral equations into matrix equations, and then solve these equations in order to get the values of CO in all the elements on which the city was discretized. The initial data and boundary conditions that were used, are the current real values, we have also considered the wind direction and measured point sources. We developed software called "Model of Environmental Pollution (MEP)" which was used to obtain the results, which are shown in graphical form. This investigation has concluded that the pollution due to carbon monoxide is in line with the environmental quality standards of the city. This methodology of simulation can be replicated in other cities, as the MEP software has already been developed.
Keywords: finite element method, carbon monoxide, air pollution, computational simulation, Petrov–Galerkin method, two dimensional, transient state, diffusion, convection, first order reaction.

1 Introduction: problematic

The atmosphere is composed essentially of nitrogen, oxygen and some noble gases. In the more densely populated areas, the main sources of pollution are due to certain human activities. One source of air pollution is the carbon monoxide (CO), in urban areas a very high percentage of the presence of CO is due to the emission of this gas from the vehicular traffic and industrial processes.

Ozone is an oxidizing gas and natural component of the atmosphere, 90% of its concentration is distributed in the stratosphere and the remaining 10% resides in the troposphere. Stratospheric ozone absorbs virtually all UV radiation from the sun, it means, acts as a protective layer for living beings and ecosystems preventing that ultraviolet radiation reach the Earth's surface. It is evident that stratospheric ozone depletion is due to the increase of CO in Earth.

In addition, emissions of CO from vehicles have a direct impact on air pollution both locally and globally. Nowadays, human activities are altering world's climate. In the atmosphere the concentration of gases that catch the reflected radiation from Earth is increasing, which amplifies the "greenhouse effect." One of the main greenhouse gas is carbon dioxide (coming mostly as a result of fossil fuel combustion and forest burning). In the third Assessment Report of 2001, the Intergovernmental Panel on Climate Change (IPCC) stated: "There is new and stronger evidence that most of the global warming observed over the last fifty years is attributable to human activities". For these reasons, the governing equations of carbon monoxide transport are solved with the finite element method to apply to the City of Arequipa.

2 Governing equations

The phenomenon of pollutant transport process in fact, has the following components: temporal variation, dispersion, convection and first order reaction or decay. These components are represented through the outlining of a differential cube [1], called control volume, and then apply the laws of physics and mathematics. In Figure 1, it is considered that the concentration (C) inside the cube is uniform because of its very small size, the x, y and z axis are analysed which are limited by the different faces of the cube, called control surfaces.

Applying the law of conservation of mass, the variation of mass per unit of time within the control volume (mass flow rate) must be equal to the rate at which the mass enters the left side of the control volume in directions of the x, y and z axis, less the same mass that is leaving on the right side, plus differential of mass, plus the mass gains due to a point source and minus the first-order kinetics also called decay [2].

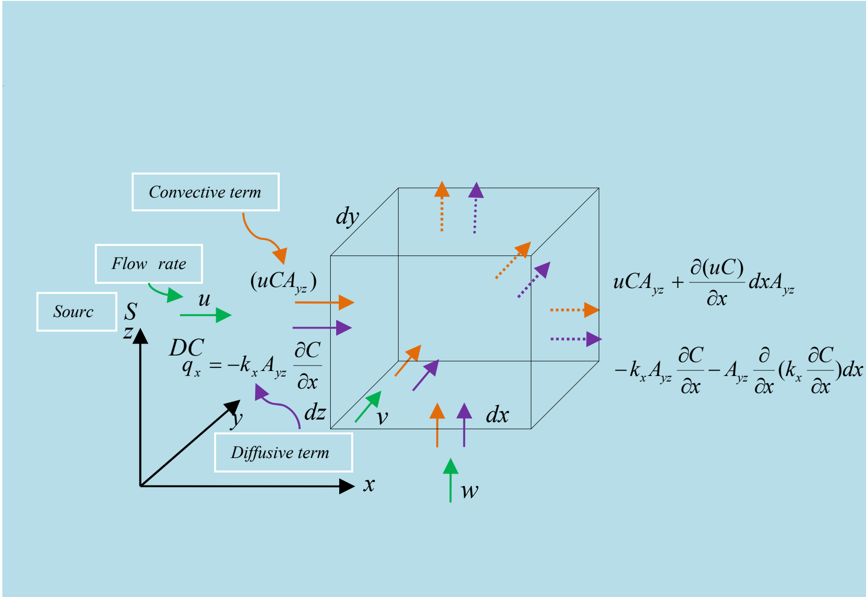

Figure 1: Diagram of the concept model for the transport of pollutants.

After applying mathematical concepts to the law of conservation of mass and make appropriate simplifications, we get to the governing equation shown below [3]:

$$\frac{\partial C}{\partial t} = -u\frac{\partial C}{\partial x} - v\frac{\partial C}{\partial y} - w\frac{\partial C}{\partial z} + \frac{\partial}{\partial x}\left(k_x \frac{\partial C}{\partial x}\right) + \frac{\partial}{\partial x}\left(k_y \frac{\partial C}{\partial y}\right) + \frac{\partial}{\partial z}\left(k_z \frac{\partial C}{\partial z}\right) \quad (1)$$

$$+S - DC$$

where,
u, flow velocity of the fluid in the direction x (m/s);
v, flow velocity of the fluid in the direction y (m/s);
w, flow velocity of the fluid in the direction z (m/s);
C, concentration of the pollutant (CO) within the fluid (mg/lit.);
k_x, diffusion coefficient in the direction x (m^2/s);
k_y, diffusion coefficient in the direction y (m^2/s);
k_z, diffusion coefficient in the direction z (m^2/s);
D, decay coefficient or first order kinetics ($1/s$);
S, point source of external pollution (mg/lit);
x, length in the main flow direction (m);
y, length in the transverse flow direction (m);
z, length in the vertical flow direction (m);
t , time (seg).

Eqn (1) is an inhomogeneous partial differential equation and has no analytical solution, therefore a solution with the finite element method will be given. In the process of transport of carbon monoxide, the air flow rate is of primary importance [4], which means that the convective component predominates in the equation [5] therefore that is why the method of Petrov–Galerkin is applied.

3 Methods and materials

3.1 Finite element method

The finite element method (FEM) is a very useful numerical tool, which is used when the mathematical model or governing equation do not admit an analytical solution. The solution process with the FEM [6] is as follows:

- Set the mathematical model and boundary conditions as well as the initial condition.
- Discretize or grid the problem domain.
- Establish the interpolation function and the function of form.
- Establish the weighting or weight (Petrov–Galerkin method) for the form function.
- Make the transformation of local coordinates (x, y, z) into global coordinates (ξ, η, ζ) as this transformation simplifies the integration of the functions involved.
- Calculate the stiffness matrix or local properties for each element and vector.
- Join local matrices and vectors in a global matrix according to netting or problem domain.
- Enter initial and boundary conditions to the global matrix and vector.
- Solve the system of equations of the global matrix [7, 8].
- Do the calibration to the solution.
- Do validation of the model.
- Calculation of secondary variables.
- Get the final results in color scale charts and tables of numerical values.

3.1.1 Petrov–Galerkin method

The Petrov–Galerkin method is used when the convective effect predominates against the dispersive effect in the pollutant transport phenomenon.

The governing equation or two-dimensional mathematical model governing the phenomenon of transport of carbon monoxide (CO) is the differential equation that is shown below:

$$\frac{\partial C}{\partial t} + u\frac{\partial C}{\partial x} + v\frac{\partial C}{\partial y} - k\frac{\partial}{\partial x}\left(\frac{\partial C}{\partial x}\right) - k\frac{\partial}{\partial y}\left(\frac{\partial C}{\partial y}\right) - S + DC = 0 \qquad (2)$$

Being C, the concentration of carbon monoxide (CO). Mathematically, in compressed form, Petrov–Galerkin method [9] for the two-dimensional case is written as:

$$\iint WR\partial A = 0 \tag{3}$$

Being A, the area of the element that the entire domain has been divided, R is the residue or errors which should tend to zero, in this method R will always represent the governing equations , that is, it will the pollutant transport equation considering the terms of convection, diffusion , source and first order reaction, that is

$$R = u\frac{\partial C}{\partial x} + v\frac{\partial C}{\partial y} - k_x\frac{\partial}{\partial x}\left(\frac{\partial C}{\partial x}\right) - k_y\frac{\partial}{\partial y}\left(\frac{\partial C}{\partial y}\right) + DC - S = 0 \tag{4}$$

Being W, the weight or weighting. The weighting functions (W_i) are defined for the Petrov–Galerkin method [9, 10] as follows:

$$W_i = N_i + \frac{\alpha h}{2|q|}\left(u\frac{\partial N_i}{\partial x} + v\frac{\partial N_i}{\partial y}\right) \tag{5}$$

where

$$\alpha = CothP_e - \frac{1}{P_e} \tag{6}$$

where P_e, is the Peclet number, this number measures the dominance of advective term over the diffusive term and is defined as [11]:

$$P_e = \frac{qh}{2k} \tag{7}$$

Being

$$q = u + v \tag{8}$$

where *h* is the longest element in the wind direction, *k* is the diffusion coefficient of the pollutant.

3.1.2 Solution of the governing equation of carbon monoxide

The first two terms in eqn (4) represent the convective part of the problem, after applying some theorems and properties, this result in the equation presented below. Due to the limited space, the details of the procedure are not presented here [12].

$$\begin{aligned} u\frac{\partial C}{\partial x} + v\frac{\partial C}{\partial y} &= \iint W\left(u\frac{\partial C}{\partial x} + v\frac{\partial C}{\partial y}\right)\partial A \\ &= \frac{A}{6A}\begin{bmatrix} y_{23}u & -x_{23}v & -y_{13}u & x_{13}v & y_{12}u & -y_{12}v \\ y_{23}u & -x_{23}v & -y_{13}u & x_{13}v & y_{12}u & -y_{12}v \\ y_{23}u & -x_{23}v & -y_{13}u & x_{13}v & y_{12}u & -y_{12}v \end{bmatrix}\begin{Bmatrix} C_1 \\ C_2 \\ C_3 \end{Bmatrix} \\ &+ \frac{\alpha h}{8A|q|}\begin{bmatrix} (y_{23}u - x_{23}v)(uy_{23} - vx_{23}) & (y_{23}u - x_{23}v)(-uy_{13} + vx_{13}) & (y_{23}u - x_{23}v)(uy_{12} - vx_{12}) \\ (-y_{13}u + x_{13}v)(uy_{23} - vx_{23}) & (-y_{13}u + x_{13}v)(-uy_{13} + vx_{13}) & (-y_{13}u + x_{13}v)(uy_{12} - vx_{12}) \\ (y_{12}u - x_{12}v)(uy_{23} - vx_{23}) & (y_{12}u - x_{12}v)(-uy_{13} + vx_{13}) & (y_{12}u - x_{12}v)(uy_{12} - vx_{12}) \end{bmatrix}\begin{Bmatrix} C_1 \\ C_2 \\ C_3 \end{Bmatrix} \end{aligned} \tag{9}$$

The solution of the third and fourth terms in eqn (4) representing the diffusive term, after following the same procedure described above, is:

$$-k_x \frac{\partial}{\partial x}\left(\frac{\partial C}{\partial x}\right) - k_y \frac{\partial}{\partial y}\left(\frac{\partial C}{\partial y}\right) = -\iint W\left(\frac{\partial}{\partial x}\left(\frac{\partial C}{\partial x}\right) + k\frac{\partial}{\partial y}\left(\frac{\partial C}{\partial y}\right)\right) dA$$
$$= \frac{1}{4A}\begin{bmatrix} k_x y_{23} y_{23} + k_y x_{23} x_{23} & -k_x y_{23} y_{13} - k_x y_{23} x_{13} & k_x y_{23} y_{12} + k_y x_{23} x_{12} \\ -k_x y_{13} y_{23} - k_y x_{13} x_{23} & k_x y_{13} y_{13} + k_y x_{13} x_{13} & -k_x y_{13} y_{12} - k_y x_{13} x_{12} \\ k_x y_{12} y_{23} + k_y x_{12} x_{23} & -k_x y_{12} y_{13} - k_y x_{12} x_{13} & k_x y_{12} y_{12} + k_y x_{12} x_{12} \end{bmatrix}\begin{Bmatrix} C_1 \\ C_2 \\ C_3 \end{Bmatrix} \quad (10)$$

The fifth term in eqn (4) is the reaction of first order kinetics or decay, the solution is:

$$DC = \iint WDCdA = \frac{DA}{3}\begin{Bmatrix} 1 \\ 1 \\ 1 \end{Bmatrix} + \frac{\alpha h D}{4|q|}\begin{Bmatrix} y_{23} - x_{23} \\ -y_{13} + x_{13} \\ y_{12} - x_{12} \end{Bmatrix}\begin{Bmatrix} u \\ v \end{Bmatrix}\begin{Bmatrix} C_1 \\ C_2 \\ C_3 \end{Bmatrix} \quad (11)$$

The sixth term is the source term, with the following solution:

$$-S = -\iint WS\, dA = -\frac{SA}{3}\begin{Bmatrix} 1 \\ 1 \\ 1 \end{Bmatrix} - \frac{\alpha h S}{4|q|}\begin{Bmatrix} y_{23} u - x_{23} v \\ -y_{13} u + x_{13} v \\ y_{12} u - x_{12} v \end{Bmatrix} \quad (12)$$

Finally, temporary or transient term is solved considering the following scheme:

$$\frac{C^{n+1} - C^n}{\Delta t} = \theta\left(u\frac{\partial C}{\partial x} + v\frac{\partial C}{\partial y} - k_x\frac{\partial}{\partial x}\left(\frac{\partial C}{\partial x}\right) - k_y\frac{\partial}{\partial y}\left(\frac{\partial C}{\partial y}\right) + DC - S\right)^{n+1}$$
$$+(1-\theta)\left(u\frac{\partial C}{\partial x} + v\frac{\partial C}{\partial y} - k_x\frac{\partial}{\partial x}\left(\frac{\partial C}{\partial x}\right) - k_y\frac{\partial}{\partial y}\left(\frac{\partial C}{\partial y}\right) + DC - S\right)^{n} \quad (13)$$

where θ is the parameter that defines the scheme that will be employ, if $\theta = 0$ the scheme is explicit, if $\theta = 1$ is an implicit scheme. For the solution of eqn (13) the Petrov- Galerkin method is used again, this paper considers the implicit scheme. The final solution of the differential eqn (2) is the sum of the partial solutions from eqns (9) to (13)

4 Model of environmental pollution (MEP) software

An own software called "Model of Environmental Pollution" in Visual Basic language while interacting with AutoCAD was elaborated. The numerical solution of the model was performed with the finite element method.

The information and data that were used as initial and boundary conditions, were provided by Regional Office of Environmental Health of Health Ministry, these data have been monitored with a mobile station in different parts and times of the city. The wind speed data were provided by the National Service of Meteorology and Hydrology [13, 14] from four stations. Values are shown in figure 2.

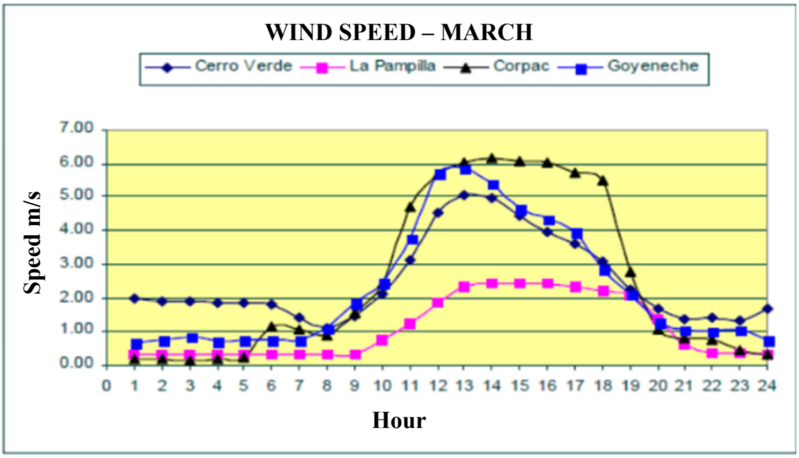

Figure 2: Variation of the wind speed in Arequipa.

The flatness of the city was drawn from the scale cadastral map of the city provided by the Provincial Municipality of Arequipa [15].

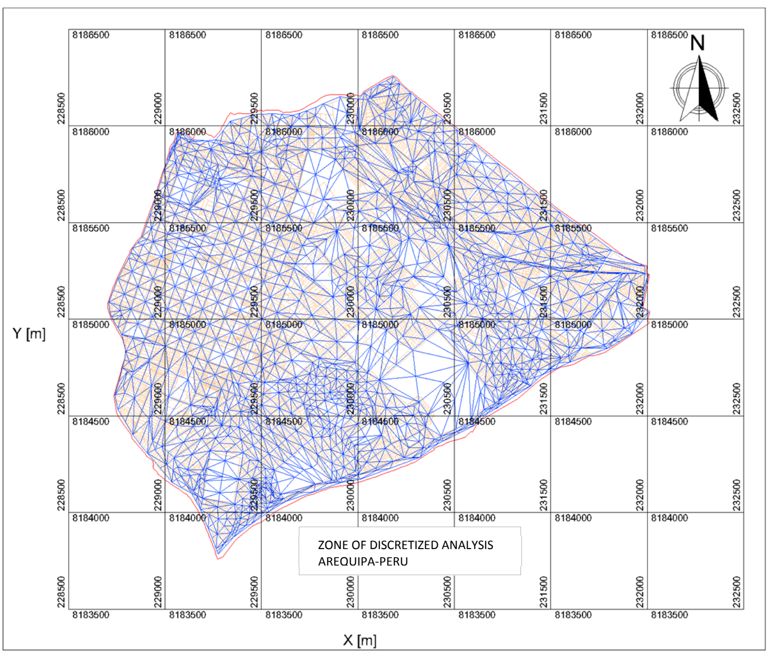

Figure 3: Discretization of the simulated zone in triangular elements.

5 Model calibration and validation

The most important step in a computer simulation is the model calibration, for it was necessary to match the simulated CO values with values measured by the health ministry. To ensure that the values match, parameters such as diffusion coefficient and source had to vary. This process is performed until a good match with the measured and simulated values is find. The final result is shown in figure 4.

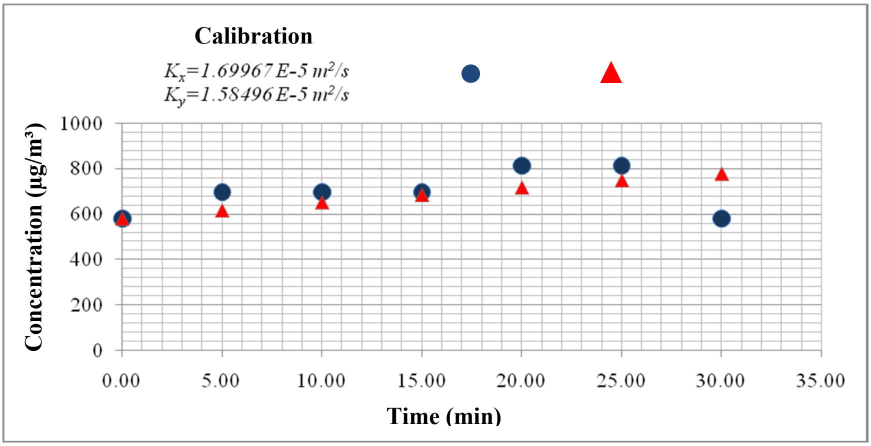

Figure 4: Results of final calibration of the model between measured and simulated values.

The values of the parameters that best matched were:

$k_x = 1.69967x10^{-5} m^2/s$: Diffusion coefficient of carbon monoxide in the direction x
$k_y = 1.58496x10^{-5} m^2/s$: Diffusion coefficient of carbon monoxide in the transverse direction y
$Q = 2.05 \mu g/m^3/s$: initial constant function source
$u = 1.26 m/s$: fluid velocity in the direction x
$v = 1.35 m/s$: fluid velocity in the direction y
$C = 580 \mu g/m^3$: initial concentration condition

With these values different and new scenarios can be generated. Validation was made after calibration, this was done with the historical records of values of CO provided by the Ministry of Health.

6 Results

The use of simulation was done in Arequipa downtown, for this the city was discretized in more than 3000 triangular elements as shown in Figure 3 and the above mentioned data were used. The first results at 9:00 am are shown in figure 5 by means of a color scale, the second results for 9:30 a.m. are shown in figure 6. It is seen that the variation in time is small since the wind speed at that time is also small as seen in figure 2. The variation of CO is oriented in the direction of the wind. The Δt employed is 5 minutes as with a longer time period the mathematical model does not converge.

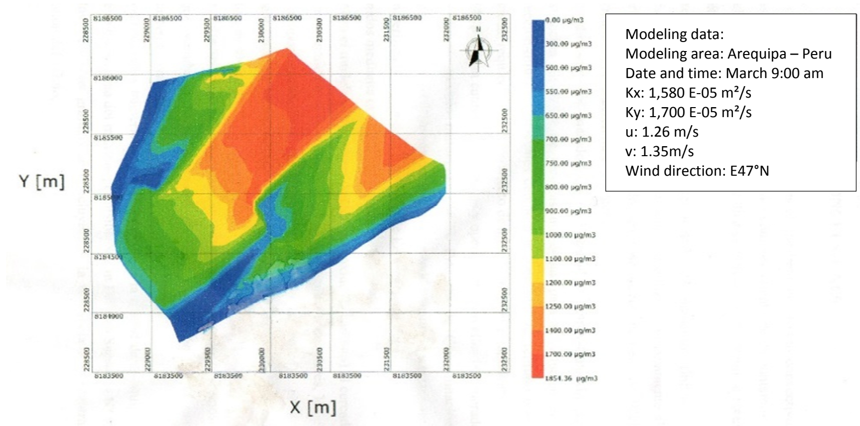

Figure 5: Simulation results of carbon monoxide in Arequipa at 9:00 am.

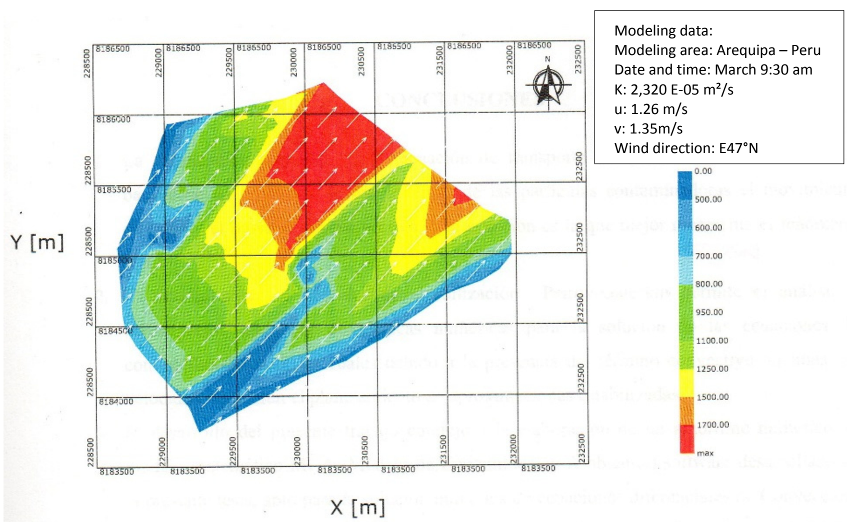

Figure 6: Simulation results of carbon monoxide in Arequipa at 9:30 am.

7 Conclusions

The results obtained from the simulation show a very good agreement with the data obtained from measurements made by the health ministry, implying that the calibrated model is good.

Once the model is established, we can generate different assumptions scenarios of pollution, for example, if vehicles increase excessively it can be inferred quantitatively how the CO will increase in the city. The usefulness of models is to predict before the event happens, if the results are bad then we can take corrective actions.

The mathematical model established, not only serves to determine the concentration of CO but also for all pollutants that have "mass" because the law used was the law of conservation of mass. Therefore, the solution of the model with the finite element method also serves to simulate the concentration of other pollutants, also the software can be used with other pollutants.

From the results of the simulation with carbon monoxide in the city of Arequipa, it is concluded that there is no contamination by carbon monoxide, as the values are below the limit of the standard of environmental quality for Peru, which is 10000. The minimum values obtained are around 3000 and peak values of 1854.36. Given these results the city of Arequipa is not contaminated with CO.

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