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Exploring Computational Fluid Dynamics Models for estimating pedestrian exposure to traffic related air pollution: A bibliometric review and critical analysis

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Abstract*– The goal of this review is to analyze the scientific work that has been carried out from 2018 to 2023 in computational modeling of exposure to air pollutants from vehicular traffic. Scopus was the database used for this research, finding a total of 555 articles to select 58 with exclusion criteria for those articles that did not focus on exposure. The bibliometric analysis concluded that this is becoming a hot topic in the scientific research community as is increasing year by year published works, and that developed countries are leading the way in this research topic. The focus of this paper is on Computational Fluid Dynamics (CFD), especially the boundary conditions, the turbulence models and its respective validation method which will indicate the physical relevance of the computational model. Results clearly indicate the that there is several physical factors, such as green infrastructure, wind conditions and traffic conditions that modify the exposure assessment, but also is evident the importance of the a social component that will also intervene within the evaluation of the exposure since both the activities and the behavior of the group of people exposed will affect the type and amount of exposure, therefore is highly recommended to integrate human exposure models into the CFD models, to evaluate how pedestrians walking near avenues are exposed to contaminants.

***Keywords*— CFD, exposure assessment, traffic-related air pollution**

I. Introduction

The World Health Organization (WHO) estimates that 4.2 million people die prematurely each year because of outdoor air pollution [1]. In urban areas, one of the main causes of this issue are the emissions air pollutants from vehicular traffic [2]. From the literature is observed, that the traffic related air pollutants are associated with higher rates of mortality, incidence of cardiovascular diseases, respiratory diseases, and lung cancer [3], [4], [5], [6].

To estimate the magnitude, frequency, and duration of exposure to a substance that a person or a population faces, the term exposure assessment arises [7]. To strengthen an exposure assessment, the following five aspects should be considered: the source of the pollutant, the environment where the pollutant is transported, the point of exposure, the route of exposure, and which people would be exposed [8].

Over the years, different techniques have been used to assess people's exposure to pollutants, from using data from fixed monitoring stations, to using wearable technological devices that allow these assessments to be more personalized [9].

In the last decades, with more computational resources available in the market, new models to simulate how pollutants behave have been developed, with one technique called Computational Fluid Dynamics (CFD), which, as the name suggests, is a combination of fluid mechanics with computational sciences, which allow for modelling, processing, and visualization of flow fields [10].

CFD models have been used to simulate the flow and transport of aerosols using an idealized respiratory system as a geometry, for children from five years old to adults [11]. It has also been evaluated with this technique; how particulate matter related to vehicular traffic affects the risk of lung cancer [12].

For the results of the computer simulations to be coherent with the phenomenon being analysed, it is important to define adequate physical parameters, such as the boundary conditions and the turbulence model to be adopted [13]. It is also necessary to establish a validation method that allows us to justify or not the results obtained from the computational model.

The air pollutants that will be discussed in this review are nitrogen oxides (NO_X), carbon monoxide (CO), and particulate matter with aerodynamic diameter less than 10 micrometers (PM_{10}), and less than 2.5 micrometers ($PM_{2.5}$).

In this review, we aim to present the current scope of CFD as a tool to evaluate exposure to air pollution and thus have a baseline on what have been done in the last five years, the gaps that have been found, and the next steps that could be taken to strengthen this research topic. The paper is divided into five main sections: Section 1 contains a brief introduction to the topic, Section 2 presents the methodology used to select the papers for this review, Section 3 presents the main results, and Sections 4 and 5 present the discussions and conclusions of this research, respectively.

II. METHODOLOGY

This research was based on a literature review of models that use CFD to estimate pedestrian exposure to traffic-related air pollutants. The exploration was conducted in the Scopus database on works published from 2018 to 2023. Two search codes were developed: (“AIR POLLUTION” AND “TRAFFIC” AND “PEDESTRIAN” AND “CFD”), known in this review as F1; while the second code known as F2 consisted of: (“AIR POLLUTION” AND “TRAFFIC RELATED” AND “PEDESTRIAN LEVEL” AND “EXPOSURE” AND “CFD”). Figure 1 shows the process of selection of the articles: a total of five hundred and fifty-five documents were obtained in the Scopus database, one hundred and fifteen were screened after the first exclusion criterion were applied and fifty-eight articles were finally selected for the confection of this manuscript following the second exclusion criterion.

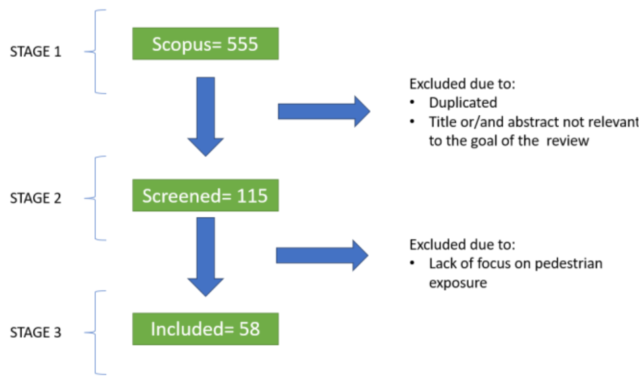

Figure 1. Selection of the articles for the review.

III. RESULTS

The results will be divided into three main aspects: a bibliometric analysis with RStudio, an exposure assessment analysis and CFD features such as boundary conditions, turbulence models and validation methods.

1. *Bibliometric analysis*

For this stage Software RStudio was employed (version 4.3.0, Boston, MA, USA. Available online: https://www.rstudio.com/, accessed on May 18, 2023), specifically the bibliometrix package. Figure 2 shows the production of scientific articles to the accessed date, and it´s evident the increase in works ins this research topic year by year, which means that this area of scientific research is becoming a hot topic as was first noted by [14].

Figure 3 Shows the countries with more research in the area, where China clearly leads this area, followed by the United States, Australia, and Western European countries such as the United Kingdom, Italy, Germany, and France. The figure also highlights regions such as Central America and Central Africa where no research has been done in Scopus in the last five years.

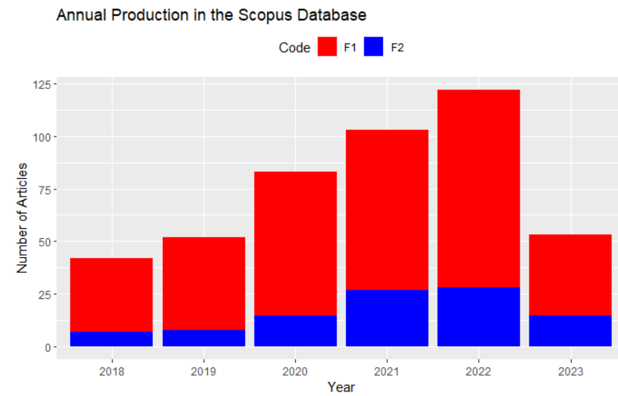

Figure 2. Publications in the Scopus database.

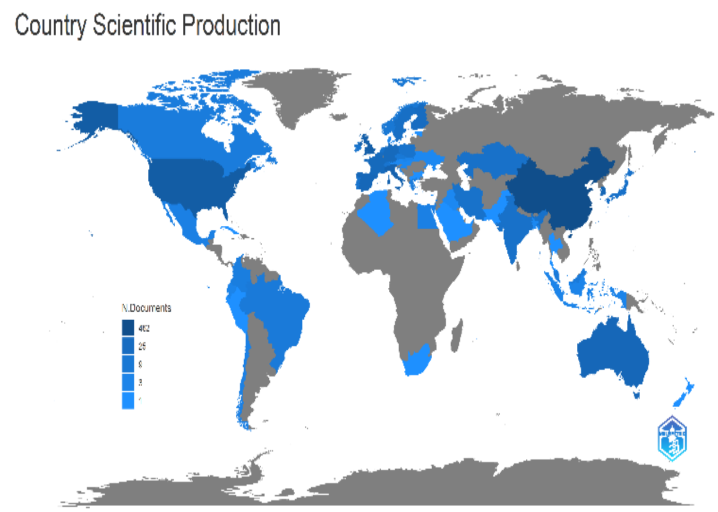

Figure 3. Scientific production by country using biblioshiny in RStudio.

The Co-Occurrence network is another exciting feature in a bibliometric analysis; it allows to see the relationship between one main circle in the center of the network, in a color, and two secondary circles at the extremes of the network and in a different color that represent different concepts. With our search codes, in Figure 4, the main circle turned out to be Computational fluid dynamics in blue. The secondary circles where the link lines are more robust with the central circle were air quality located below the central circle, and atmospheric pollution to the left, and both in red, which means that our codes lead to articles where CFD is intensely used to study air quality, and therefore atmospheric pollution appears to be relevant, and other words associated with, like concentration, air pollutants, particulate matter, etc.

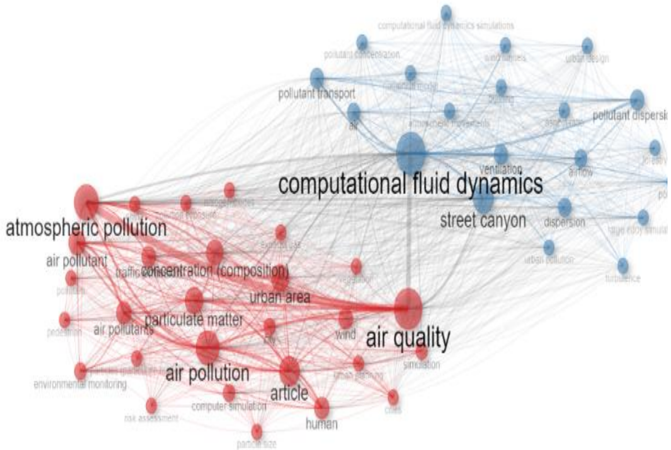

Figure 4. Co-occurrence Network obtained from biblioshiny in RStuido

2. *CFD simulations features*

2.1 Boundary conditions

Boundary conditions are important because they should represent the real physical conditions of the analyzed phenomena. In this review the focus will be on the inlet and outlet boundary conditions.

Significantly, the most used inlet boundary condition is to define velocity at the entrance of the domain, either with a constant value or with a vertical profile, both of which are usually obtained from experimental data. In this review, fifty articles used this condition, as seen in Figure 5. Four articles did not specify the inlet boundary condition used, and other four specified periodic boundary conditions, with the intention of an infinite and periodically repeating model domain; all these works use transient simulation with the Large Eddy Simulation approach (15-18).

Meanwhile in the outlet, the Zero gradient outlet boundary condition is used in twenty-four articles, this condition means that all the flow derivatives are set to zero to accomplish a fully developed flow. Eighteen articles preferred the pressure outlet, where constant static pressure is defined, and all the other flow derivatives are zero. In both cases, flow cannot re-enter the domain because this could generate numerical instability in the solution of the respective model. Twelve articles did not specify, and the same four articles that set periodic boundary conditions at the inlet did it also at the outlet.

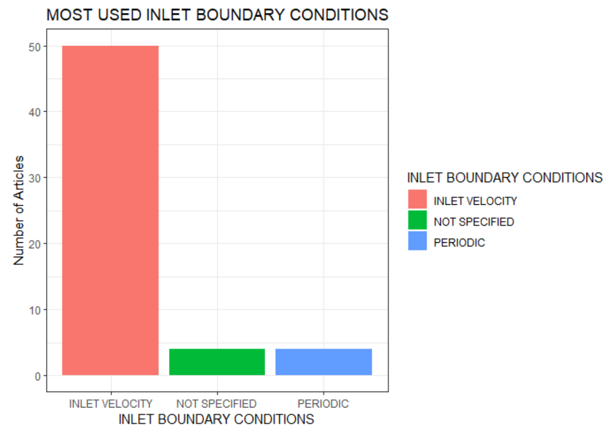

Figure 5. Inlet boundary conditions in the reviewed articles.

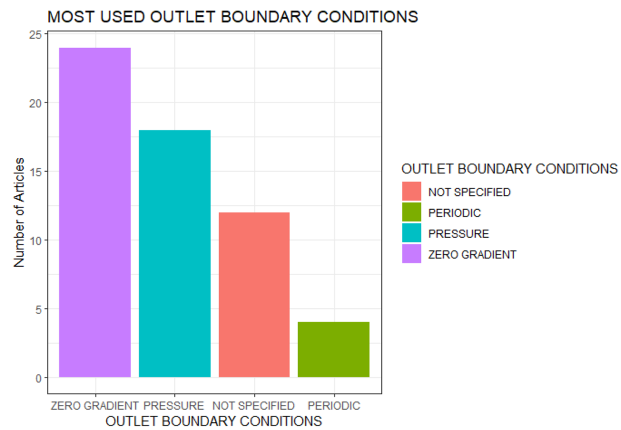

Figure 6. Inlet boundary conditions in the reviewed articles.

2.2 Turbulence models

This review focus in two turbulence simulation approaches: The Large-Eddy Simulation, and the Reynolds-averaged Navier Stokes equations. The former is used to model large- and small-scale vortices in the flow, and it´s recommended when high computational requirements are met, also the LES presents better results for the mean concentration distribution, comparing with the best RANS model [15], however the latest is most widely used in the reviews papers as seen in Figure 7.

Figure 8 shows that the three RANS turbulence models most used are derived from the κ-ε two equations model, where the κ represents the turbulent kinetic energy, and the ε represents the rate of dissipation of the turbulent kinetic energy. Only one of the papers used the κ-ω two equations model, where the k represents the same turbulent kinetic energy as the κ-ε, however the ω represents the specific rate of dissipation of the turbulent kinetic energy.

Table 1 compares the advantages and disadvantages of the five RANS turbulence models.

Table 1. Advantages and disadvantages of the RANS turbulence models.

Turbulence model	Advantages	Disadvantages
Standard κ-ε	Recommended to confined flows, and thin boundary layers.	Hard to describe flows with curves, eddies, sudden acceleration, and separated flows.
RNG κ-ε	Improves simulations with eddies and with separation compared with the standard model.	Does not have the stability in the flow compared with the standard model.
Realizable κ-ε	Additional to the RNG modifications, help to describe jets flows.	Does not have the stability in the flow compared with the standard model.
Standard κ-ω	Recommended to predicts flows in the boundary layer with adverse pressure gradients.	Have difficulties to predict shear flows.
SST κ-ω	Good to predict shear flows near the boundary layer.	Needs more mesh refinement.

Table 2 shows the mathematic formulation for the rate of dissipation of the turbulent kinetic energy in case of the three κ-ε turbulence models and the specific rate of dissipation of turbulent kinetic energy in case of the two κ-ω turbulence models.

$$\frac{\bar{D}\kappa}{\bar{D}t} = P_\kappa - \varepsilon + \frac{\partial}{\partial x_j}\left[\left(\frac{\nu_T}{\sigma_k} + \nu\right)\frac{\partial \kappa}{\partial x_j}\right] \quad (1)$$

$$\frac{\bar{D}\kappa}{\bar{D}t} = P_\kappa - \beta^* k\omega + \frac{\partial}{\partial x_j}\left[\left(\frac{\nu_T}{\sigma_k^*} + \nu\right)\frac{\partial \kappa}{\partial x_j}\right] \quad (2)$$

From (1), P_κ represents the production of turbulent energy, ε the rate of kinetic energy dissipation per unit of mass, ν_T is the eddy viscosity that can be expressed as:

$$\nu_T = C_\mu \frac{\kappa^2}{\varepsilon} \quad (3)$$

C_μ and σ_k are constants that depends on the model itself.

From (2), P_κ represents the production of turbulent energy, ω the specific rate of kinetic energy dissipation per unit of mass, ν_T is the eddy viscosity that can be expressed as:

$$\nu_T = \frac{\kappa}{\omega} \quad (4)$$

Table 2. Advantages and disadvantages of the RANS turbulence models.

RANS turbulence model	Mathematic formulation of the dissipation rate of the kinetic turbulent energy	References using the model
Standard κ-ε	$\frac{\bar{D}\varepsilon}{\bar{D}t} = (C_{\varepsilon 1} p_\kappa - C_{\varepsilon 2}\varepsilon)\frac{\varepsilon}{\kappa} + \frac{\partial}{\partial x_j}\left[\left(\frac{\nu_T}{\sigma_\varepsilon} + \nu\right)\frac{\partial \varepsilon}{\partial x_j}\right]$ (5)	[9], [16], [17], [18], [19], [20], [21], [22], [23], [24], [25], [26], [27], [28], [29], [30]
RNG κ-ε	$\frac{\bar{D}\varepsilon}{\bar{D}t} = (C_{\varepsilon 1} p_\kappa - C_{\varepsilon 2}\varepsilon)\frac{\varepsilon}{\kappa} - R + \frac{\partial}{\partial x_j}\left[\left(\frac{\nu_T}{\sigma_\varepsilon} + \nu\right)\frac{\partial \varepsilon}{\partial x_j}\right]$ (6)	[31], [32], [33], [34], [35], [36], [37], [38], [39], [40], [41]
Realizable κ-ε	$\frac{\bar{D}\varepsilon}{\bar{D}t} = \left(C_{1\rho} 2S_{ij}^{2\,1/2}\right)\varepsilon - C_{2\rho}\frac{\varepsilon^2}{\kappa+\sqrt{\nu_T\varepsilon}} + \frac{\partial}{\partial x_j}\left[\left(\frac{\nu_T}{\sigma_\varepsilon} + \nu\right)\frac{\partial \varepsilon}{\partial x_j}\right]$ (7)	[42], [43], [44], [45], [46], [47]
Standard κ-ω	$\frac{\bar{D}\omega}{\bar{D}t} = \alpha\frac{\omega}{\kappa}P_\kappa - \beta^* k\omega + \frac{\partial}{\partial x_j}\left[\left(\frac{\nu_T}{\sigma_\omega} + \nu\right)\frac{\partial \omega}{\partial x_j}\right]$ (8)	[48]
SST κ-ω	$\frac{\bar{D}\omega}{\bar{D}t} = \Upsilon\frac{\omega}{\kappa}P_\kappa - \beta^* k\omega + \frac{\partial}{\partial x_j}\left[\left(\frac{\nu_T}{\sigma_\omega} + \nu\right)\frac{\partial \omega}{\partial x_j}\right]$ (9)	[49]

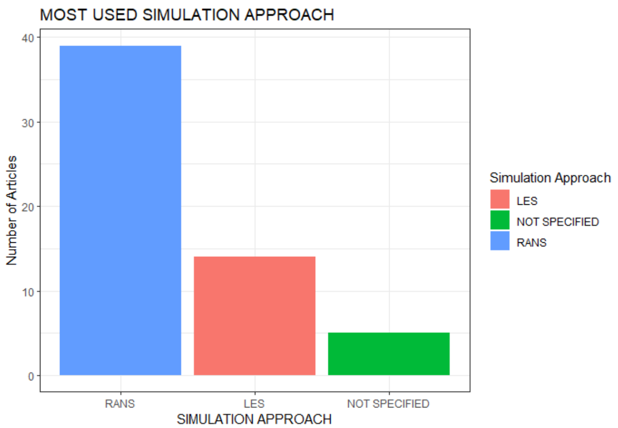

Figure 7. Turbulence simulation approaches in the reviewed articles.

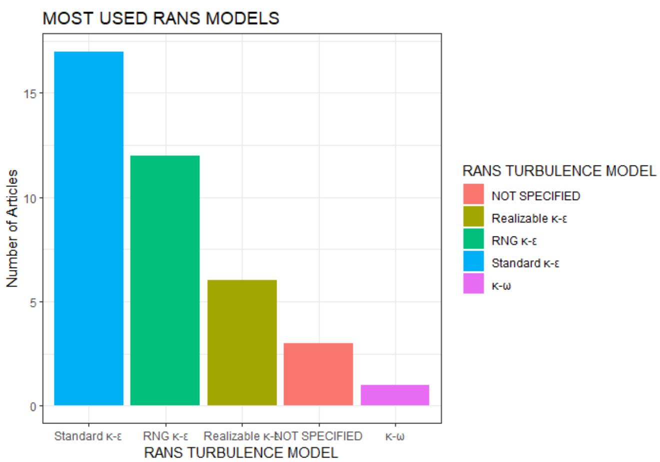

Figure 8. RANS Turbulence models in the reviewed articles.

2.3 *Validation Methods*

From Figure 9, the use of wind tunnel data in the validation of CFD simulations of air pollutants is used in thirty seven articles, and its common practice because it provides a solid foundation for assessing the accuracy of models and ensuring their usefulness in real-world applications, because in a wind tunnel, researchers can precisely control experimental conditions, such as wind speed and direction, pollutant source geometry, and other relevant parameters. This allows for the creation of reproducible and well-defined test scenarios. Another technique commonly used to validate is the use of low-cost and portable sensors that allows more spatial resolution of the data, and with a tripod they can be placed at the desired height depending on the goal of the respective exposure assessment. Ten articles used this method, while eight didn't specified whether they use a validation method, infringed what the ASME points out in its validation manual [50].

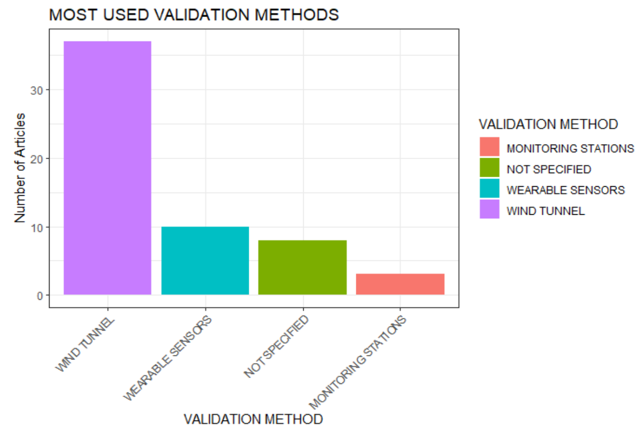

Figure 9. Validation methods in the reviewed articles.

3. *Assessment of pedestrian exposure*

CFD models, as we have seen in this review, offer significant advantages to study the dispersion of air pollutants; few studies have considered the exposure of people to these pollutants through this technique. The main reason for this gap could be the complexity of including people´s activity variables in the models that accurately represent their location and behavior in a specific environment, as people behave differently depending on the given circumstances. This can be difficult and costly in terms of resources and time. One solution to this issue will be to wisely select the group of persons that the evaluation exposure will consider; for example, in the case of pedestrian exposure to air pollutants, a distinction could be done between simple pedestrians that only walk briefly on sidewalks or near avenues, and that their exposure periods are generally short; and street vendors who spend several hours a day near the avenues selling their products and therefore their exposure periods are longer. A 2019 study showed that street vendors in commercials sites are more exposed to particulate matter than street vendors in residential sites [51]. Another recommendation will be to segment the population according to age groups, as children, adults, and the elderly may have different vulnerabilities to air pollutants. There is a clear need to have some standards that allow us to quantify exposure and consider the factors that have been mentioned.

However, in addition to all the factors that have been mentioned that can be framed within the field of physical sciences, there is a social component that will also intervene within the evaluation of exposure, since both the activities and the behavior of the group of exposed people will affect the type and amount of exposure [8]. That's why several techniques have been introduced in recent years to establish patterns of activity, such as asking potentially exposed people to keep diaries, recording video, and using telemetry to monitor vital information about people, which can then be used for exposure assessment models. For example, heart rate and ventilation were studied by [52], and the results obtained there were signed in several exposure studies [53], [54].

When we talk about the group of people exposed, there are intrinsic factors of each individual that are going to affect the inhaled dose of a given pollutant, for example, the age of the individual and their body weight. The formulas for calculating exposure will vary depending on the duration of that exposure. For short periods of exposure, the following general equation is recommended:

$$E\ (kg/min) = C\ (kg/m3) * IR\ (m3/min) \quad (10)$$

Where E is the exposure in units of mass per time, C is the concentration of the pollutant in units of mass per volume, and IR is the rate of inhalation in units of volume per time.

The above equation would only consider exposure at the entrance of the respiratory system, for a more robust exposure assessment would be considering how the inhaled doses of certain pollutants are deposited in the different regions of the respiratory system, for this the respiratory deposition dose (RDD) is presented, which consists of the following formula found in [55]

$$RDD = IR * PM_i * DF_i \quad (11)$$

Where IR is the inhalation rate and is a variable that depends on the physical activity that the person is doing at the time[56]. It has also been found in the literature that this variable is related to the age and weight of the person [57]; DFi is the deposition fraction of particulate matter for the different diameters and has been found to depend only on the aerodynamic diameter of the particle being analyzed ; while PMi is the mass concentration of particulate matter for the different diameters, and its variability is spatiotemporal, so it is recommended to analyze this variable using statistical techniques and take properly averaged values.

Because of all the amount of data that is required, making a good exposure assessment is going to be only as good as the quality of the data that is available [8]. It is important that the data meets certain criteria:

- The data must be curated, this means that the technical procedures, measurements, methods or models used generate reasonable information consistent with the desired application.
- The data must be relevant, meaning that the information is applicable to the required use.
- The data and the methodology must be clear and complete, this means the degree of clarity and complete documentation of the data, assumptions, methods, quality processes and everything that generates information.
- The data must be accompanied by a state of uncertainty and variability, that is, both qualitative and quantitative information on the degree of uncertainty and variability included in the information must be included.
- The data should be reviewed and evaluated, so that the exposure information can be verified and validated.

Quantifying exposure due to vehicular traffic remains very complex, as there are many factors involved, leading to uncertainty in the health effects caused by vehicle fleets.

The first factor that is more resalted in the articles, is how some types of vegetation near the avenues, does not necessarily mean better pollutants distribution, since meteorological factors such as wind speed and direction must be considered, for example when areas of low wind speed were identified the dispersion of the NO is high related to wind direction [49], Also depending on the side relative to the wind that is being studied, the pollutants may behave differently. When the wind direction is perpendicular to the axis of the road, the concentration is increased windward, but the leeward is reduced at pedestrian level [28].

Other factor is the dynamics and the flow patterns of both: vehicles and pedestrians; reduction of CO levels near the pedestrian zone has been related with vehicle speed increasing [33]. Similar results were obtained comparing a continuous flow of vehicles, with a discontinuous flow, where exposure of pedestrians resulted higher in the latter because the vehicle speed was varying, versus the former where the vehicle speed was kept constant [20].

The benefits of a good CFD model go directly hand in hand with the computational requirement that is available. For instance, for a better representation of the vehicle speed, a dynamic updating mesh can be adapted [31] It is also possible to use models with high spatial and temporal resolution to assess in which areas within the selected domain pedestrians are most exposed [45]. Another novelty introduced in this area was the use of virtual walkers as mobile agents in LES simulations with an average walking speed of a person, and with a wind speed measured in the pedestrian region [58], [59].

The coupling of CFD models with chemical models, for a better detail of the behavior of gases and particles is also a trend seen in some studies, and the results show that a coupled model reflects greater agreement with the experimental data than using a conventional CFD model [39].

A hot topic in the current days. as is the artificial intelligence is combined with CFD models in a 2022 paper for calculate the exposure to traffic related air pollutants using the respiratory deposition dose [60].

IV. CONCLUSIONS

From the bibliometric analysis, the evolution of scientific research around computational models to estimate exposure due to pollutants related to vehicular traffic is highlighted, it is also noted the disparity that exists in scientific research in this area between the most developed countries such as the United States, Japan, and the members of the European Union. against Latin American countries and the African continent.

Regarding turbulence models, no model is universally acceptable even for the case of evaluating the concentration of pollutants resulting from vehicular traffic since it will depend on the available computational capacity, as well as the characteristics of the flow and the geometry of the domain that has been selected.

The validation methods are something like the turbulence models, but it's clear that the preferred technique is using data from wind tunnel experiments. The issue with this selection is the discrepancy between the wind tunnel data and the conditions that the CFD model seeks to accomplish.

Analyzing the ways to estimate the pedestrian exposure and the factors that take primary consideration in the papers, respiratory deposition dose appears to be A complete way of estimating pollutants, particularly PM penetrates throughout the respiratory system, and combines information from the environment as well as personalized information about each individual.

It's interesting the discrepancy in the topic of vegetation and green infrastructure; some studies consider that it helps to increase concentrations, while other studies show that under certain circumstances it can help to reduce them. One article recommends that if you want to introduce trees near avenues, they should have variability in heights.

Another factor to take into consideration is the dynamics of the traffic, highlighting interesting that the more continuous the vehicular flow, the greater the dispersion of pollutants in the respiratory zone of pedestrians.

There is a social component that will also intervene within the evaluation of the exposure since both the activities and the behavior of the group of people exposed will affect the type and amount of exposure, therefore is highly recommended to integrate human exposure models into the CFD models, to evaluate how pedestrians walking near avenues are exposed to contaminants.

CFD models offers great advantages in comparison with other tools such as data for monitoring stations, since the spatial variation of the concentration and dispersion of pollutants at the pedestrian level cannot be observed in these, meanwhile in a computational model with a sufficient requirement is possible to Analise this variation.

It is recommended that the experimental or computational data obtained for the assessment of exposure be carefully reviewed, both statistically and physically, to ensure that the results generate reasonable information consistent with the desired application.

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