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Spatial Modeling of Extreme Concentrations of Carbon Monoxide Pollution in Urban Regions

José del Carmen Jiménez Hernández¹, Humberto Vaquera Huerta², Paulino Pérez Rodríguez²

¹Instituto de Física y Matemáticas, Universidad Tecnológica de la Mixteca, Huajuapan de León, Oaxaca, México

²Departamento de Estadística, Colegio de Postgraduados, Texcoco, Edo. De, México

Email address

jcjim@mixteco.utm.mx (J. del C. J. Hernández) *Corresponding author

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Abstract

Extreme value models has been applied in environmental studies for modeling air pollution data. Recently, the max-stable processes have become a useful tool for statistical modeling of spatial behavior of extremes. In this article, the max-stable processes models are applied to data of extreme concentration levels of carbon monoxide in order to investigate spatial trends of this air pollutant in one of the largest urban zone in the world (Mexico City). The proposed approach uses the Smith and Schlather dependence models which are fitted in each year and, based on the Takeuchi information criterion, the Schlather model was chosen as the best fitted for these data. Subsequently, we propose a trend surfaces parameter nested into the parameters of the extreme values distribution, that allows to obtain predictive maps for this pollutant. The results of the studied case indicate that Schlather dependence models shows the best fit, and predictive maps shows an increase in the levels of this pollutant in the south region of the urban studied area.

1. Introduction

Throughout its history mankind has looked for the enjoyment of a life with a higher level of well-being and comfort. However, the development it has experienced to reach it has been accompanied with massive consumption of natural and power resources, as well as the generation of a large variety of waste and emissions to the atmosphere which have caused a large environmental degradation.

A good example of environmental problems which have implications, both local and global, are the atmospheric ones, from which, the most important ones, due to their effects on the health of the population and the natural ecosystems, are the decrease of the air quality, the phenomenon of global climate change and the reduction of the stratospheric ozone layer.

The atmospheric pollution has effects at local, regional and global levels. Several countries like Japan, China and Mexico face, for some time now, problems of air quality in their principal metropolitan areas; in the particular case of Mexico, the Valley of Mexico stands out as the most known and commented one.

In the Valley of Mexico Metropolitan Zone (VMMZ) the atmospheric concentration of the principal pollutants is monitored: sulfur dioxide (SO₂), carbon monoxide (CO),

nitrogen dioxide (NO₂), ozone (O₃), suspended particles (PM_{10} and $PM_{2.5}$), total suspended particles (PST) and lead (Pb). Of these pollutants, the CO has been, steadily, the most emitted pollutant in the VMMZ, with values that have been between 66% and 79% of the total of emissions [21].

Many works studying some of these pollutants may be found in the literature, for example, [13] study the NO_2 in Portugal in the spatio-temporal approach using geostatistical tools, from the view point of the extreme value theory, [2] study the occurrence and duration of ozone exceedances in Mexico City through a model of queuing theory, [22] use the Dagum distribution to modeling ozono levels in Mexico City. But none related to the present study. Reason for which this work focuses on the spatial extreme analysis of CO in the VMMZ.

Carbon monoxide is an odorless and colorless gas, highly toxic, mainly emitted from burning fuels or any organic material when done in an oxygen-limited atmosphere. Its presence in the atmosphere in high concentrations is fatal to humans. Road traffic is the main source of carbon monoxide. Intoxication from this pollutant is one of the most common types of poisoning; it can inhibit oxygen from being transported to the cells and cause dizziness, headache, nausea, unconsciousness, and even death [10], [26]. The NOM-021-SSA1-1993 norm establishes that this pollutant must not surpass the permissible value of 11.00 ppm, equivalent to 12595 μ g/m³ in a mobile 8 hours mean once a year, as protection to the health of the susceptible population [20].

For our study, the max-stable processes are applied, which are natural models for modeling spatial extremes [12], these are a natural generalization of multivariate extreme value distribution in infinite dimensions. Nowadays, different spectral representations have been developed for stationary max-stable processes; see [8], [9] and [18]. Max-stable processes have been recently used for statistical modeling of spatial data; for example, [4] modeled extreme rainfall data using these processes. Another application to rainfall data can be found in [14], who modeled rainfall and proposed a practical estimation procedure based on pairwise likelihood. Other modeling approaches for spatial extremes, based either on copulas or on latent processes, are presented by [7].

Currently, different classes of max-stable processes have been introduced; herein we will mention two of them, which will be used with our data. [24] used the [8] spectral representation and proposed a max-stable spatial model which is known as storm profile model. The different variables used in its construction can be interpreted as storm components, including shape and intensity. The process is based on points of a Poisson process together with a *f* kernel function, which can be a centered Gaussian density function. In this case, [23] explicitly found the bivariate distribution function for two locations; in this model, the dependence structure is obtained using Gaussian densities.

In real applications, the measurements are taken at various locations, in some cases on a mesh, at specific time intervals. To do the inference, the observations are assumed to be independent in time.

More recently, [18] proposed using a stochastic process as the kernel function. This generates a great variety of models when varying said process. He suggests using a Gaussian stochastic process, in this case, also obtaining an explicit bivariate distribution function. In both cases, using the [15] dependence function, the extreme coefficient can be obtained, which in this type of process is used as the function that allows to measure spatial dependence. Spatio-temporal aspects on extreme modeling are treated by [6] and [12].

The objective of the present paper is to use the max-stable stationary process to study the multivariate maximum concentrations of carbon monoxide in the spatial context to investigate spatial trends of this contaminant.

2. Spatial Extremes and Max-Stable Processes

2.1. Max-Stable Processes and Spatial Models

Max-stable processes are the result of a natural extension of the multivariate extreme value theory in infinite dimensions. They provide a natural generalization of the extreme dependence structure in continuous spaces. Thus, the bivariate distribution function can be derived.

Let *T* be a set of indices and let $\{Y_i(x)\}_{x \in T^*} i=1,...,n$, be *n* independent replicates of a continuous stochastic process. Assume there are sequences of continuous functions $a_n(x)>0$

and $b_n(x) \in R$ so that

$$Z(x) = \lim_{n \to +\infty} \frac{\max_{i=1}^{n} Y_i(x) - b_n(x)}{a_n(x)}, \quad x \in T$$
(1)

If this limit exists, the limit process Z(x) is a max-stable process [8].

Not that (1) does not guarantee that the limit exist; however, it always happens and can be observed that this type of processes can be appropriate to model maximum spatial extremes. Without loss of generality if $a_n(x)=n$ and $b_n(x)=0$, the marginal distributions have a Fréchet distribution; this is $F(z)=\exp(-1/z)$, z>0. There are currently two different characterizations for this type of processes. The first of them, often referred to as the storm profile model, was introduced by [24] and the second was proposed by [18], who introduced a new characterization allowing a random shape.

2.1.1. The Smith Model

Let $\{(\xi_i, y_i), i \ge 1\}$ denote the points of a Poisson process on $(0, +\infty) \times R^d$ with an intensity measure of $\xi^{-2} d\xi v(dy)$, where v(dy) is a positive measure on R^d . Then a characterization of a max-stable process with Fréchet marginal distributions is

$$Z(x) = \max_{i} \left\{ \xi_i f(y_i, x) \right\}, \quad x \in \mathbb{R}^d$$
(2)

where $\{f(x, y), x, y \in \mathbb{R}^d\}$ is a non-negative function such that $\int_{\mathbb{P}^d} f(x, y) \nu(dy) = 1$, $\forall x \in \mathbb{R}^d$. To see that equation (2) defines a stationary max-stable process with Fréchet marginals, the marginals have to be proven to actually be Fréchet and that

$$\Pr[Z(x_1) \le z_1, Z(x_2) \le z_2] = \exp\left[-\frac{1}{z_1}\Phi\left(\frac{a}{2} + \frac{1}{a}\log\frac{z_2}{z_1}\right) - \frac{1}{z_2}\Phi\left(\frac{a}{2} + \frac{1}{a}\log\frac{z_1}{z_2}\right)\right]$$

where $\Phi(\cdot)$ is the standard normal distribution function and, for two given locations 1 and 2, $a^2 = \Delta x^T \Sigma^{-1} \Delta x$, where Δx is the distance between both locations.

2.1.2. The Schlather Model

Let $Y(\cdot)$ be a stationary process on \mathbb{R}^d such that $E[\max\{0, Y(x)\}]=1$ and let $\{\xi_i, i \ge 1\}$ be realizations of Poisson process on R^+ with $\xi^{-2}d\xi$ intensity measure. Then, Schlather proves that the max-stable stationary process with unit Fréchet marginals can be defined as,

Z(x) satisfies the properties of a max-stable process. The process defined in (2) is more general and Smith considers a particular case where v(dy) is the Lebesque measure and $f(x,y)=f_0(y-x)$, where $f_0(y-x)$ is the multivariate normal density function with zero mean and Σ covariance matrix. With these assumptions, we can prove that the cumulative distribution function for two locations is given by,

$$\Pr[Z(x_1) \le z_1, Z(x_2) \le z_2] = \exp\left[-\frac{1}{z_1}\Phi\left(\frac{a}{2} + \frac{1}{a}\log\frac{z_2}{z_1}\right) - \frac{1}{z_2}\Phi\left(\frac{a}{2} + \frac{1}{a}\log\frac{z_1}{z_2}\right)\right]$$

 $Z(x) = \max_{i} \xi_{i\max}\{0, Y_i(x)\}$ (3)

Where $Y_i(\cdot)$ are independent and identically distributed realizations of $Y(\cdot)$.

Equation (3) is general and needs additional assumptions to obtain practical models. Schlather proposed taking $Y_i(\cdot)$ to be a stationary standard Gaussian process with correlation function $\rho(h)$, with $E[\max\{0, Y_i(x)\}]=1$. With these

assumptions, we can prove that the bivariate cumulative distribution function of process is,

$$\Pr[Z(x_1) \le z_1, Z(x_2) \le z_2] = \exp\left[-\frac{1}{2}\left(\frac{1}{z_1} + \frac{1}{z_2}\right)\left(1 + \sqrt{1 - 2(\rho(h) + 1)\frac{z_1z_2}{(z_1 + z_2)^2}}\right)\right]$$

where $h \in R^+$ is the distance between locations 1 and 2. Usually, $\rho(h)$ is choosen from a valid parametric family (See Table 1); in this case c_2 and v are the range and the smooth parameters of the correlation function, $\Gamma(\cdot)$ is the gamma

function, $J_{\nu}(\cdot)$ and $K_{\nu}(\cdot)$ and third type ν order modified

Bessel functions and d is the dimension of the random field. In this case, it is possible to add a sill c_1 and a nugget effect α to these correlation functions, as follows,

$$\rho_*(h) = \begin{cases} \nu + c_{1,} \, h = 0 \\ c_1 \rho(h) \, h > 0 \end{cases}$$

Tał	ole	1.	Some	correl	ation	functions
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Family	Correlation function	Range of validity
Whittle-Matern	$\rho(h) = \frac{2^{1-\nu}}{\Gamma(\nu)} \left(\frac{h}{c_2}\right)^{\nu} K_{\nu}\left(\frac{h}{c_2}\right)$	$c_2 > 0, \nu > 0$
Cauchy	$\rho(h) = \left[1 + \left(\frac{h}{c_2}\right)^2\right]^{-\nu}$	$c_2 > 0, \nu > 0$
Powered Exponential	$\rho(h) = \exp\left[-\left(\frac{h}{c_2}\right)^{\nu}\right]$	$c_2 > 0, 0 < \nu \le 2$
Bessel	$\rho(h) = \left(\frac{2c_2}{h}\right)^{\nu} \Gamma(\nu+1) J_{\nu}\left(\frac{h}{c_2}\right)$	$c_2 > 0, \nu \ge \frac{d-2}{2}$

2.1.3. Spatial Dependence

Let $Z(\cdot)$ be a stationary max-stable process with Fréchet margins the extremal dependence between N locations fixed in R^{d} can be summarized in the extremal coefficient defined as

$$Pr[Z(x_1) \le z, \dots, Z(x_N) \le z] = \exp\left(-\frac{\Theta_N}{z}\right)$$
(4)

where $1 \leq \Theta_N \leq N$, with lower and upper bounds corresponding

to a complete dependence and independence, respectively. Thus, we get a measure of the degree of spatial dependence between two stations. Given the properties of the max-stable process with unit Fréchet margins, the cumulative distribution function belongs to the multivariate extreme value distributions class, this is,

$$Pr[Z(x_1) \le z, ..., Z(x_N) \le z] = \exp(-V(z_1, ..., z_N))$$

where V is a -1 order homogeneous function, called the exponent measure [15], [3], and consequently the homogeneity property of V implies a strong relationship between it and the extremal coefficient. Thus, we get,

$$\Theta_N = V(1, \dots, 1)$$

A special case of equation (4) is considering pairwise extremal coefficients, this is,

$$Pr[Z(x_1) \le z, Z(x_2) \le z] = \exp\left\{-\frac{\Theta(x_1 - x_2)}{z}\right\}$$
 (5)

 $\Theta(\cdot)$ is known as the extremal coefficient function and provides sufficient information about the extreme dependence for many problems, although it does not characterize the whole distribution [19].

The $\Theta(\cdot)$ function for the previously described models can be derived directly from the bivariate distribution function, taking $z_1 = z_2 = z$, this is

$$\Theta(x_1 - x_2) = 2\Phi\left(\frac{\sqrt{(x_1 - x_2)^T \Sigma^{-1}(x_1 - x_2)}}{2}\right)$$

For the Smith model, while for the Schlather model it is,

$$\Theta(x_1 - x_2) = 1 + \sqrt{\frac{1 - \rho(x_1 - x_2)}{2}}$$

2.2. Inference in Max-Stable Processes

2.2.1. Parameter Estimation

For this type of processes, only the bivariate distribution function is known analytically, thus data fitting is not simple. In this paper, we consider estimation based on composite maximum likelihood, particularly the estimation of pairwise maximum likelihood [11]. In this case, the pairwise log-likelihood function is given by,

$$l_p(\boldsymbol{z};\boldsymbol{\psi}) = \sum_{i < j} \sum_{k=1}^{n_{ij}} \log f(\boldsymbol{z}_k^{(i)}, \boldsymbol{z}_k^{(i)}; \boldsymbol{\psi})$$
(6)

here z are the available data on the whole region, $n_{i,j}$ is the number of observations common between *i* and *j* locations, and $z_k^{(i)}$ is the *k*th observation of the *i*th location, and $f(\cdot, \cdot)$ is the bivariate density of the max-stable process. The properties of the composite maximum likelihood estimators are well known [4] and belong to the class of maximum likelihood estimators under misspecification.

2.2.2. Model Comparison

Selecting the model plays an important role in statistical modeling. Given various models that adequately fit our data, we should choose the simplest and no the most complex model. There are several approaches to select the model, depending on the models that are going to be compared. In this paper, we chose the Takeuchi Information Criterion (TIC) [25], given by,

$$TIC = -2 l_p(\widehat{\psi}) - 2 t_f \{\widehat{J}H^{-1}\}$$
(7)

and as in the case of the AIC criterion [1], the best model will be that whose TIC is lowest. Recently, [27] rediscovered this information criterion and proved its use to select models when composite maximum likelihood estimation is used.

3. Methodology for Modeling Spatial Extremes

For modeling spatial extreme data, the following approach is proposed:

- a. Use of block maxima approach for each year. The maximum were taken from each block, made up of three-day consecutive observations, to guarantee their independence [3].
- b. To perform an exploratory analysis for each station for every year and fit a GEV distribution, and verify the assumption.
- c. Transform the data to get a unit Fréchet distribution in each location as follows: if $Y \sim \text{GEV}(\mu,\sigma,\xi)$, then the

random variable defined as $Z = \left(1 + \xi \frac{Y - \mu}{\sigma}\right)^{1/\varsigma}$ follows a unit Fréchet distribution.

- d. Fit the Smith and Schlather max-stable models for each year, obtaining the parameter estimations in each model.
- e. To produce predictive maps by introducing a linear trend surfaces into the GEV distribution parameter.

To perform the data analysis a code in R statistical software was written, by using specifically, SpatialExtremes [16] and [17].

3.1. CO Data from Mexico City

We present an application example of the max-stable processes described in the previous sections. The data set to be analyzed is made up of daily measurements of carbon monoxide registered hourly in VMMZ. The data were obtained from the Mexico City Environmental Meteorological System, which consist of daily measurements of the carbon monoxide levels registered every hour in 9 meteorological stations, from 2008 to 2013, available at http://www.aire.df.gob.mx.

Table 2 shows the list of stations, their geographical locations, and their altitudes. Figure 1 shows the study area, the VMMZ consists of 16 delegations of Mexico City and 29 municipalities in Mexico State.

Table 2. Meteorological stations under study.

Code	Station	Longitude	Latitude	Altitude
MER	Merced	-99°7' 10.52"	19°25' 28.59"	2245
PED	Pedregal	-99°12' 14.90"	19°19' 30.54"	2326
SAG	San Agustin	-99°1' 49.15"	19°31' 58.69"	2241
SUR	Santa Ursula	-99°8' 59.96"	19°18' 52.12"	2279
TLA	Tlalnepantla	-99°12' 16.55"	19°31' 44.68"	2311
TLI	Tultitlan	-99°10' 37.81"	19°36' 9.14"	2313
UIZ	UAM Iztapalapa	-99°4' 25.96"	19°21' 38.84"	2221
VIF	Villa de las Flores	-99°5° 47.72"	19°39' 29.59"	2242
IZT	Iztacalco	-99°7' 3.50"	19°23' 3.88"	2238



Figure 1. Study region.

3.2. Results for CO in Mexico City

Figure 2 shows the time series for Pedregal station from 2008 to 2013, in which the behavior of three-day block maxima of carbon monoxide is illustrated in each year.



Figure 2. Carbon monoxide for Pedregal station from 2008 to 2013.

For the Smith model, the estimated spatial dependence parameters are shown in Table 3.

0.0011950(0.0001059)

Year	$\widehat{\sigma}_{11}$	$\widehat{\sigma}_{12}$	$\widehat{\sigma}_{22}$
2008	0.0003051(0.0000996	-0.0015313(0.0004490)	0.0131039(0.0022439)
2009	0.0023020(0.0001546)	-0.0021882(0.0002323)	0.0057172(0.0003743)
2010	0.0029670(0.0006931)	-0.0102894(0.0023580)	0.0360046(0.0080169)
2011	0.0009467(0.0000489)	0.0010138(0.0000732)	0.0104137(0.0000307)
2012	0.0013960(0.0003106)	0.0077026(0.0017259)	0.0444249(0.0096874)

Table 3. Spatial dependence parameters estimated for the Smith model, the standard errors is shown in parentheses.

The Schlather model was adjusted using the Whittle-Matérn (WM) correlation function and exponential (Exp). The results show that the model with the lower TIC was that where we used the exponential correlation function. Table 4 shows the results.

T-11- 1 T-1----

-0.0040738(0.0003724)

0.0220853(0.0016569)

Table 4. Takeuchi Information Criterion.							
	2008	2009	2010	2011	2012	2013	
IC WM	37049.25	36668.09	36914.81	37256.32	36933.39	36812.45	
IC Exp	37048.90	36667.56	36911.75	37233.72	36932.95	36803.19	

The spatial dependence parameters for the Schlather model using this correlation function are shown in Table 5. Note that in every case, the smooth parameter is near two, this suggests decreasing the dimensionality of the model and doing a hypothesis test on this parameter.

Table 5. Spatial dependence parameters estimated for the Schlather model, the standard errors is shown in parentheses.

Year	â	ĉ ₂	Ŷ
2008	0.7723(0.1033)	0.3141(0.1283)	1.9999(3.26)
2009	0.7000(0.1178)	0.2315(0.0698)	1.9998(1.84)
2010	0.5562(0.3162)	0.0950(0.0398)	1.9887(2.43)
2011	0.1384(0.1708)	0.0342(0.2616)	1.9902(8.82)
2012	0.7818(0.2594)	0.1113(0.0732)	1.9997(4.34)
2013	0.9999(0.1274)	0.1066(0.0492)	1.9814(1.48)

To analyze the spatial dependence, the non-parametric extremal coefficients in each year were graphed. Figure 3 shows these coefficients for 2008, 2009, 2012, and 2013. Note that as time advances, the dependence tends to decrease.



Figure 3. Non-parametric extremal coefficient. The continuous line estimates the trend of the spatial dependence.

2013

Т

TIC Exp

Table 6 summarizes the Schlather model fitted to the 2012 data with the four correlation functions; they all have similar TIC, but the adjustment with the exponential function gives the lowest TIC. Similarly, the value of the log-likelihood function is similar in these cases.

Table 6. Summary of the Schlather model fitted to the 2012 data. Standard errors are shown in parentheses. TIC is the Takeuchi information criterion and l_p isthe maximized composite log-likelihood.

Correlation	â	ĉ ₂	Ŷ	TIC	l_p	
Whitmat	0.7545(0.1704)	0.0235(0.2351)	7.3450(140.30)	35897.60	-17943.46	
Cauchy	0.7578(0.1518)	0.6800(24.1971)	30.1698(2105.10)	35897.68	-17943.44	
Exponencial	0.7617(0.2202)	0.1252(0.0637)	1.9994(3.58)	35897.09	-17943.43	
Bessel	0.7574(0.1335)	0.0051(0.7280)	150.3081(4347.12)	35897.42	-17943.43	

To do the forecasts, it is convenient to define trend surfaces in the GEV distribution parameters as it is probable that the parameters show marginal spatial variation. In this case, for every $x \in X$, we assume that $Y(x) \sim \text{GEV}(\mu(x), \sigma(x), \xi(x))$, and thus we can define, for example $\mu(x)=h(x;\beta_{\mu})$, $x \in X$, for a $h(\cdot;\beta_{\mu})$ parametric function. To detect an adequate tendency, an exploratory analysis was done on the data. Figure 4 shows a symbol graph for the 2012 data. The circles are centered on the location of each station whose radius is proportional to the output value in that location and the mean value of the area. This suggests the following surfaces for our parameters: $\mu(x)=\beta_{\mu,0}+\beta_{\mu,1}lon(x)+\beta_{\mu,2}lat(x)$, $\sigma(x)=\beta_{\sigma,0}+\beta_{\sigma,1}lon(x)+\beta_{\sigma,2}lat(x)$ y $\xi(x)=\beta_{\xi,0}$.



Figure 4. Symbol plot for 2012 data.

Other ways to select these marginal structures can be applied, for example, by adjusting several plausible models and choosing the one that has the lowest compound likelihood information criterion. In this case, the assumption of having Fréchet marginal distributions in each location can be omitted and the max-stable model can be fitted to the original data. Thus, the Schlather model was fitted to the 2012 data with the exponential correlation function and with the tendencies of the GEV distribution parameters. Table 7 shows the estimated parameters and their respective standard errors, also, Figure 5 shows the validation of the model; the diagonal graphs the return levels and under it, the probability graphs in the Gumbel scale between the observed maximums for each block and those obtained through simulations of the adjusted model. The upper graph compares the extreme coefficient adjusted with the semi-parametric model. The other two graphs are the locations of the stations and the maximum probability graph by blocks, where the block size is four; this validates the goodness of fit of the model. Punctual predictive maps where then made for the location, shape, and return level at one week parameters; this is shown in Figure 6 - 8.



Table 7. Estimated parameters and standard errors of the Schlather model fitted to 2012 data, assuming trend surfaces in the GEV distribution parameters.



Figure 6. Punctual forecasts for the Schlather process fitted, location parameter.



Figure 7. Punctual forecasts for the Schlather process fitted, scale parameter.



Figure 8. Punctual forecasts for the Schlather process fitted, return level at one week.

Finally, predictive maps were made using the trend surfaces estimated from the GEV distribution parameters. Return levels 1 and 2 week were used. Figure 9 - 10 shows these maps. Note that an increase in the levels of the pollutant is forecasted in the south region of the Mexico valley, while in the north region it remains low. It is worth mentioning that in this case, spatial dependence is not taken into account.



Figure 9. Forecast of the return level, 1 week.



Figure 10. Forecast of the return level, 2 week.

4. Conclusions

A methodology based in the max-stable processes by using a bivariate dependence model was implemented for investigating spatial trends in CO extreme concentrations. The methodology applied to carbon monoxide pollution data in the Valley of Mexico Metropolitan Zone from 2008 to 2013 showed to be a good way to make inferences on the behavior of extreme concentrations. The max-stable models were fitted to these data and the best fit was observed to be with the Schlather model, likewise defining trend surfaces in the GEV distribution parameters. Fitting the Schlather model to the year 2012, we got predictive models for the following years, noting that higher levels of this pollutant are expected in the south region of the City.

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