Influence of mixing height and atmospheric stability conditions on correlation of NO2 columns and surface concentrations in a Mexico-United States border region

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Abstract
The objective was to analyze how representative tropospheric NO2 column densities are of surface NO2 measurements under different atmospheric stability conditions in the air basin of two border cities: Calexico, United States, and Mexicali, Mexico. NO2 columns were measured by the Ozone Monitoring Instrument (OMI) on the NASA Aura satellite. NO2 concentrations and meteorological parameters were also measured on the surface for comparison. Specifically, the correlations between OMI and surface NO2 concentrations under different atmospheric stability conditions according to the Pasquill-Gifford (P-G) and Monin-Obukhov (M-O) classification schemes were determined for 2017 and 2018. During the passage of the satellite through the study area (11:00–13:00 UTC−8), unstable conditions were documented in both years. Good correlation was found between the surface NO2 and OMI NO2 column observations in the second semester of each year, particularly under unstable conditions as diagnosed by the P-G and M-O schemes applied in the first and second year, respectively. However, a weakening of these conditions occurs during the autumn–winter period. In both cases, the highest determination coefficients were found for Calexico, with values of 0.48 and 0.36 in 2017 and 2018, respectively; for Mexicali, the determination coefficients were 0.23 and 0.35, respectively. Under each atmospheric stability scheme, the mechanical and convective turbulence caused a decreasing trend in wind speed and solar radiation over the course of second semester of 2017 and in friction velocity, temperature, and sensible heat flux over the course of the same period for 2018. The negative trend of these parameters during the analyzed time frames helped to reduce the influence of unstable atmospheric conditions, favoring better correlations between satellite and surface NO2 measurements. The methodology applied and results obtained herein can enable us to better understand the representativeness of OMI NO2 data in arid border zones with extreme meteorological conditions.
1 | INTRODUCTION

Atmospheric stability conditions play an important role in the mixing of air pollutants. This is more markedly observed under extreme weather conditions or during the changes in the convective process that occur from season to season (Szep et al., 2017; Yuval et al., 2020). One example of this phenomenon occurred in winter 2004 in Logan, Utah, United States: Temperatures reached $-23.6^\circ$C, favoring thermal inversion and causing the worst air pollution episode ever recorded in the country (Malek et al., 2006). In other metropolitan zones such as Mexico City (Mexico), Los Angeles (United States), and the Kathmandu Valley (Nepal), the transport of pollutants has shown to be affected by variability in temperature, wind speed, solar radiation, and relative humidity (Shaw et al., 2007; Cohan et al., 2011; Mues et al., 2017).

The generation of nitrogen dioxide (NO$_2$) by anthropogenic emissions on the Earth’s surface and its involvement in chemical reactions in the atmosphere affects the creation of tropospheric ozone (O$_3$) during photochemical reactions. Specifically, in urban areas, solar radiation and wind speed conditions impact available energy and pollutant levels (Sillman, 1999; Habeebullah et al., 2015). Both of these latter parameters can modify the mixing layer height of pollutants and, consequently, their concentration levels.

Satellite data on pollutants have enabled a greater understanding of their behavior and distribution at different temporal and spatial scales. Previously, these data were integrated with surface NO$_2$ data in Central Mexico in order to generate tropospheric NO$_2$ columns with greater representativeness of the spatial distribution of this pollutant near the surface (Rivera et al., 2013). The sensitivity of NO$_2$ data from the Ozone Monitoring Instrument (OMI) to vertical atmospheric conditions has been studied in recent years. In Hamilton, Canada, OMI and surface NO$_2$ data were compared: The highest regression coefficients were found during inversion days ($R^2 = 0.35$) under stable atmospheric conditions (Wallace and Kanaroglou, 2009). One study showed good correlations ($R$) between the seasonal variation of both measurements in the European cities of Berlin (0.86), Madrid (0.81), and Paris (0.69) (Paraschiv et al., 2017).

The air basin of Mexicali in Baja California, Mexico, and neighboring Calexico in California, United States, is shared due to the similar orographic conditions of these cities. Wind conditions can cause pollution episodes in either city throughout the year, mostly in winter and summer (Kelly et al., 2010; Secretaría de Protección al Ambiente, Baja California [SPABC], 2011a). One case study (Mendoza et al., 2011) showed that, in August 2001 (summer), an influence area of nitrogen oxides (NO$_x$) originating in Mexicali spread to the Imperial Valley of California and Arizona. Also, in January 2002, PM$_{2.5}$ originating in Los Angeles, California, and Las Vegas, Nevada, was transported to the air basin of Mexicali and Calexico (MXL-CLX).

Pollutant concentrations are monitored in both Mexicali and Calexico by the California Air Resources Board (CARB; “IADAM Air Quality Data Statistics”) and Subsecretaría de Protección al Ambiente (SPABC), respectively (California Air Resources Board, n.d.; SPABC, 2011b). However, there is not enough information on the mixing height of pollutants and the influence of atmospheric stability on vertical NO$_2$ tropospheric columns. The present study first aimed to estimate (a) the height of the mixing layer and (b) local atmospheric stability. Then, it aimed (c) to evaluate how representative OMI NO$_2$ values are of surface NO$_2$ measurements under different atmospheric stability conditions in 2017 and 2018.

2 | STUDY AREA AND DATA

The city of Mexicali is located in northwestern Mexico near the border with the United States. It has a total area of 149 km$^2$ (Figure 1) and an arid climate. The average maximum temperature in the summer is $42^\circ$C, and the average annual rainfall is 75 mm. The wind comes mainly from northwest, west-northwest (winter, spring, and autumn), and south-southeast (summer) (SPABC, 2011b; Canales-Rodríguez et al., 2015; Villanueva-Solis, 2017). One of the main climate hazards during the summer is heat waves during which temperatures significantly higher than the average are presented for several days. The heat waves occur more frequently within the city limits (Instituto Nacional de Estadística y Geografía [INEGI], 2009; García Cueto et al., 2015).

The neighboring city of Calexico is located in southern Imperial County, California, United States. Its climatic conditions are extremely similar to Mexicali, except for perceptible differences in wind behavior (Kelly et al., 2010). The Mexicali Valley-Imperial Valley area is an important economic zone, with Mexicali spanning 58% of...
the total area (Figure 1) (Mungaray-Moctezuma and Calderón Ramírez, 2015). The average elevation above sea level of Calexico and Mexicali is 8 m and 156 m, respectively, although some elevations below sea level are presented in northern Imperial County and western Mexicali. The main NO₂ emission sources in this region are the result of combustion processes, including the burning of agricultural crops, vehicles, and power plants (San Diego County Air Pollution Control District [SDAPCD], 2012; Sánchez-Duque et al., 2015; Montero et al., 2018).

Ground-level data were obtained from meteorological and air quality monitoring stations for the following meteorological parameters: wind speed and friction velocity (m⋅s⁻¹), solar radiation (W⋅m⁻²), relative humidity (%), and temperature (°C). These data were obtained from the monitoring stations indicated in Figure 1: (a) the EMA_MXL station administrated by the National Meteorological Service (SMN for its acronym in Spanish; smn.conagua.gob.mx/es/estaciones-meteorologicas-automaticas), (b) the II_UABC station located in the Engineering Institute of the Autonomous University of Baja California (UABC for its acronym in Spanish), and (c) the ICA station (Imperial County Airport) belonging to the CARB (www.arb.ca.gov/adam/index.html) located around 18 km north of Calexico. Local sensible heat flux values (Q艾滋, in W⋅m⁻²) and friction velocity were measured at the II_UABC station. No data were available for some months for these last parameters; thus, surface measurements from the ICA station were used to estimate its respective value using the AERMET model (United States Environmental Protection Agency [US-EPA], 2019).

The sensor used to obtain the friction velocity and sensible heat flux in the UABC station, was a Campbell Scientific CSAT3 sonic anemometer (Haro-Rincón et al., 2013), which, through its temperature sensor (T) and the vertical component of the velocity (w), calculates the sensible heat flux with the equation \( Q艾滋 = \rho C_p (wT) \) (Burns et al., 2012). The friction velocity is obtained by the sensor using their components of the velocity through the covariance values (Grare et al., 2016).

Given the similarity of the air temperature distribution in the cities of Mexicali and Calexico (García-Cueto et al., 2007, 2009), it is inferred that the sensible heat flux must be extremely similar; This seems to be caused because the ground cover materials, native and anthropogenic, keep a similar proportion, in such a way that the amount of heat absorbed and released by the surfaces, which depends on the thermal properties of those surfaces (Oke, 1988), in diurnal and seasonal cycles are similar. Regarding the friction speed (u*), which was estimated for
unstable conditions by an iterative process using the AER-MET model, the correlation that was found between the measured values of II-UABC and the values estimated in ICA, was 0.70, which as a first approximation is considered an acceptable result. The values of $u_*$ are less than one; the maximum overestimated magnitude was 0.33, and the minimum underestimated was 0.45. Since $u_*$ is cubed to estimate the Monin-Obhukov Longitude, the error made when using the estimated values is very small, and therefore they are considered to be representative of air quality monitoring sites.

The vertical column densities (VCDs) of NO$_2$, in molecules cm$^{-2}$ units (from now on as: molec cm$^{-2}$), were measured by the OMI instrument (OMI NO$_2$) administrated by the National Aeronautics and Space Administration (NASA) at a spatial resolution of 13 × 24 km at nadir. Their values represent the number of NO$_2$ molecules from the surface to the top of the troposphere in grids of 0.25° × 0.25°. These were obtained from Goddard Earth Sciences Data and Information Services Center (Giovanni) for cloud radiance fractions less than 30% (giovanni.gsfc.nasa.gov/giovanni/). The NO$_2$ sensor measures the vertical column of this pollutant in the corresponding swath of the study area once per day, in some moment between the local time interval of 11:00 to 13:00 hr (UTC–8). Accordingly, the daily averages of all considered parameters were obtained during this time. About 40% of the OMI measurements were missing due to anomalies caused by the partial blocking of the measuring instrument. A detailed explanation can be found at the following website: http://projects.knmi.nl/omi/research/product/rowanomaly-background.php. However, valid data were available for 215 and 219 days in 2017 and 2018, respectively. NO$_2$ surface concentrations (ppb) were obtained from the air quality monitoring stations of SPABC14 (Mexicali) (www.spabc.gob.mx/calidad-del-aire/) and Ethel_Street (Calexico) (www.arb.ca.gov/adam/index.html) (Figure 1).

As might be expected in a hot arid dry climate, representative of the urban areas Mexicali-Calexico, of the available energy ($Q^*$ it was found that 56% is used to heat urban air ($Q_H$), followed by storage ($Q_S$) in the urban fabric (33%), leaving only 11% for evaporation ($Q_E$) from vegetated areas (García-Cueto et al., 2004); The above indicates that, given the lack of vegetation in the study area, the humidity distribution does not seem to be relevant, or it is only marginally important. On the other hand, according to studies carried out on the spatial distribution of air temperature for the urban areas of Mexicali-Calexico (García-Cueto et al., 2007; 2009), thermal differences were found from 0.2°C to 0.9°C in an annual period taking into account extreme values. Regarding the wind, given the similarity of the urban layout between Mexicali and Calexico, its homogeneity in the vertical sense (two-level constructions are common), wide streets (urban canyon ratio $H/W = 0.5$), and proximity between the sites of the air quality monitoring stations and the meteorological stations (the maximum distance is 3.5 km), it is inferred that the magnitude of the wind speed should not be significantly different. Therefore, it is considered that the error caused by not having simultaneous measurements in the same place, of NO$_2$ and meteorological, should not be significant, and that it could even be within the sensitivity errors of the measurement instruments.

### 2.1 Meteorological conditions and local NO$_2$ data

From January to February of 2017, winter storms were recorded, favoring humid conditions and low temperatures. In summer (July, August, and September), temperatures above 40°C were recorded, which are not unusual during this season. In 2018, the winter storms and cold fronts lasted until May, resulting in humidity levels of 40–50%. In summer and early fall of the same year, the North American Monsoon brought moisture to the state of Baja California. From October to December, synoptic
events continued to favor humid conditions (60%), causing short periods of rain (Comisión Nacional del Agua [CONAGUA], 2017; 2018).

Increases in humidity and temperature, which occurred frequently during winter season in 2018, favor a reduction in NO₂ concentrations (Wu and Chen, 2012; Habeebullah et al., 2015). In the Mexicali-Calexico (MXL-CLX) air basin, the minimum NO₂ values are shown hourly in Figure 2, with the lowest values being presented in 2018. Overall, Mexicali had the highest pollutant levels. In both cities, the maximum NO₂ concentrations were reached in the morning and evening, while the minimum concentrations occurred from 10:00 to 15:00 hr.

3 | METHODOLOGY

The atmospheric stability classes were determined in two ways using (a) the modified Pasquill-Gifford stability analysis scheme and (b) the inverse of the Monin-Obukhov length \( \frac{1}{L} \) (Essa et al., 2013). Both methods consider mechanical and convective turbulence and have diurnal stage classes. This was relevant because the OMI data corresponded with specific hours of the day in the study area (Table 1). In the Pasquill-Gifford classification, net radiation and wind speed values are considered (Asharafi and Hoshyaripour, 2010). In the Monin-Obukhov classification, the length \( L \) was estimated as follows:

\[
L = -\frac{\rho C_p T u^3}{kg Q_H}
\]

where \( \rho \) is the density of dry air (1.2 kg m\(^{-3}\)), \( T \) (K) is the temperature, \( C_p \) (1,010 J kg\(^{-1}\) K\(^{-1}\)) is the specific heat of air at constant pressure, \( k \) (0.4) is the Von Karman constant, and \( g \) (9.81 m s\(^{-2}\)) is the gravitational acceleration (Bonan, 2015; Haro Velastegui et al., 2018). The temperature and sensible heat flux \( (Q_H) \) were obtained from the meteorological station of II_UABC (Figure 1).

In 2018, \( Q_H \) and \( u^* \) values were incomplete and complemented with estimations from the AERMET model. In this latter model, the input meteorological data were obtained from ICA station (Figure 1). The net radiation estimation require solar radiation, temperature, and cloud cover data. \( Q_H \) is estimated through a parameterization of this parameter and air temperature according to the methodology of Holtslag and Van Ulden (1983). Friction velocity was estimated with a iterative procedure that depends of \( Q_H \) and Monin-Obukhov length described by Paine (1987). In the AERMET, both methods can be use because surface meteorological data are available (US-EPA, 2019).

**FIGURE 2** Average hourly concentrations of NO₂ in Calexico (left column) and Mexicali (right column) during 2017 (a, b) and 2018 (c, d), respectively. The red rectangles identify the study period.
Previous studies in Oklahoma City, United States, and different regions of Cuba show that the AERMET model produces reliable results for these parameters during the diurnal period (Simpson et al., 2007; Turtos Carbonell et al., 2013; Rodriguez Valdés et al., 2015).

The atmospheric stability directly affects the mixing height (MH) because this parameter depends on the convective process and wind dynamics (Aliabadi et al., 2016). MH was calculated using the Lagrangian HYSPLIT 4 model in the VMIXING program (https://www.ready.noaa.gov/HYSPLIT_vmixing.php). This model calculates the MH from potential temperature data, locating the height at each grid point of NAM12 data (North American meso-scale model) every 3 hr at a horizontal resolution of 12 km. It is assumed that the mixing layer height can be equal to the height at which the potential temperature first exceeds the surface value by 2 K. The temperature profile is analyzed from the surface up to determine the height of the mixed layer. This kind of data have been used to evaluate the confidence of planet boundary layer estimations (Garcia et al., 2007; Yu et al., 2010; Coniglio et al., 2013).

The periods with the highest determination coefficients ($R^2$) between the tropospheric OMI NO$_2$ columns and surface NO$_2$ concentrations were identified at each air quality monitoring station (SPABC14 and Ethel_Street) (Boersma et al., 2008; Kim et al., 2016). This let to know the reliability of the data extracted from the satellite images. Also, the monitoring station that was best represented was determined considering that both stations are located in the same satellite observation area. Finally, the stability classes under which the best correspondence was found between both parameters were recognized.

### RESULTS AND DISCUSSION

Considering for this estimation only the diurnal period of 11–13 hr (UTC–8), the atmospheric basin of Mexicali and Calexico had and average monthly mixing height ranging between 753–1774 magl and 748–1785 magl, respectively, in 2017 and 716–1615 magl and 735–1598 magl, respectively, in 2018. The results obtained are comparable with those that were estimated for the daytime period by Bei et al. (2013) in 2010 at the Parque Morelos in Tijuana, and also with the values obtained by Salcido et al. (2020) in Mexicali Valley for July 2010, January 2012, and October 2016. The maximum values in 2017 were reached during May and August and in 2018 during July and August, which correspond with the months of highest atmospheric instability according to the Pasquill-Gifford (A, A-B) and Monin-Obukhov (A, B) classifications (Figure 3a,d,g,j). The increasing temperature trend before and during these latter months favors convective turbulence and the vertical mixing of pollutants, causing a decrease in the NO$_2$ concentrations (Figure 3c,i) below the annual average of 6.53 ppb in Calexico and 7.56 ppb in Mexicali in 2017 and 6.65 ppb in Calexico and 9.93 ppb in Mexicali in 2018.

The OMI and surface NO$_2$ concentrations in Calexico and Mexicali show a similar average monthly trend, with a determination coefficient ($R^2$) of 0.41 and 0.74 for 2017 and 2018, respectively, at a significance level of $\alpha = 0.05$ and $p$ value $< 0.05$. Specifically, the VCD of NO$_2$ in the troposphere (OMI NO$_2$) had a similar behavior as the surface NO$_2$ measurements during both years, mostly around mid-year (June–July) and in the final third (October–November) (Figure 3c,i). The unstable atmospheric cases were higher in 2017 than in 2018 (Figure 3a,d,g,j). It has been found that during the periods of major convective turbulence, the largest mixing height favor the OMI NO$_2$ detection in the troposphere (Boersma et al., 2007; Schaap et al., 2013; Laughner et al., 2016).

From January–May and June–November 2017, Mexicali showed a lag in reaching the highest daily values near 30 ppb in comparison to Calexico, whose
maximum values ranged from 10 to 20 ppb (Figure 3b). From January–June and July–December 2018, similar high values were found (Figure 3h). In the first year, the maximum daily values were reached in December in Calexico and Mexicali, corresponding with 31 ppb and 59 ppb, respectively, which could negatively affect the correlation between OMI and surface NO₂ concentrations, because they are the furthest values in the data distribution.

The OMI NO₂ data distribution indicated that the highest levels in 2017 and 2018 occurred in June–November and January–June, respectively. The decrease...
of minimum values during the second semester of each year, according to the probability density graphs (Figure 3e,k), favored higher determination coefficients between the VCDs of OMI NO2 levels and surface NO2 concentrations. Specifically, the higher determination coefficients were found on days characterized by the A and B stability classes according to the Monin-Obukhov (M-O) method and the A, A-B, and B classes according to the Pasquill-Gifford (P-G) method. In particular, in 2017, the highest $R^2$ was found for the P-G atmospheric classes during days with combined A and A-B conditions in Calexico (0.48) and Mexicali (0.23) and considering the average of NO2 concentrations between both cities (0.34) (Figure 3f). In 2018, the highest $R^2$ was found for the M-O classes during days with A conditions with the averages (AVG) concentrations between both cities (0.41), followed by Calexico (0.36) and Mexicali (0.35). Overall, in 2018, similar $R^2$ values were found under the combined A and B classes in each city (Figure 3l).

In 2017, the P-G classification was more sensitive: The best correlation between OMI NO2 and surface NO2 concentrations was identified under this classification scheme. In 2018, the highest correlation was identified under the M-O (A) classification scheme. In each year, it was important to reduce the influence of the minimum concentrations. The highest concentrations occurred in 2017. Atmospheric synoptic phenomena affected the study area differently, directly influencing the variability of the physical and meteorological parameters used to determine the atmospheric stability classes (Jiang et al., 2013).

As previously mentioned, in 2017, the highest $R^2$ was identified for the June–November period using the P-G classification. The correlation was highest at 12:00 hr from October to November, with Calexico having the highest $R^2$ (0.41) (Figure 4a). At this hour, the mechanical and convective turbulence in both cities were governed by similar wind patterns and a decreasing trend of solar radiation, respectively (Figure 4b). Although the latter parameter was only measured in Mexicali, the proximity of both border cities and their location in a single atmospheric basin (SPABC, 2011a) allowed us to explore its behavior. The highest number of emission sources due to combustion processes is located in Mexicali (Kelly et al., 2010), and pollutants in this city have a lower mixing height on average during the June–

![Figure 4](image-url)
November period (Figure 3a), causing higher daily concentrations in most cases (Figure 4c) and the lowest $R^2$ value.

In 2018, the M-O classification was more sensitive, enabling a better correlation to be detected during the July–December period. This result reflects the concentrations measured at 11:00 hr from October to December in which $R^2$ values of 0.38 and 0.31 were obtained for Calexico and Mexicali, respectively (Figure 4d). In the M-O classification, mechanical and convective turbulence can be analyzed by identifying decreasing trends of friction velocity and temperature, respectively (Figure 4e). The convective behavior is influenced by the sensible heat flux due to more unstable atmospheric conditions, mostly during October. However, there were two dates in November during which the sensible heat flux ($Q$) decreased and NO2 concentration increased in both cities (Figure 4f). A previous study on heat islands in the study zone showed that the spatial temperature distribution favors higher $Q$ values in Mexicali, allowing for major heat transfer from the surface to the atmosphere (García-Cueto et al., 2007).

In other border cities such as Tijuana and San Diego, the orographic conditions are not as homogenous as Mexicali and Calexico, and different atmospheric stability conditions are observed. For example, wind speeds of around 1–4 m s$^{-1}$ have been documented in Tijuana. Although Calexico and Mexicali have a similar range of wind speeds, the relief is more homogeneous, and the meteorological conditions are more extreme (Vanoye and Mendoza, 2009; Rivera et al., 2015). In Ontario, Canada, significant correlations were found between OMI and surface NO2 concentrations during days of thermal inversion ($R^2 = 0.35$) when wind speeds fluctuated between 1.3 and 4.4 m s$^{-1}$. In comparison with the study case, better correlations were found during more stable atmospheric conditions (Wallace and Kanaroglou, 2009).

5 | CONCLUSIONS

In Mexicali and Calexico, the highest mixing heights were founded during 2017, 1774 magl and 1785 magl, respectively. For both years, Calexico had the highest. Atmospheric instability during the analyzed time frame (11:00–13:00, GMT−8) was strong to moderate. The minimum NO2 concentrations in both Mexicali and Calexico were found during these hours. The variability of the considered meteorological parameters influenced the atmospheric stability classes, enabling a greater understanding of the atmospheric conditions under which the most reliable correlations between OMI and surface NO2 data were found in 2017 and 2018. The monthly average OMI NO2 densities ranged from $1.73 \times 10^{15}$ to $2.3 \times 10^{15}$ molec cm$^{-2}$ and from $1.70 \times 10^{15}$ to $2.6 \times 10^{15}$ molec cm$^{-2}$ in 2017 and 2018, respectively. Their correlation with monthly average surface NO2 concentrations was greater in Mexicali (0.39 and 0.55 in 2017 and 2018, respectively) than in Calexico (0.20 and 0.42 in 2017 and 2018, respectively). The variability of surface concentrations due to their transport in the atmosphere was not considered; nevertheless, the meteorological parameters observed at specific points reliably explained turbulence and convective phenomena. The highest correlations between OMI and surface NO2 concentrations were obtained during the second semester of each year due to lower variation in the daily maximum and minimum NO2 concentrations. The Pasquill-Gifford classification was more sensitive and enabled the highest correlations in 2017 to be detected under unstable atmospheric conditions (A, A–B); determination coefficients of 0.48 and 0.23 were found for Calexico and Mexicali, respectively. The Monin-Obukhov classification performed better for 2018 (A); under these conditions, determination coefficients of 0.36 and 0.35 were found for Calexico and Mexicali, respectively. The correlations are obtained in this way because the OMI data present limitations when compared to the surface concentrations, particularly during the daytime period where the effects of convective turbulence are present in an urban arid zone. The decreasing trend of solar radiation and wind speed during October–November 2017 and of temperature and friction velocity during October–December 2018 favored a similar pattern of behavior between OMI and surface NO2 concentrations. In conclusion, different atmospheric schemes explain better the satellite data behavior because of the NO2 variability not only was it affected by atmospheric local conditions, but also had an impact for the synoptic phenomena of winter storms and cold fronts, which represent an opportunity area for future research. The methods applied and results obtained herein enable a better understanding of the representativeness of OMI NO2 data in arid border zones with extreme meteorological conditions.

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