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PARTICLE DEPOSITION MODELING AND ATMOSPHERIC AEROSOL QUANTIFICATION: A CASE STUDY IN FORTALEZA (CEARÁ) - BRAZIL

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ABSTRACT

Fortaleza is currently a large metropolis located in northeastern Brazil, the city goes through a constant demographic growth and significant increase of the local vehicular fleet. Currently, public policies for urban mobility in the city are being developed, such as encouraging the use of bicycles in cycle lanes, however these cycle-lanes are located in major high traffic routes in the city. In view of the above, the present study aims to simulate the deposition of atmospheric particles in users of cycle lanes (cyclists), in the vicinity of a large vehicular traffic road in Fortaleza.The concentrations of particles (0.3 µm, 0.5 µm, 1.0 µm, 2.5 µm, 5.0 µm and 10 µm) were measured with a portable particle sizer (DT 9881 CEM) and the concentration distributions for the sized particles were measured in the Dosimetry of Multiple Path Particles (MPPD).The measured particles had higher concentrations at peak times (6:00a.m. - 9:00 a.m.) and (5:00 a.m. 7:00 p.m.), from 5:00 p.m. to 7:00 p.m. in average values 29% ± 8.3% higher, with the days of Saturday registering the lowest concentrations. In cyclists, particle deposition was more significant, with particles of 0.3 µm and 0.5 µm depositing more representatively in the tracheobronchial (TB) and pulmonary (PUL) regions. Particles of diameter 1.0 µm, 2.5 µm, 5.0 µm and 10 µm were most representative deposited in the extrathoracic (ET) and TB regions. Our results suggest that the use of cycle lanes, in the vicinity of traffic routes, may exacerbate the deposition of particles in the respiratory system, possibly leading to health risks.

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INTRODUCTION

Due to the relationship between the high levels of pollutants in the atmosphere and social well-being, several studies have been developing problematizing environmental issues around the world. For the most part, these studies turn to the regions of large urban centers. There are 3.7 million premature deaths worldwide annually due to the effects of urban pollution (WHO, 2015).

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In large urban centers, traffic-generated pollution represents an important contribution to particulate matter (PM), which is released through the exhaust gas and emissions of organic and inorganic gaseous precursors from the combustion of fuels and lubricants (Amato, 2009). The harmful effects on human health due to the high concentrations of PM present in the atmosphere is evident all over the world. Studies have shown a correlation between lung cancer (Nielse *et al*, 2016, Leroux *et al*, 2015), cardiovascular diseases (Delfino *et al*, 2005) and respiratory diseases (Pope *et al*., 2011; Carmo *et al*., 2010; Wichmann *et al*., 2000). In addition, it has been reported that the number of hospital visits due to respiratory problems has increased (Bakonyi *et al*., 2004). Control of pollution generated by vehicles is a challenge for Brazil and developing countries. Cities with intense vehicular traffic areas have higher PM levels in the atmosphere when compared to rural areas (Notter, 2015). Particularly, the state of Ceará has a vehicle fleet of more than 2.7 million cars, specifically the city of Fortaleza, with just over 1 million vehicles (DENATRAN, 2016).In the annual reports presented by the national traffic department (DENATRAN), it is possible to observe a significant increase in the vehicular fleet of the city of Fortaleza between 2015 and 2016, with an increase of approximately thirty thousand vehicles in circulation (DENATRAN, 2016). This is a potential increase in emissions of air pollutants. In view of the above, the present work aims to measure the concentration of atmospheric particles and its relative deposition in the human respiratory system, considering concentrations obtained in the vicinity of an intense traffic route in Fortaleza, Brazil.

MATERIAL AND METHODS

Description of study area and collection flow

The study was conducted in an area for meteorological studies developed by the State University of Ceará (UECE) - Itaperi Campus, located on the banks of Dr. Silas Munguba Av. In Fortaleza-Ceará at coordinates 3º 47 '09,3 "S e 38 ° 33'08.8 "W (Figure 1).

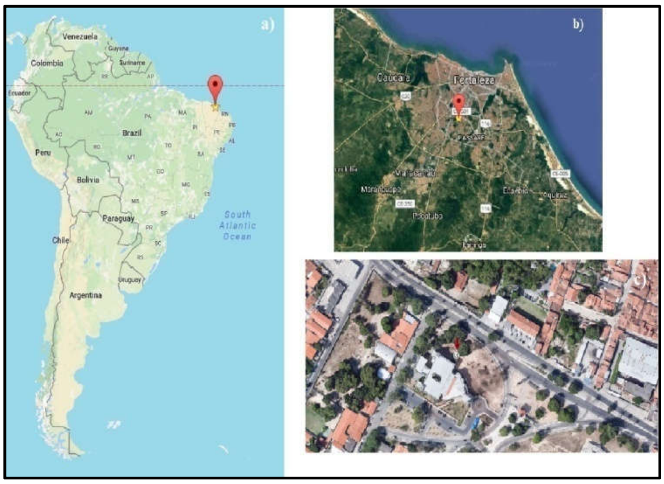

Figure 1. Place of collection. Maps of (a) Fortaleza - Ceará in South America, (b) State University of Ceará, and (c) Location of study in Fortaleza – Ceará. The pictures were taken from Google maps (https://maps.google.com/)

According to the Fortaleza urban transport company, 21 bus lines and an average daily volume of approximately 14,700 vehicles (cars, buses, motorcycles) circulate daily (ETUFOR, 2016). The samplings were conducted from Monday to Saturday for five weeks interspersed: August 15-20, August 29 to September 3, September 12 to 17, September 26 to October 1, and October 10 to 15, 2016. The sampling site was 100 m from the avenue and 20 m from the entrance of the university, in addition to being positioned 50 cm above ground level. In addition to the traffic streets, the sampling site is surrounded by educational buildings, offices and commercial airships. Parameters with aerodynamic diameter of 0.3 µm, 0.5 µm, 1.0 µm, 2.5 µm, 5.0 µm and 10 µm were measured and modeling of their deposition in the human respiratory system was performed considering two scenarios: physical activity (cycling) and baseline situation. These scenarios were considered according to the urban mobility policies implemented in the city of Fortaleza. Among these policies, exclusive tracks are being implemented for the use of bicycles, which are located in the vicinity of vehicle flow routes, which may exacerbate exposure to pollutants from vehicular emissions.

Sampling Devices

For the determination of the relative concentrations, a portable particle sizer (DT 9881 CEM) was used, which was arranged at a height of 1.70 m above ground level, in 13 h trials comprising the time of 6: The parameters of temperature, relative humidity, rainfall, wind speed and direction were constantly measured using a meteorological station (weather center - Instrutemp - ITWH - 1080), which allowed us to evaluate possible associated meteorological influences measures.

Particle deposition modeling

For the modeling related to the deposition of particles in the human respiratory system, the software Multiple-Path Particle Dosimetry model (MPPD) was used. MPPD estimates particle deposition fractions in the lungs of adult human rats and children for monodisperse and polydisperse aerosols with aerodynamic size that can range from ultrafine to coarse (Li *et al*., 2016); (Anjilvel and Asgharian, 1995). In this study, among the MPPD airway models, the multipath model was used due to its formalism, considered to be the closest to the actual structure of the human respiratory tract (Li *et al*, 2016). For the human airway, there are five model options, including the Yeh-Schum Single Path, the Yeh-Schum 5 Lobe, the stochastic model, the age-specific symmetric model, and the age-specific 5-lobes model. The stochastic model (lung size - total 60th percentile of the airways) was used to estimate the deposition of particles in the adult respiratory system. The model's input parameters include functional residual capacity (FRC, mL), upper respiratory tract volume (URT volume, mL), respiratory rate (BF, min-1) and tidal volume (TV, mL). The respiratory parameters used in the modeling were those proposed by Panis (2010) for people in physical activity and by Martins *et al*. (2010) for people in a baseline situation (Table 1).

Table 1. Respiratory parameters. Respiratory parameters used in modeling for simulation at baseline according to (Martins *et al*, 2010) and respiratory parameters used in modeling for exercise simulation (cycling) according to Panis and collaborators (2010)

Input Parameter	FRC (mL)	URT (mL)	TV (mL)	BF (min^{-1})
Basal	3.300 mL	50 mL	625 mL	12 min^{-1}
Physical Activity	3.300 mL	50 mL	2.200 mL	28 min^{-1}

For the concentration values used in MPPD, we consider a monodisperse distribution of particles with spherical surface area and density of 1.0 g / cm³ (Sracic, 2016).

RESULTS AND DISCUSSION

Meteorological Aspects

An evaluation of the meteorological variables during the study allows us to have a better representation of the observed data. A number of studies have reported that meteorological factors such as wind speed and direction (Hossein *et al*, 2006 and Wehner and Wiedensohler, 2003), temperature (Hossein *et al*, 2006), relative humidity (Hamed, 2011) and precipitation influence the concentrations of particles in the atmosphere. Variations in wind speed, temperature, air humidity and precipitation were constantly measured (Figure 2).

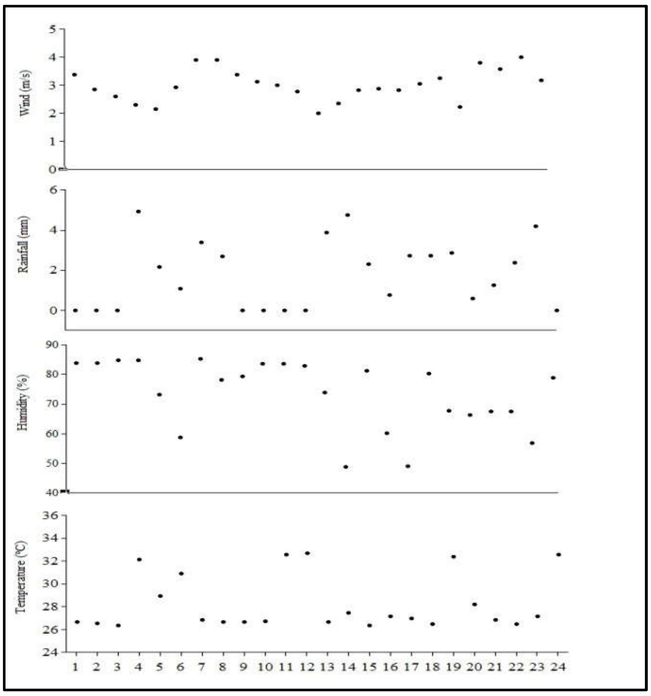

Figure 2. Meteorological variables in the study period. Representation of the meteorological variables observed during the study period. In the (x) axis are presented, on average, the collections made during the study period

During the study period, the average temperatures presented low amplitudes, varying between 26.4 °C and 33.1 °C. The nocturnal period presented lower temperatures when compared to the diurnal period. In situations of high temperature inversions, an increase in the concentrations of pollutants in the atmosphere may occur (Kukkonen *et al*, 2015). Relative humidity presented variations between 49% and 85.3%, at the end of August and at the beginning of September, values below those considered adequate by WHO. This low humidity occurred throughout the state of Ceará due to a mass of dry air that settled over almost all of Brazil (FUNCEME, 2016a). In the early morning and late night air humidity had the highest averages, with 79.2% in the morning (6:00 a.m. - 8:00 a.m.) and 76.6% in the evening (5:00 p.m. 7:00 p.m.). Wind velocities varied between 1.9 m / s and 4.5 m / s throughout the test period, with higher daytime values between the hours of 9:00 am and 4:00 pm. tests coincided with the season of strong winds in the coast of Ceará, which favored a higher incidence of high intensity winds at the study site. A factor that influenced the increase of the intensity of the winds during this period was the displacement of high atmospheric pressure from the South Atlantic Ocean towards the Brazilian Northeast (FUNCEME, 2016b). Among these factors, wind speed and direction have a great influence on PM levels. Studies indicate a lower concentration of particles when these are measured in situations of higher wind speeds (Zhao *et al*, 2015). The direction and velocity of the wind change the concentrations of particles in the atmosphere, however this dependence differs with the particle size class (Wehner and Wiedensohler, 2003).

Variation by day of the week for the particles under study

We observed a constant behavior in relation to the concentration values of the particles as a function of time during the entire period of data collection (6:00 a.m. - 7:00 p.m.). On average, peak evening hours (5:00 p.m. - 7 p.m.) showed higher concentrations than the morning peak time (between 6:00 a.m. and 9:00 a.m.). Just considering the averages on Saturdays, the concentrations of the two peak times are similar. Considering the flow of vehicles as the main source of particulate emissions in the study region, a better representation of particle concentrations is presented in the averages of Wednesdays. This is justified, because Wednesday better represents the profile of the flow of vehicles of a region. The profile of the flow of vehicles on Mondays is slightly lower than its average and the Fridays profile is slightly higher (DNIT, 2006). Figures 3 and 4 show the concentration profiles for atmospheric aerosols measured during the day.

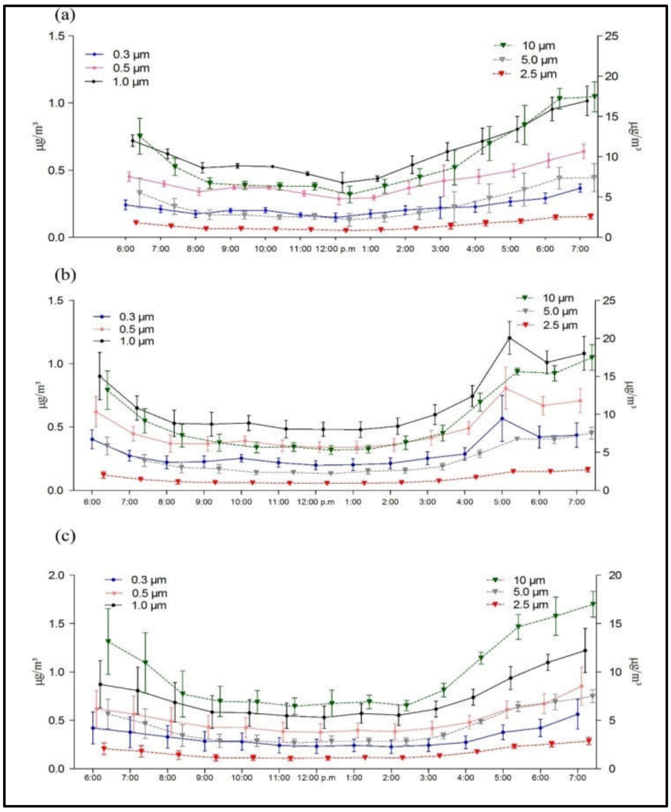

Figure 3. Concentration of second, third and fourth particles. Representation of the particle concentration profile considering the averages of the days studied. The results are plotted with two axes (y) relative to particle concentration, the left axis being representative of the particles of 0.3 µm, 0.5 µm and 1.0 µm and the right (y) axis representative of the particles of 2.5 µm, 5.0 µm and 10 µm and the (x) axis represents the time of day. Results are presented as mean ± standard error of the mean. (a) averages of concentrations on Mondays; (b) averages of concentrations on Tuesdays; (c) Concentration averages on Wednesdays

Peak times are characterized by the fact that they contain the largest volumes of single-lane vehicles on a given day and may vary from place to place, but tend to remain stable in the same place, most of which from work (DNIT, 2006). This diurnal variability of the particles in the atmosphere is justified by the intense traffic of vehicles, which peaks during the morning and decreases during the day, favoring a greater dispersion of the pollutants in the atmosphere between the hours of 9:00 a.m. - 4:00 p.m. During the peak hours of the afternoon, there is an increase in the concentration of particles due to also the flow of vehicles and the decrease of the atmospheric boundary layer, which results in a lower dispersion of the particles (Tiwari, 2016). On weekdays, there are 305 buses in the morning between 6:00 am and 9:00 am and 377 buses between the hours of 4:00 pm and 7:00 pm, this represents an increase of 23.6% between one period and another (ETUFOR, 2017). On average, concentrations for all particle sizes were 2.3% higher on Wednesdays compared to Saturdays. This is probably justified by the greater number of mid-week circulating diesel vehicles, mainly buses and trucks (Alizadeh-Choobari, 2016).

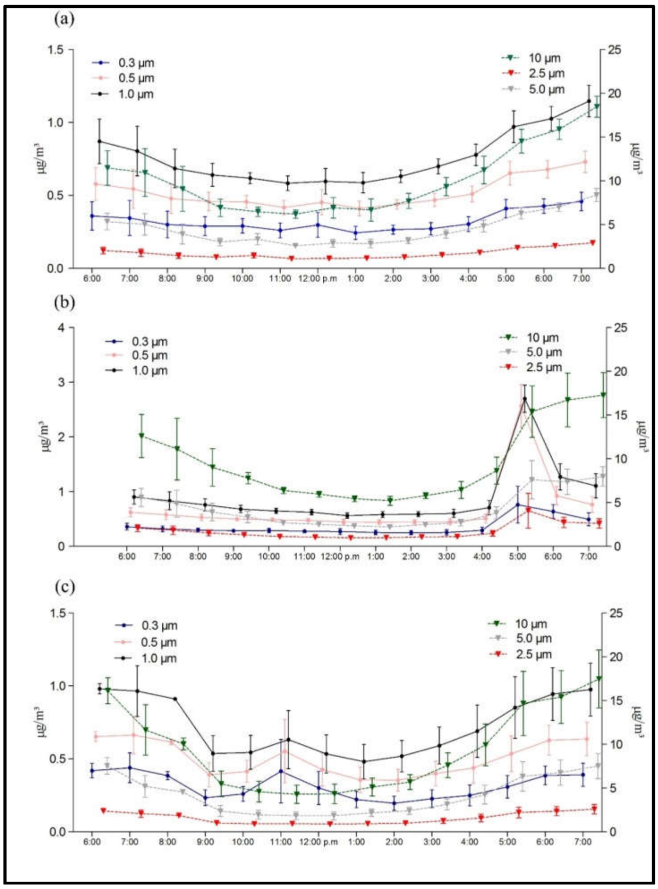

Figure 4. Concentration of particles on Thursdays, Fridays and Saturdays. Representation of the particle concentration profile considering the averages of the days studied. The results are plotted with two axes (y) relative to particle concentration, the left axis being representative of the particles of 0.3 µm, 0.5 µm and 1.0 µm and the right (y) axis representative of the particles of 2.5 µm, 5.0 µm and 10 µm and the (x) axis represents the time of day. Results are presented as mean ± standard error of the mean. (a) averages of concentrations on Thursdays; (b) Meetings averages on Fridays; c) Means of concentrations on Saturdays

For the 0.3 µm particles, on Saturdays, concentrations higher than the other days of the week were recorded. For the other particles measured on average, Saturdays presented differences 10% lower in comparison to the other days. On Saturdays, on Dr. Silas Munguba avenue, 270 buses run on average during the morning peak hours, with 88 buses between 6:00 am and 7:00 pm, 104 between 7:00 pm and 8:00 pm, and 78 between 8:00 p.m. and 9:00 p.m., this represents a decrease of 35 vehicles over the weekday average. In the peak hours of the afternoon there is also a decrease in the number of buses in circulation, with an average of 286 vehicles between 4:00 pm and 7:00 pm on Saturdays, representing a decrease of 24.1% in average weekday vehicles (ETUFOR, 2017). The daily particle profile presented a more variable pattern on Saturdays, this is justified because Saturdays are atypical days of vehicular flow, due to the weekend (DNIT, 2006). On Tuesdays, atypical peaks occur at concentrations as shown in Fig. 3b. A significant increase in the concentrations of all particles between 4:00 p.m. and 5:00 p.m. is noticeable. This increase is most evident in particles with a diameter of 1.0 µm and 0.3 µm. On Tuesday, September 27, between 4:00 p.m. and 5:00 p.m., the aforementioned particles recorded an increase of 66% and 35%, respectively, in comparison with the other weeks, for the same time and day. This can be justified because, at that time, the relative average wind speeds were 50% lower than the average of the other Tuesdays, this fact can be related to a smaller dispersion combined with a greater accumulation of the pollutants, as explained by Kim and collaborators (2015). In the particle concentration profile for Fridays (Figure 4b), a similar increase is seen in the same time interval. On Friday 19/08, between 4:00 p.m. and 5:00 p.m., particles with a diameter of 1.0 µm and 0.5 µm registered a 10% and 7% increase, respectively, compared to other Fridays in study. This increase can also be justified considering that on that day, the winds also presented mean velocity 60% lower when compared to the other sixths. In short, between the hours of 9:00 a.m. and 4:00 p.m. the winds had speeds 63% higher than the winds in the hours between 6:00 a.m. and 8:00 a.m. and between 4:00 p.m. and 7:00 p.m.

Wind speed and particle concentration

Measurement of air pollution levels in the vicinity of vehicle traffic routes are indicators of the impact of vehicular emissions on urban air quality; however, weather conditions, in particular wind speeds, need to be taken into account due to transportation and dilution of pollutants under study (Kim, 2015).

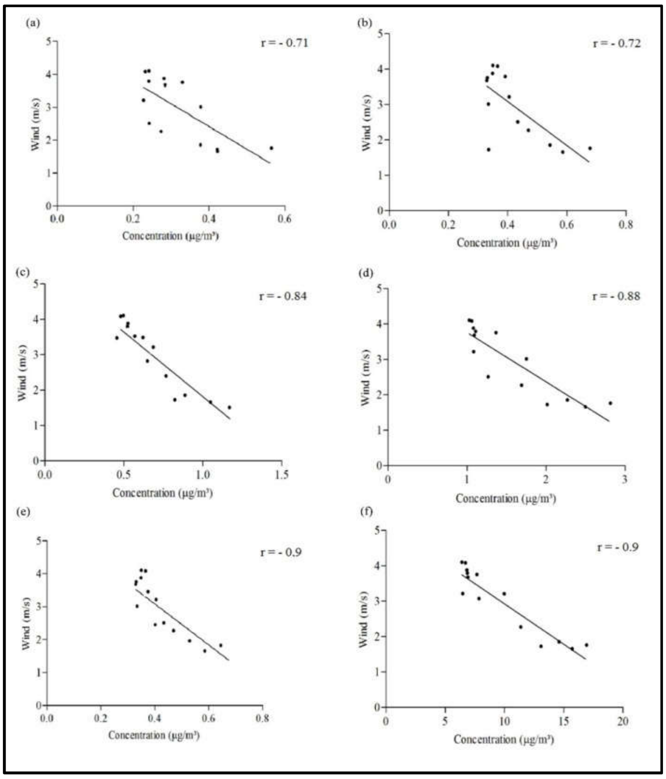

Figure 5. Correlation between particle concentration and wind velocity. Pearson's correlation between the measured concentrations and the velocities of the winds. a) Correlation relative to particles of 0.3 µm; b) Correlation relative to 0.5 µm particles; c) Correlation relative to particles of 1.0 µm; d) Correlation relative to particles of 2.5 µm; e) Correlation relative to particles of 5.0 µm; f) Correlation relative to 10.0 µm particles.

Considering the relation between the concentrations of particles and the aforementioned dispersion of the pollutants, figure 5 shows correlations between the concentrations and the velocities of the winds for the study period. A strong negative correlation was observed for the averages presented, between the concentrations measured in the study period and the wind velocities.

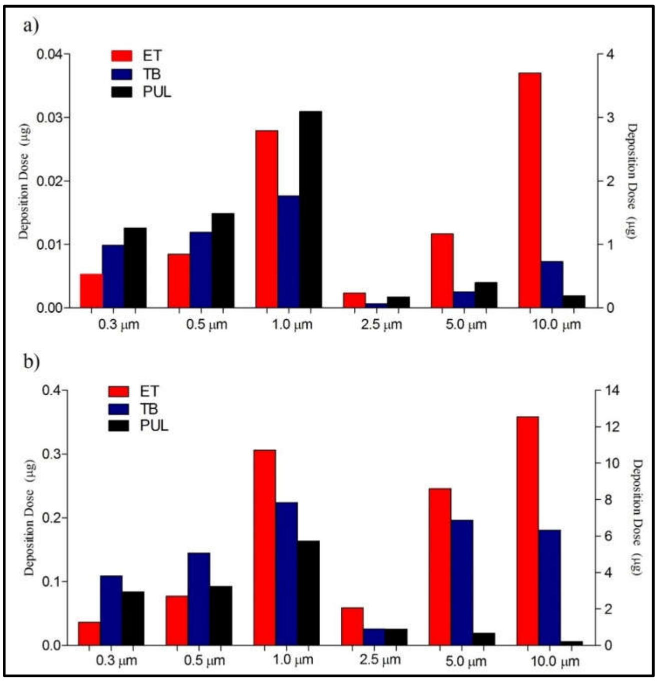

Figure 6. Estimation of particle deposition for the mornings studied. Estimation of deposition in the respiratory system (a) Mass deposited in different lung regions, considering the peak hours of the mornings for a situation of basal respiration; (b) mass deposited in different lung regions, considering the peak hours of the mornings for a situation of physical activity (cycling). The left (y) axis is relative to the particles of 0.3, 0.5 and 1.0 µm and the right (y) axis is relative to the particles of 2.5, 5.0 and 10.0 µm

Deposition of particles

Calculations of the probability of particle deposition in different lung regions are of great value in view of which lung diseases caused by inhalation of particles have often been reported to occur at specific sites in the lung, particularly in specific lobes (Holfmann, 2011;Subramaniam *et al*., 2003). The results on particle deposition are presented considering the average morning and afternoon peak hours of Wednesdays. Peaks occur in the use of the bicycle system in the periods between 6:00 am and 9:00 am due to the standard entrance of schools and companies and between 4:00 pm and 7:00 pm due to the companies and schools (Andrade, 2016). It was established a period of one hour of exposure to the measured atmospheric particles, this time of exposure was defined considering the average time of use of the bicycle system in Fortaleza in the two schedules described. Figures 7 and 8 express the mass quantity of particles deposited in the respiratory system, considering three pulmonary regions (extrathoracic, tracheobronchial and pulmonary) and differing in the exercise and rest situation. The pattern of deposition of the particles is shown according to the division of lung regions proposed by the model (MPPD): extrathoracic (ET); tracheobronchial (TB); pulmonary (PUL). Vehicle emissions are typically considered the greatest anthropogenic threat to athletic performance, due to the high levels of air pollution often found in environments that coincide with sports practices (Sracic, 2016). The difference between particle deposition in basal and exercise situations, in all lung regions and among all particle sizes, is notorious, reinforcing the idea of how harmful sports practice in the vicinity of traffic routes, such as case of the use of the bicycle system in Fortaleza. Studies have shown that ultrafine particles presented a much higher mass fraction of deposition in peripheral regions of the human lung, due to the fact that they are deposited by Brownian diffusion, a process that occurs more frequently in alveolar regions due to the smaller diameter of the particles (Sracic, Sanders *et al*., 1979, Patton and Byron, 2007). The particles with a diameter of 1.0 µm already have a higher mass deposition in the upper airways due to the impaction process in the first generations of airways (Patton and Byron, 2007). For 0.3 µm particles at baseline, the pulmonary region recorded a two-fold mass deposition of the particles deposited in the upper airways (Figures 7a and 8a).

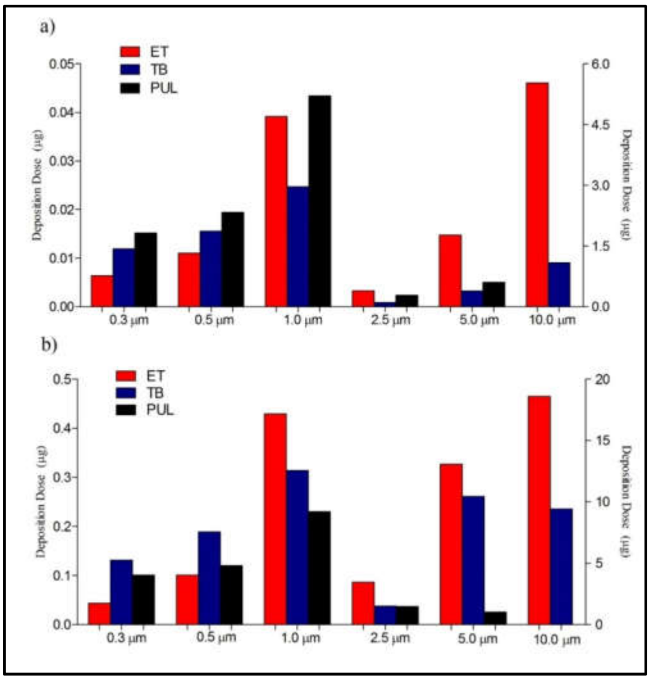

Figure 7. Estimation of particle deposition for the afternoons studied. Estimation of deposition in the respiratory system (a) Mass deposited in different lung regions, considering the peak hours of the afternoons for a situation of basal respiration; (b) mass deposited in different lung regions, considering the peak hours of the afternoons for a situation of physical activity (cycling). The left (y) axis is relative to the particles of 0.3, 0.5 and 1.0 µm and the right (y) axis is relative to the particles of 2.5, 5.0 and 10.0 µm

In the lung regions, the mass deposited in the exercise situation registered an increase of 665% in relation to the baseline situation. The 0.5 µm particles showed an increase in the ET region, when baseline and exercise conditions were compared, and the TB region presented values in the deposited mass of 0.14 µg in a physical activity situation (Figures 7a and 8a). The particles of 1.0 µm recorded the highest deposited mass concentrations in comparison with the particles of 0.3 and 0.5 µm (Figures 7a and 8a), with a mean of 58% higher. An eleven-fold increase was recorded between the two situations, in the ET region, for particles of 1.0 µm. For the 0.3, 0.5 and 1.0 µm sizes in lung regions, there was a six-fold increase in baseline and exercise scores. During the exercise, the amount of particles deposited in the alveolar region is approximately ten times higher than the resting state, this deposition is more exacerbated in children from 5 to 10 years old (Oravisjarvi *et al*., 2011). In the afternoon (Figure 8), concentrations higher than the peak morning hours were recorded, averaging 25% higher. Considering the particle distribution profile during the day (Figures 3 and 4), the late afternoon hours recorded concentrations 13% higher than the early morning periods. In summary, particles with aerodynamic diameters of less than 1.0 µm are of great importance in studies aimed at understanding the effects of air pollution on human health. This is true, since most diesel particles can range from 0.001 µm to 1.0 µm and more than 90% of these are less than 0.05 µm (Kittelson, 1998). Vehicle traffic is the largest source of exposure to particulate matter for cyclists in large cities, the level of exposure may vary at different locations in the city, depending sometimes on the intensity of vehicular traffic, wind speed and the fact that vehicles slow down and, then accelerate again at traffic lights (Bergmans, 2009).

Compared with other sites, the use of bicycles in cycle tracks was associated with an increase of 11% in the concentration of particles inhaled by users (Boogaard *et al*, 2009). During the hours between 06:00 a.m. and 8:00 p.m., the 2.5 µm particles recorded an average of 1.7 µg / m 3 and between the hours of 5:00 a.m. and 7:00 p.m. average of 2.85 µg / m 3. Already 5.0 µm particles recorded a mean of 4.5 µg / m³ in the same period of the morning and 6.8 µg / m³ in the same period of the afternoon. Particles with a diameter of 10.0 µm recorded the highest concentrations, averaging 10.5 µg / m³ during peak morning hours and 15.7 µg / m³ during peak afternoon hours. A study carried out in the vicinity of Pequin University in China identified the same deposition pattern, with night peak times being the most significant for particle deposition, also justifying this deposition pattern due to the increase of vehicle emissions during the peak time (Li *et al*, 2016). As already explained above, said particles having diameters greater than 1.0 µm, mostly, deposit in the upper airways due to impaction and sedimentation processes. This behavior is also observed in the deposition profile of the exposed particles. For particles with a diameter of 2.5 µm, the largest difference is in the ET region, with deposition in the upper airways during exercise corresponding to nine times the mass deposited in the upper airways at baseline. In upper airways, the total mass deposited for particles of 5.0 µm corresponds to 57.1% of the simulated mass total. In exercise situations, there is a seven-fold increase when the physical activity and rest scenarios for upper airway deposition are compared. In 10.0 µm particles, 98% of inhaled particles are deposited in the respiratory system, 78% of which are deposited in the upper airways, 15.3% in the lower airways and only 4% are deposited in the alveolar region. Sracic (2016) also showed a higher deposition in the upper and lower airways for particles with a diameter of 10 µm. In the afternoon, the particles had more significant concentrations compared to the morning period. Sracic (2016) demonstrated in athletes, in the practice of physical activity, a mass deposition that varied between 28 and 37 µg in the lower airways for particles of 10 µm. Users of cycle ranges, in the vicinity of traffic routes, may present a deposition of MP_{10} ranging from 1.9 to 2.6 µg of mass deposited per kilometer pedaled and for $MP_{2.5}$ a deposition between 3.4 can be estimated and 5.2 µg of mass deposited per kilometer pedal (Panis, 2010). The collected data show the greater exposure to atmospheric particles in people who practice physical activity in the vicinity of vehicle flow pathways.

Conclusion

We showed that the use of cycle lanes, in the vicinity of traffic routes, can exacerbate the deposition of particles in the respiratory system of cyclists, leading to health risks. There was a notable increase of about 9 times in mass concentrations deposited in cyclists when compared to people in rest situations. We can conclude that the urban mobility policies implemented by the public power in the city of Fortaleza - Ceará are of extreme importance for the city, however, such policies must be accompanied by more intense actions aimed at reducing the intense and increasing flow of vehicles, mitigating the emissions of particulate matter into the atmosphere. This paper highlights the importance of being allied, public policies of urban mobility and social welfare. Every year, 3.7 million deaths occur worldwide due to exposure to air pollution (WHO, 2016). In May 2015, WHO established a resolution, highlighting the key role of the authorities in saving lives and reducing health costs by treating air pollution effectively. Countries need to develop air quality monitoring systems, air quality related disease registries, develop clean technologies and fuels for domestic use, heating and lighting and strengthen the international transfer of specialized scientific knowledge on air pollution (WHO, 2015).

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