International Journal of Latest Research in Engineering and Technology (IJLRET)
ISSN: 2454-5031
www.ijlret.com || Volume 05 - Issue 04 || April 2019 || PP. 01-17

Prediction of Concentrations of Suspended Particle Levels of 2.5 micrometers (PM2.5) in Mexico City with Probability Distribution Functions and its Trend

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Abstract: The study includes a data analysis from 2010 to 2018, it was proposed to obtain the best or better probability distribution functions that Model PM2.5 concentrations in mexico city, using the following PDF, Gama Distribution Function, Extreme Value Distribution Function, Gumbel Distribution Function and Weibull Distribution Function, the maximum likelihood and moments method was used to obtain the estimators, and with the aid of the Matlab 2017 program, RMSE, MSE, were used to assess the forecast model, determination coefficient, prediction approximation and approximation index, in turn, an analysis is made to observe its trend within the period using the method of obtaining new functions of normal probability distribution and extreme value by bayesian inference to concentration data of daily highs later corroborating with the official air page of mexico city.

Keywords: 2.5 Micrometer Particulate Material, Probability Distributions, Fit Indicators, Bayesian Inference.

The particulate material of aerodynamic diameter less than or equal to 2.5 micrometers is referred to as PM2.5 and PM0.1 refers to particulate material of aerodynamic diameter less than or equal to 0.1 micrometer. Another common way of referring to these particles is the designation of coarse particulate material (PM 2.5-10), fine particulate material (PM 0.1-2.5) and ultra-fine particulate material (PM <0.1). These classifications are important from the point of view of composition, from the point of view of behavior (transport and disposal) in the atmosphere and from the toxicological point of view.

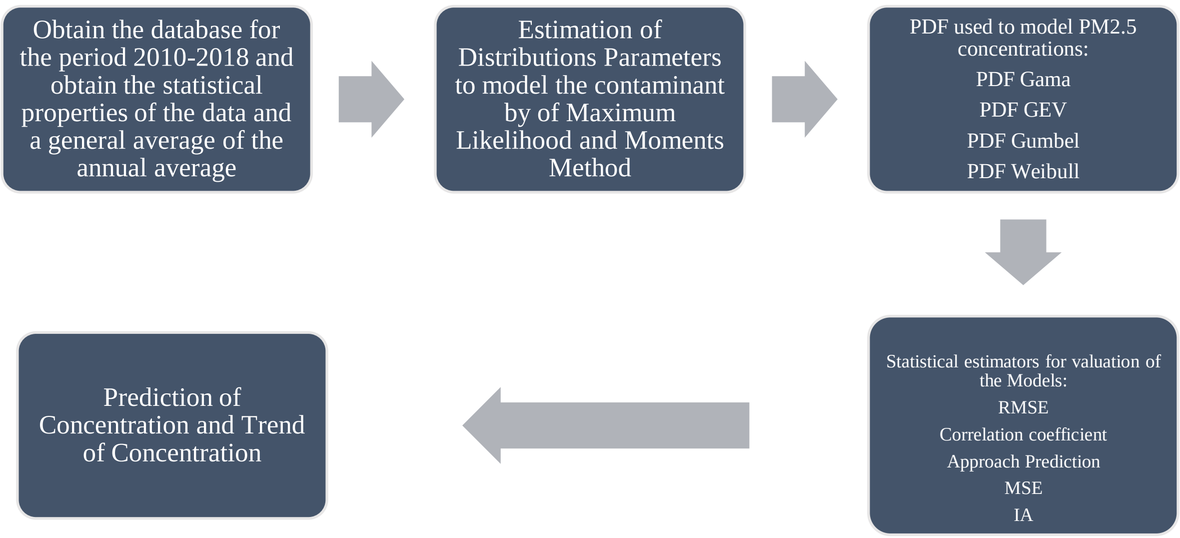
During breathing, the suspended particles can evade natural defenses, lodge in the lungs for a long time and even dissolve and enter the bloodstream, which makes it one of the most dangerous air pollutants for health. The particles have any shape and size, there are spherical, cubic, fibrous, scaly, irregular, they can also be liquid, like steam that comes off when bathing or solid, like those thrown by trucks through their escapes. It is also considered that, in terms of health effects, particulate matter is more important than other common air pollutants. The World Health Organization estimates that PM2.5 particles contribute to approximately 800,000 deaths per year globally; Indeed, there is evidence that particulate matter pollution causes: premature death in people with heart and lung diseases, nonfatal heart attacks, irregular heartbeat, respiratory tract irritation, coughing, difficulty breathing, aggravates asthma, and decreases asthma. Pulmonary function. In Mexico City the main sources of particles are the exhaust of automobiles, the burning of diesel, the dusting during the dry season of the year and the constructions.

Given the stochastic nature of atmospheric processes, concentrations of air pollutants can be treated as random variables with measurable statistical properties. If certain conditions are the statistical characteristics of pollutant concentrations, they can be described by probability density functions. Probability density functions (pdf) have been widely used in recent years in a variety of applications, where smoothing data,

Interpolation or extrapolation is needed (Wilks, 1995). Specifically, in the atmospheric sciences the most characteristic applications include the approximation of the frequency of exceedances of the critical levels of concentration and the estimation of the reduction of emissions, required for the standard of air quality objectives (Georgopoulos and Seinfend, 1982; Abatzoglou et al., 1996; Burkehardt et al., 1998; Morel et al., 1999).

The maximum likelihood method is considered advantageous for estimating parameters compared to moment methods (which is also occasionally used). On the other hand, the maximum likelihood method requires a great processing power due to the complex numerical calculations involved, when large data sets are analyzed, computational time increases substantially.

Probability Distribution Functions and Methodology



Four Probability Distribution Functions were used, which are the Gama Distribution Function, the GEV Distribution Function, the Maximum Gumbel Distribution Function, and the Weibull Distribution Function.

Table1. Probability Distribution Functions and their Parameters.

Distribution	ProbabilityDensityFunction	Parameters
GEV	$f(x) = \left(\frac{1}{\sigma}\right) exp^{-\left((1+kz)^{\left(-\frac{1}{k}\right)}\right)(1+kz)^{\left(-1-\frac{1}{k}\right)}}$	***K*** **shape** $\boldsymbol{\sigma}$ **scale** **µ location**
Gumbel	$f(x) = \left(\frac{1}{\sigma}\right) exp^{(-z-exp^{-z})}$ $z = \frac{x-\mu}{\sigma}$	$\boldsymbol{\sigma}$ **scale** **µlocation**
Weibull	$f(x) = \frac{\alpha}{\beta}\left(\frac{x}{\beta}\right)^{\alpha-1} exp^{\left(-\frac{x^{\alpha}}{\beta}\right)}$	**The □ shape** **The □ scale**
Gama	$f(x) = \frac{Beta^{alfa}}{\Gamma(alfa)} x^{alfa-1} e^{-Betax}$	$Beta = \frac{\sum x_i^2}{\sum x_i} - \frac{\sum x_i}{N}$ $Alfa = \frac{(\sum x_i)^2}{N\sum x_i^2 - (\sum x_i)^2}$

Statistical Adjustment Estimators

The deviation indicators of a group of data in relation to a model can be used to assess the goodness of fit between the two. Among the most common indicators are the following: RMSE, MAE, NRMSE, CV-MRSE, SDR, and $\boldsymbol{R^2}$. Those that were used to determine the distribution that best fit gave the data. They are the mean square error (RMSE), mean square error (MSE), prediction accuracy (AP) and coefficient of determination ($\boldsymbol{R^2}$) Table2 gives the equations for the adjustment indicators that have been used by Lu (2003) and Junninen et al. (2002).

Table2. AdjustmentEstimator

Estimator	Equation
Error Measures **Root Mean Square Error**	$RMSE = \sqrt{\left(\frac{1}{N-1}\right)\sum_{i=1}^{N}(Pi - Oi)^2}$
Error Measures **Mean Square Error**	$MSE = \left(\frac{1}{N}\right)\sum_{i=1}^{N}(Pi - Oi)^2$
Accuracy Measures **Coefficiente of Determination**	$R^2 = \left(\frac{\sum_{i=1}^{N}(Pi - P)(Oi - O)}{NS_pS_o}\right)^2$
AccuracyMeasures **PredictionAccuracy**	$AP = \frac{\sum_{i=1}^{N}(Pi - O)^2}{\sum_{i=1}^{N}(Oi - O)^2}$
AccuracyMeasures **Index of Accuracy**	$IA = 1 - \frac{\sum_{i=1}^{N}(Pi - Oi)^2}{\sum_{i=1}^{N}(\lvert Pi - O\rvert - \lvert(Oi - O)\rvert)^2}$

Notation: N = number of observations, P_i= predictive valúes, O_i= observed values, P = average of predicted values, **O** = average of theobservedvalues, S_p= Standard Deviation of Predicted valúes, S_o = Standard deviation of theobserved valúes.

Studio of Área

The Mexico City in its geographical location is located in a closed or almost closed basin, which in all directions is north, south, east or west, adjoins a mountain range or mountain pass, which is the highest altitude with volcanoes to the east the Popocatepetl and the Iztaccihualt, which the circulation of wind and the dispersion of pollutants makes it difficult, both for suspended particles and for other pollutants.

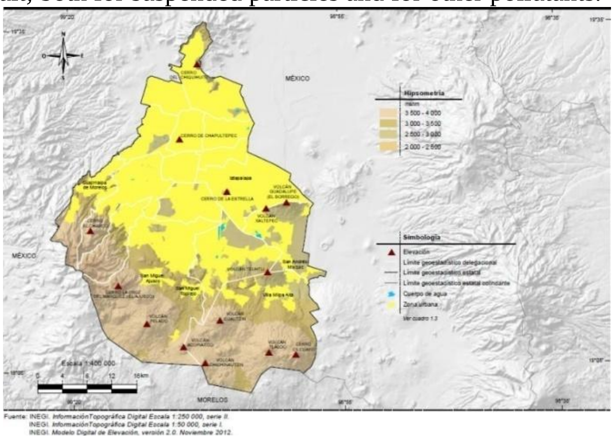


Figure 1. Relief of Mexico City (Source: https://www.paratodomexico.com/)

Statistical Description of the Data

In the following table we can see the characteristics of the database which show 5% of null or unread values.

Table3. Statistical Description of the Average Concentration of PM2.5 Data Trend 2010-2018

Numbers of Data	78888
Mínimum	0.4286 µgr/m^3
Máximum	131.28 µgr/m^3
Mean	13.92 µgr/m^3
Variance	64.32 µgr/m^3
Standard Deviation	8.02 µgr/m^3
Median	12.38 µgr/m^3

Result

Table4. Estimation Parameters and Trend Adjustment Indicators 2010-2018

Distribution	Estimatedparameters	RMSE	MSE	R^2	IA	Kolmogorov–Smirnov	Chi Test
GEV	K = 0.0937 Sigma=5.53 Mu=10.17	0.4617	0.2131	0.9884	0.6216	0	h = 0 p =0.6918
Gumbel	Al =0.159 U = 10.311	0.6362	0.4047	0.6717	0.4468	-	h =0 p =0.6225
Weibull	A = 15.309 B = 1.7937	0.4689	0.2198	0.7747	0.6160	0	h =1 p = 0.0022
Gama	Alfa= 3.39 Beta= 4.17	0.4664	0.2175	0.9689	0.6188	0	h =0 p =0.6331

In the previous table we can see that the best adjusted probability distribution function was the GEV, followed by the distribution function Gama, with an R^2 of 0.98 and that of the Gama with a 0.96, we can also see that the RMSE of both are similar and the Approach Index is higher in the GEV than the others, and the Gama follows it.

The kindness tests used were the Kolmogorov - Smirnov test and the Chi square test, the K - S test was accepted, except the Weibull pdf in the Chi test.

The outliers were removed, which cause that the goodness tests do not adjust, causing the rejection of the adjustment with an alpha value of 5% or less, the adjustment can be checked also with the statistical estimators and with the graphs of the empirical and theoretical cdf, then the QQ plot graphs are given to observe that the theoretical distribution function follows the input or concentration data.

Temporary Series of the Trend of PM2.5 of the 2010-2018

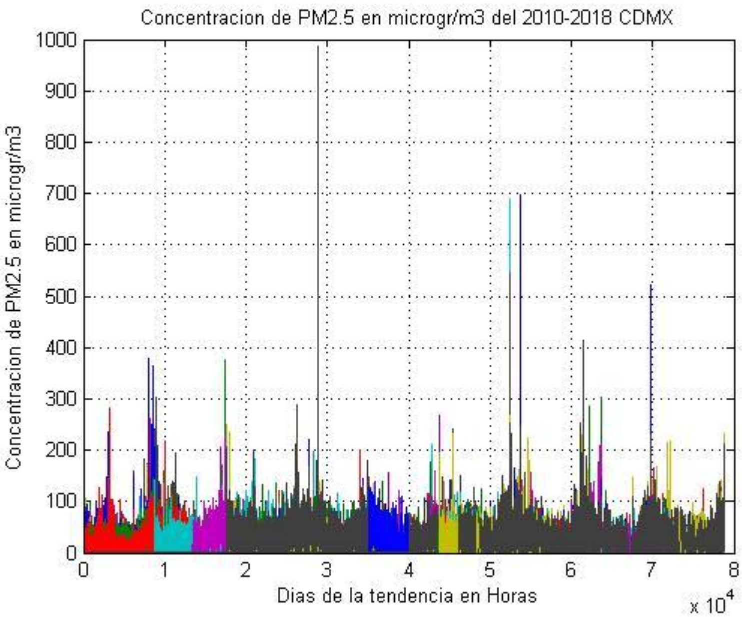
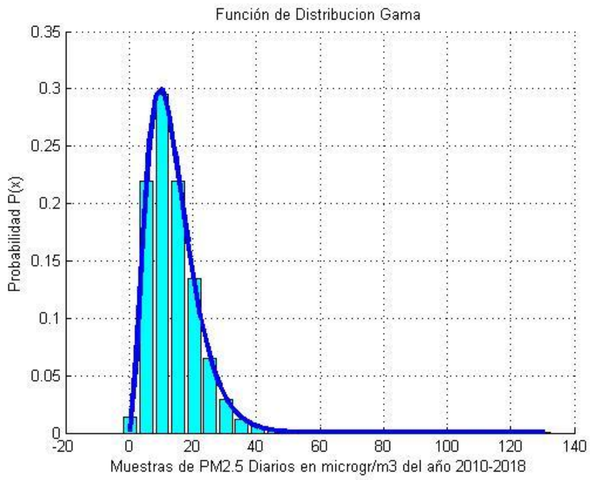
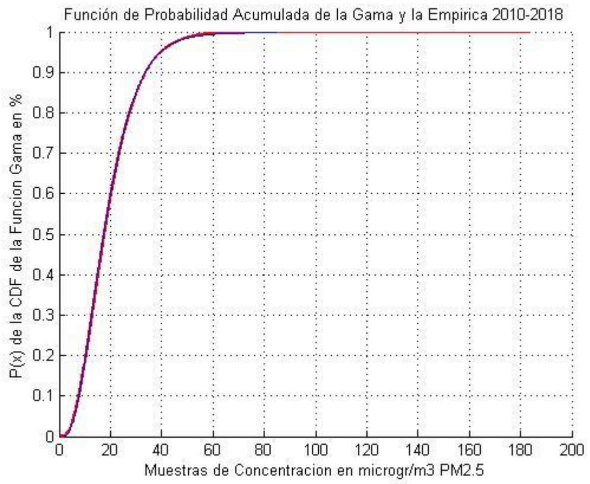


Figure 2. Temporary Series of the Concentration of PM2.5 in μgr/m^3 in Mexico City Trend 2010-2018 in hours

Table5. Adjustments to the 2010-2018 Tendency

<table>
<tr><th>PDF</th><th>CDF</th></tr>
<tr><td>
</td><td>
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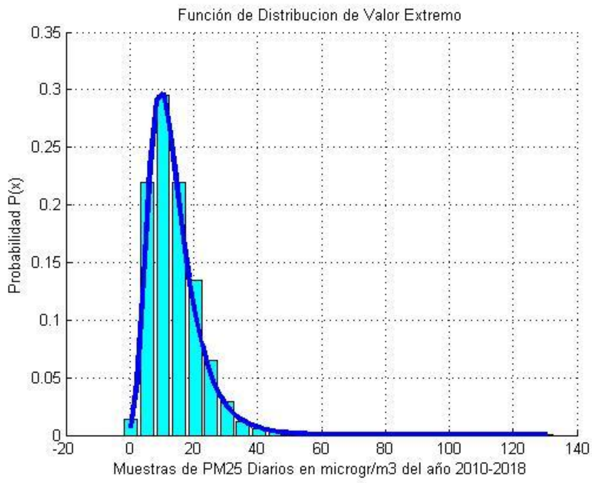
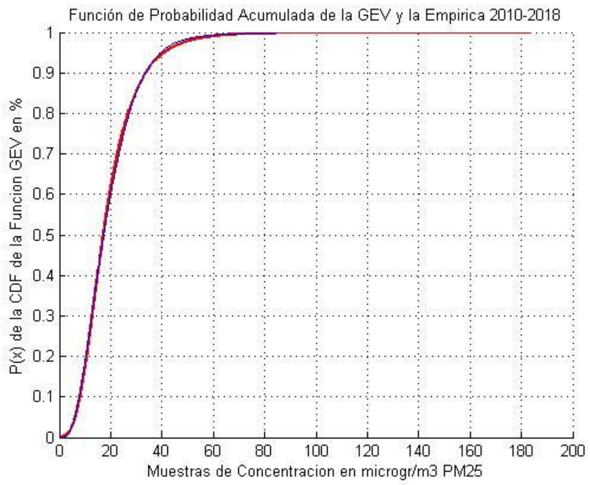
<tr><td>
</td><td>
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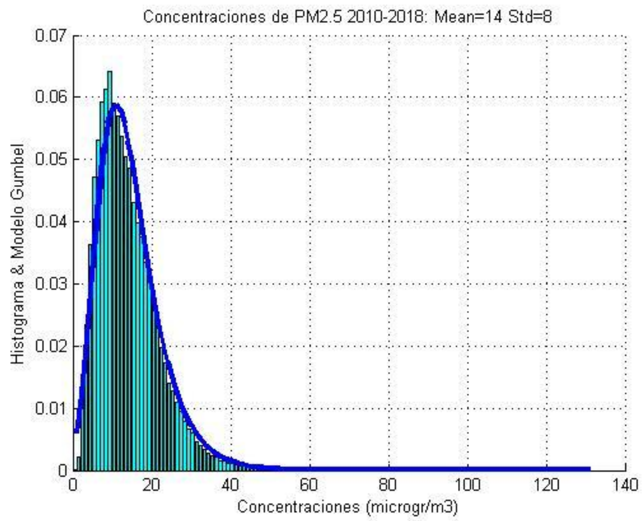
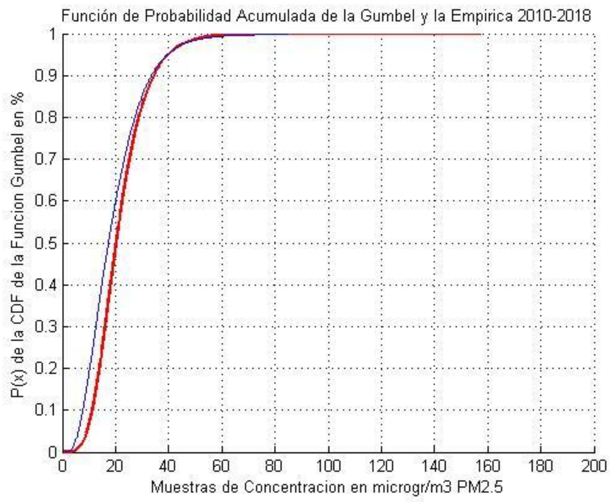
<tr><td>
</td><td>
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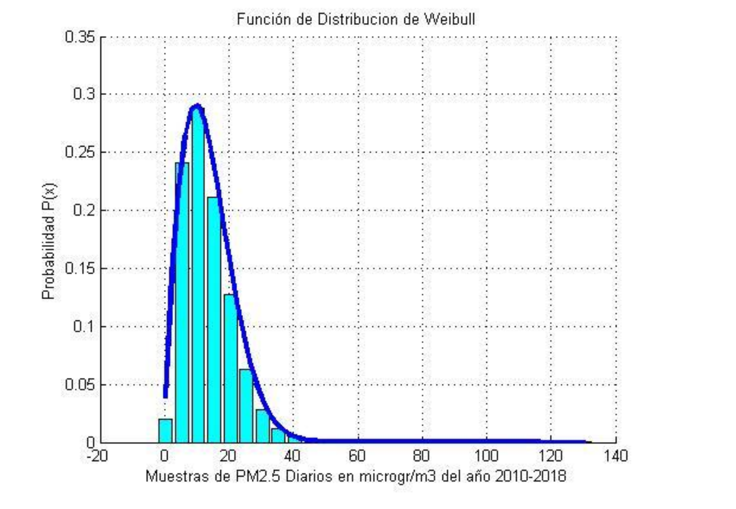
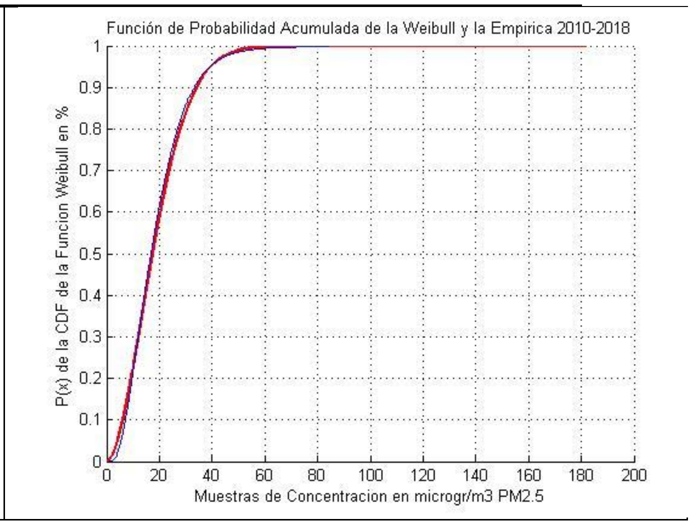
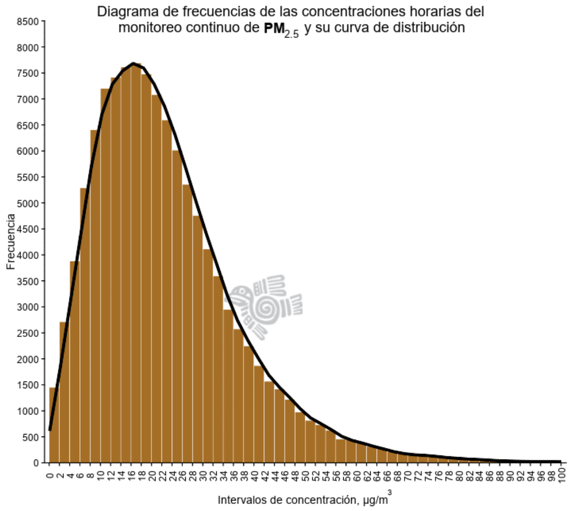




Comparing Against the Data Shown from the Official Website of Mexico City.



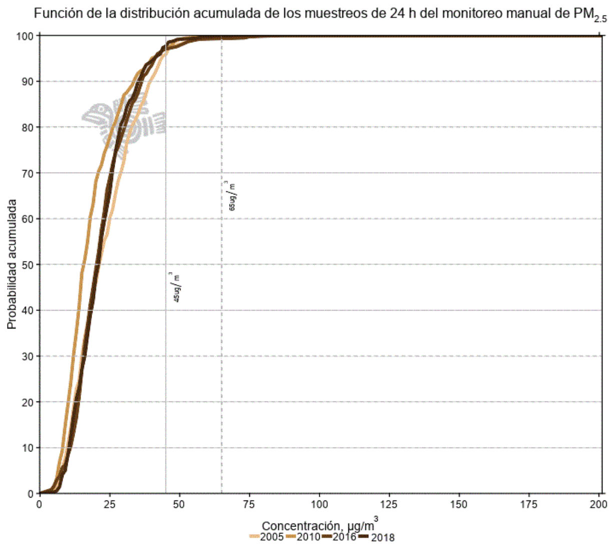
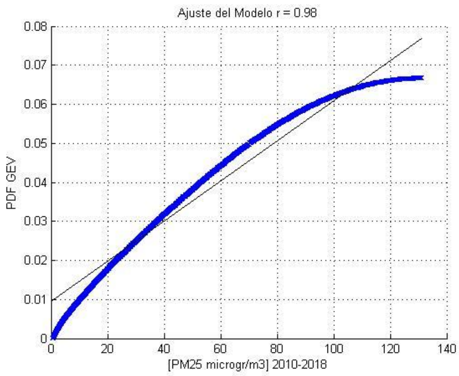
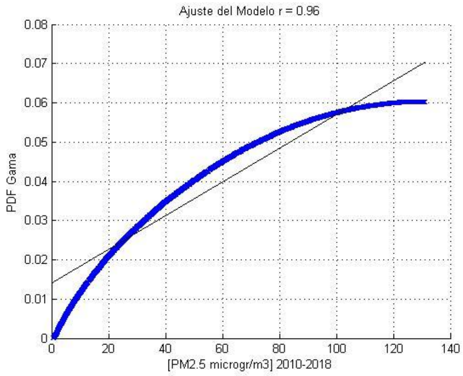
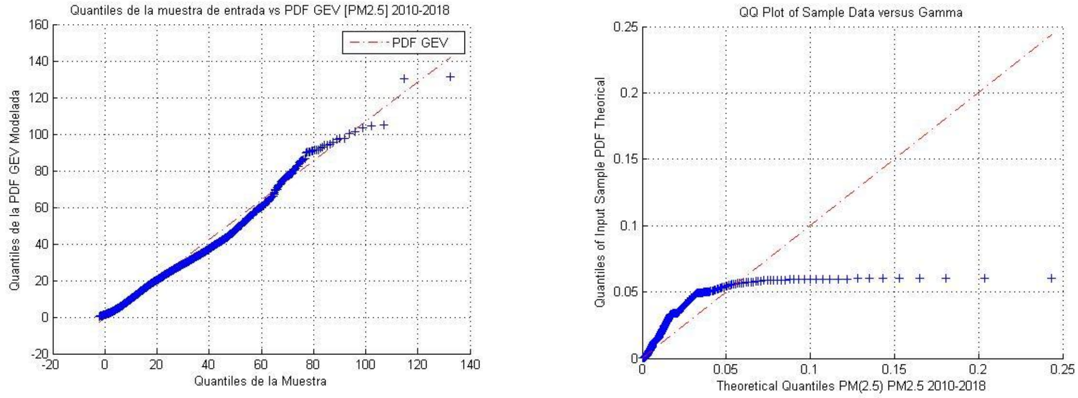


Figure 3. Histogram of the Concentration of PM2.5 in **µ**gr/m^3 and the FDC in Mexico City Trend 2010-2018 (Source: **http://www.aire.cdmx.gob.mx**)

GEV and Gama Adjustment Data Graphics







Graphs of the Gumbel (EV) and Weibull Fit Data

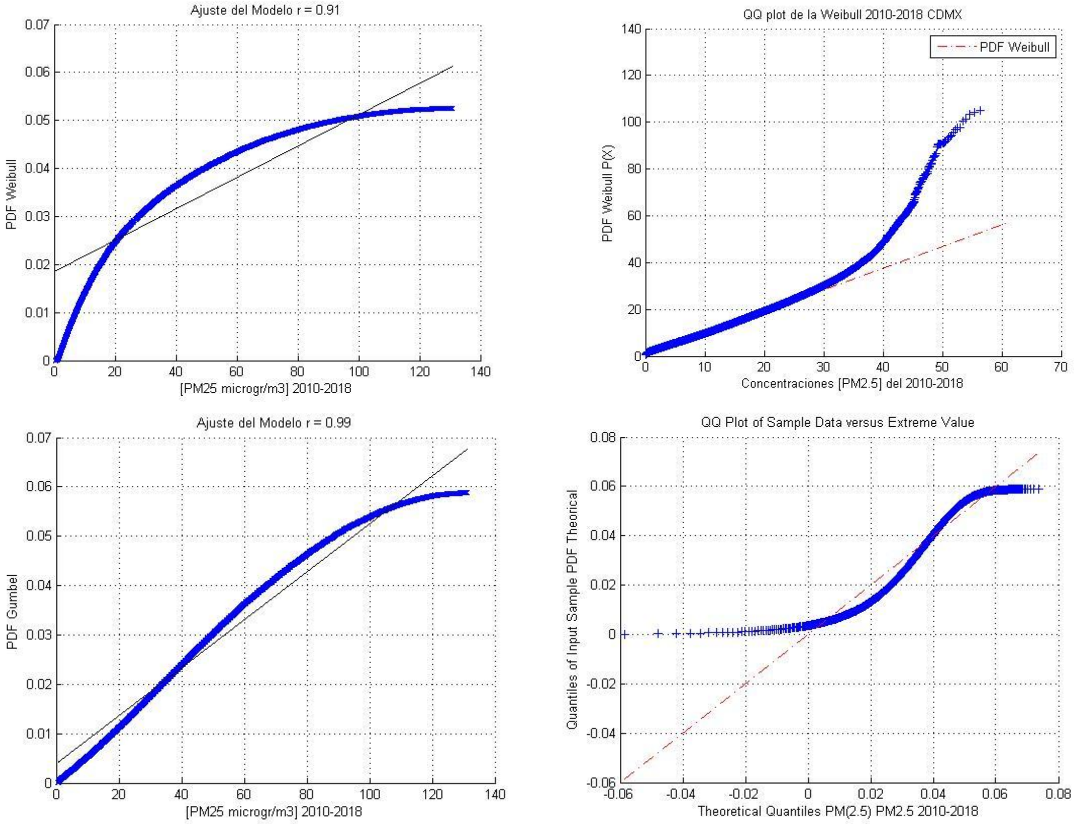


Figure 4.Graph of the adjustment and QQ plot of the GEV model, Gama, Gumbel and Weibull of the Concentration of PM2.5 in μgr/m^3, Mexico City Trend 2010-2018.

TheLastYear 2018

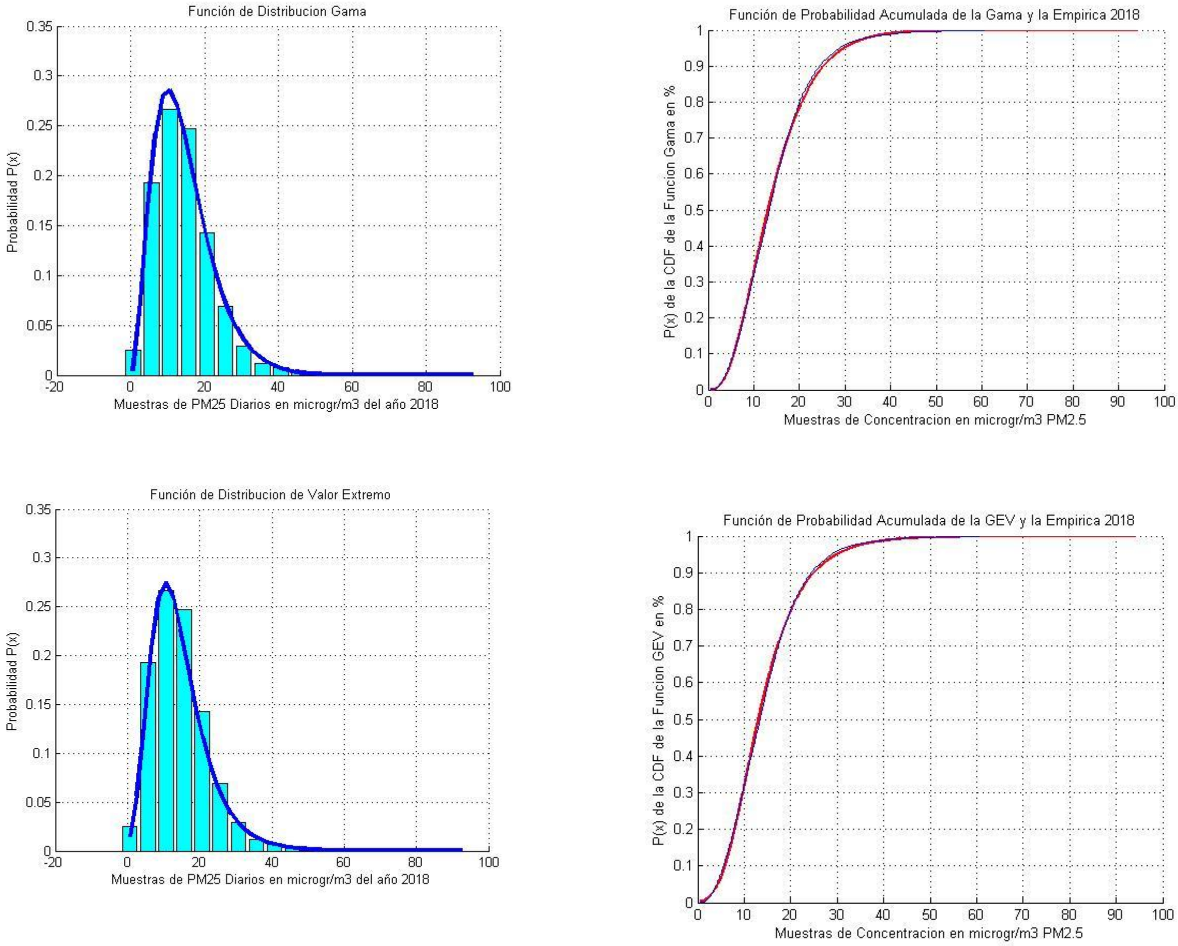


Figure 5.Graphic of the adjustment of the GEV and Gama Model Concentration of PM2.5 in **μ**gr/m^3 and its CDF, Mexico City of 2018.

Analysis of Trend of the PM2.5 of the Mexico City 2010-2018

Table 5. Average of the Adjustments of the Tendency was included the Weibull 2010-2018

Trend Years	AveragePM2.5 μgr/m^3 aprox. http://www.aire.cdmx.gob.mx	Mean GEV PM2.5 μgr/m^3	Mean Weibull PM2.5 μgr/m^3	Mean Gama PM2.5 μgr/m^3
2010	18	19.7103	19.7613	19.6658
2011	20	18.9931	19.0419	18.9895
2012	21	20.2941	20.3533	20.2902
2013	23	23.1892	23.2672	23.1815
2014	18	18.4819	18.5401	18.4783
2015	22	16.9081	16.7433	16.9053
2016	22	16.0381	16.0879	16.0238
2017	22	15.5354	15.5915	15.5593
2018	22	14.55	14.33	14.54

Daily Maximum Concentrations of PM2.5

In the previous table we can see the trend that is decreasing and the comparison is made against the data obtained from the official website of Mexico City. An analysis is now made to observe its trend within the period using the method of obtaining new functions of Normal Probability Distribution and Extreme Value by Bayesian Inference to data of Daily Maximum Concentrations, which have a skewed Gaussian behavior, see in [18] we can also see if with a function of the GEV type one with greater variance than the other obtained, the concentration will decrease or increase.

The New GEV or GEV One and Two are found with the following expressions

$$\boldsymbol{GEV}\left(\sum_{i=1}^{n}\frac{\boldsymbol{\mu_i}}{\boldsymbol{n}},\frac{\mathbf{1}}{\boldsymbol{n}-\mathbf{1}}\sum_{i=1}^{n-1}\boldsymbol{\sigma_i}\ ,\boldsymbol{k}\right) \tag{1}$$

With

$$\boldsymbol{k} > 0 \quad x \in \left[\boldsymbol{\mu} - \frac{\boldsymbol{\sigma}}{\boldsymbol{k}}, +\infty\right] \qquad\qquad k < 0 \quad x \in \left[-\infty, \mu - \frac{\sigma}{k}\right]$$

New GEV

$$\boldsymbol{k} = \left(\frac{\boldsymbol{GEVk} + \boldsymbol{GEVkA}}{\sum_{i=1}^{2}\boldsymbol{pn}}\right) \tag{2}$$

$$\boldsymbol{Sigma} = \left(\frac{\boldsymbol{GEVsd} + \boldsymbol{PostSD}}{\sum_{i=1}^{2}\boldsymbol{pn}}\right) \tag{3}$$

$$\boldsymbol{Mu} = \left(\frac{\boldsymbol{GEVmu} + \boldsymbol{Postmean}}{\sum_{i=1}^{2}\boldsymbol{pn}}\right) \tag{4}$$

This expression was the one that worked best, approaching the function of distribution of input, through the Bayesian Inference we are looking for the values above the official standard of annual average concentration.

Table 6. Means of Trend Adjustments 2010-2018

Year	PDF Gaussiana	New GEV	Estimators Statistics of the Gaussian	Estimators Statistics of the New GEV
2010	Mean=13.05 sdt=6.10	k =-0.1816 sigma =5.17 mu = 11.62 Mean =13.80	MSE = 0.0011 RMSE = 0.032 AP=0.985 ÍA=0.997 $\boldsymbol{R}^2$=0.9900	MSE =0.0023 RMSE= 0.0490 AP= 0.5304 ÍA= 0.9874 $\boldsymbol{R}^2$=0.86
2011	Mean=15.22 sdt=6.02	k =-0.2287 sigma =5.38 mu =13.85 Mean =15.95	MSE = 0.00051379 RMSE = 0.0227 AP=0.9740 $\boldsymbol{R}^2$=0.9971 ÍA=0.9990	MSE =0.00088966 RMSE= 0.0302 AP= 0.9805 ÍA= 0.9933 $\boldsymbol{R}^2$=0.85
2012	Mean=19.82	k = -0.2433	MSE = 0.00027592	MSE =0.00049893

	sdt=6.64	sigma =6.09 mu =18.2885 Mean = 20.59	RMSE = 0.0166 AP=0.9700 $\boldsymbol{R^2}$=0.9977 ÍA=0.9994	RMSE= 0.0226 AP= 1 ÍA= 0.9927 $\boldsymbol{R^2}$=0.88
2013	Mean=22.40 sdt=8.74	k =-0.2358 sigma =7.84 mu =20.1873 Mean = 23.19	MSE = 0.00061524 RMSE = 0.0252 AP= 0.9696 $\boldsymbol{R^2}$=0.9969 ÍA=0.9989	MSE =0.0008826 RMSE= 0.0302 AP= 1 ÍA= 0.9907 $\boldsymbol{R^2}$=0.9
2014	Mean=19.12 sdt=7.07	k=-0.2410 sigma =6.45 mu =17.443 Mean =19.89	MSE = 0.0002276 RMSE = 0.0157 AP= 0.990 $\boldsymbol{R^2}$=0.9976 ÍA=0.99	MSE =0.0005734 RMSE= 0.0238 AP= 0.7023 ÍA= 0.9957 $\boldsymbol{R^2}$=0.9
2015	Mean=19.50 sdt=8.27	k =-0.2048 sigma = 6.89 mu =17.2495 Mean =20.04	MSE = 0.0009697 RMSE = 0.0312 AP= 0.94 $\boldsymbol{R^2}$=0.99 ÍA=0.9977	MSE = 0.0023 RMSE= 0.0480 AP= 0.6598 ÍA= 0.9924 $\boldsymbol{R^2}$=0.78
2016	Mean=18.59 sdt=8.27	k=-0.2178 sigma = 7.13 mu = 16.40 Mean =19.23	MSE = 0.0006312 RMSE = 0.0252 AP= 0.9521 $\boldsymbol{R^2}$=0.9963 ÍA=0.9986	MSE = 0.0010 RMSE= 0.0322 AP= 0.7844 ÍA= 0.9962 $\boldsymbol{R^2}$=0.81
2017	Mean=18.21 sdt=7.05	k=-0.2694 sigma =6.636 mu =16.68 Mean =19.08	MSE = 0.0002111 RMSE = 0.0146 AP= 0.999 $\boldsymbol{R^2}$=0.9956 ÍA=0.99	MSE = 0.0002051 RMSE= 0.0145 AP= 0.8673 ÍA= 0.99 $\boldsymbol{R^2}$=0.96
2018	Mean=16.50 sdt=6.38	k =-0.2249 sigma =5.74 mu =15.03 Mean =16.59	MSE = 0.00071506 RMSE = 0.0268 AP = 0.9659 $\boldsymbol{R^2}$= 0.9946 IA = 0.9987	MSE = 0.0020 RMSE = 0.0458 AP = 0.7538 $\boldsymbol{R^2}$= 0.8732 IA = 0.9960

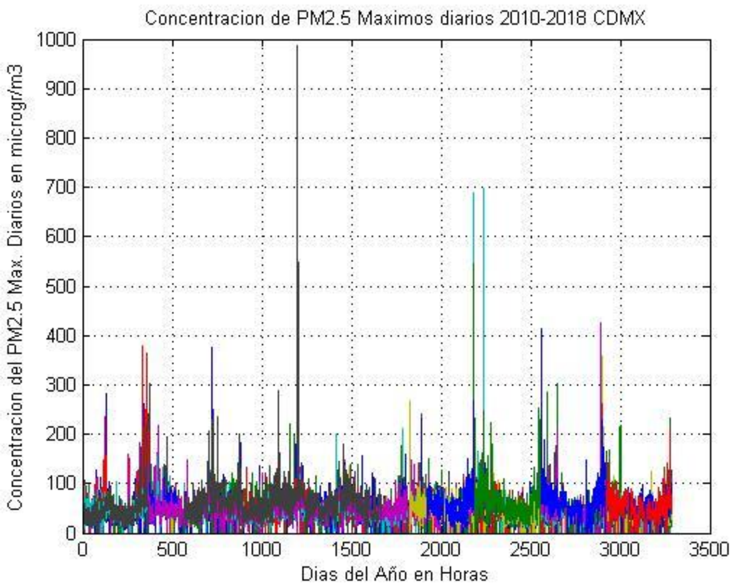


Figure 6.Concentration Time Series PM2.5 $\mu gr/m^3$ Mexico City 2010-2018.

Graphics of Gaussian and GEV obtained

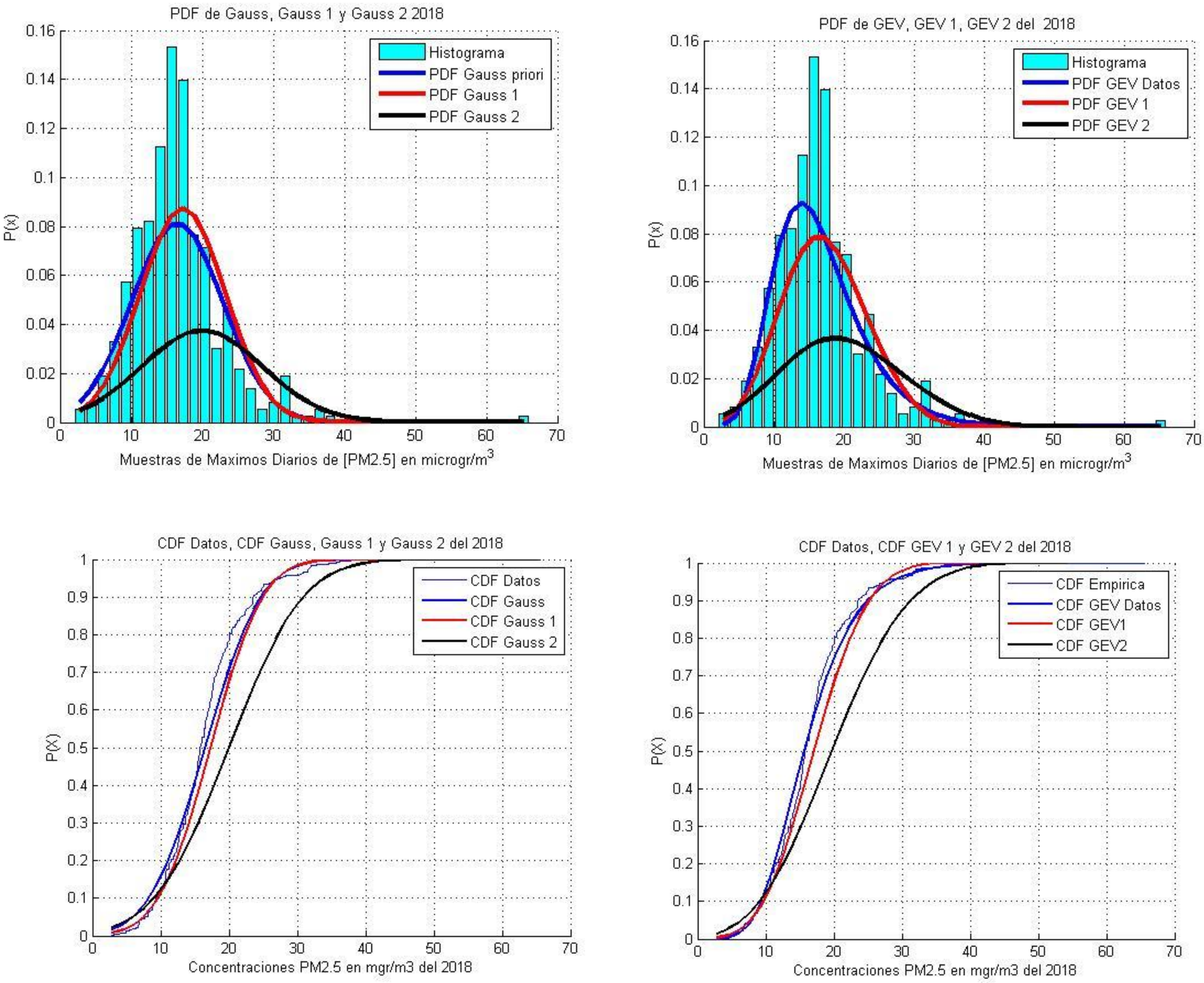


Figure 6.Graphic of the adjustment of the GEV and Gama model Concentration of PM2.5 in **µ**gr/m^3 and its CDF, Mexico City of 2018.

Statistics of the Maximum Concentrations of PM2.5**µ**gr/m^3

Mean = 15.17**µ**gr/m^3

Std = 6.82**µ**gr/m^3

Máximum = 100**µ**gr/m^3

Mínimum = 2.5**µ**gr/m^3

Variance = 46.70**µ**gr/m^3

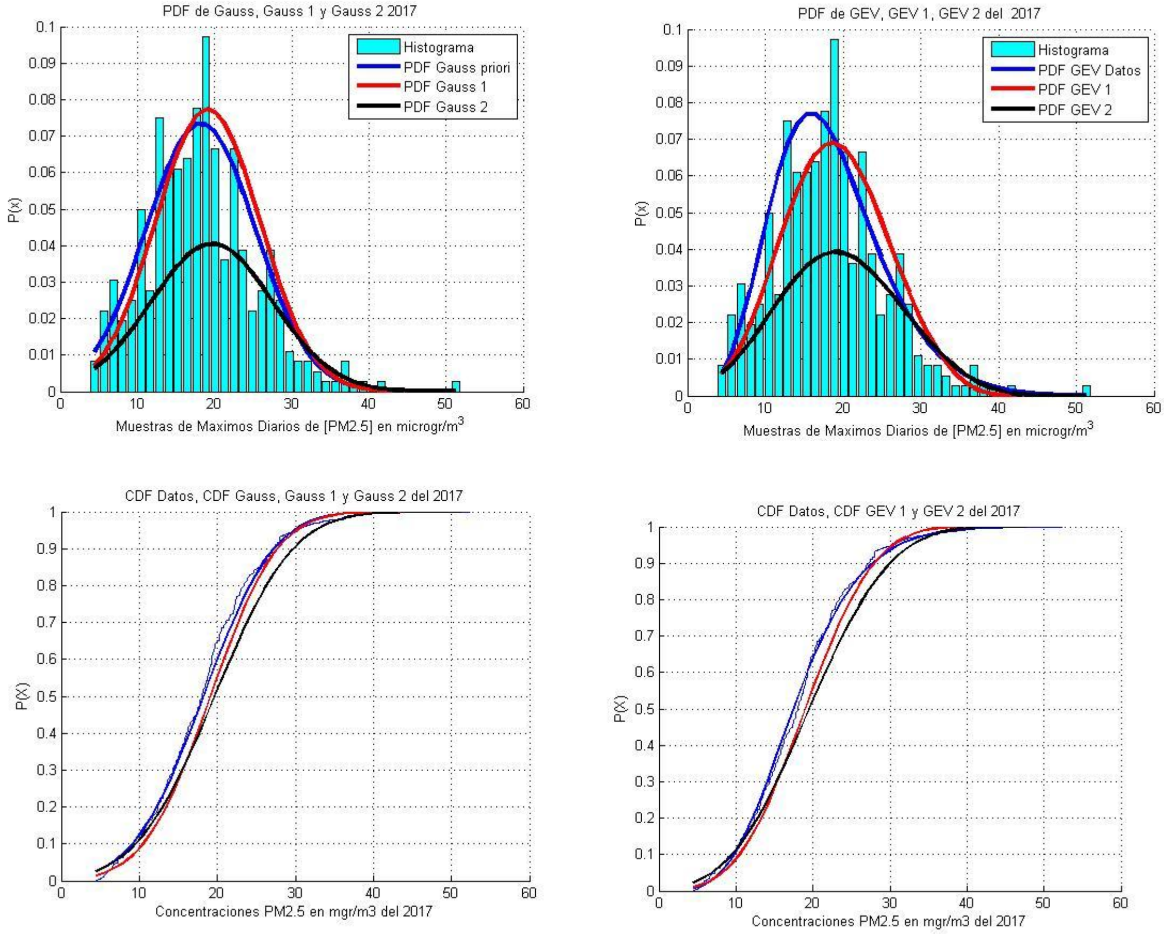
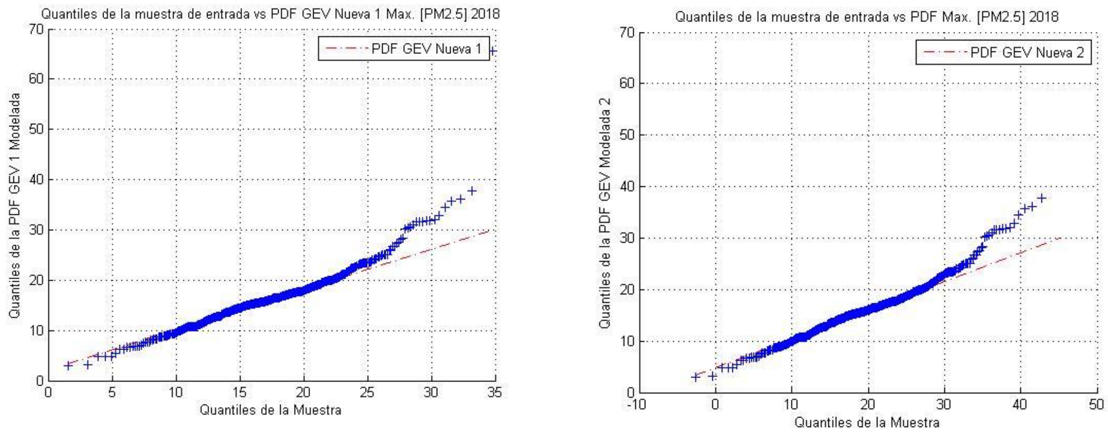


Figure 7. Graphic of the adjustment of the GEV and Gama model Concentration of PM2.5 in µgr/m^3 and its CDF, Mexico City of 2018



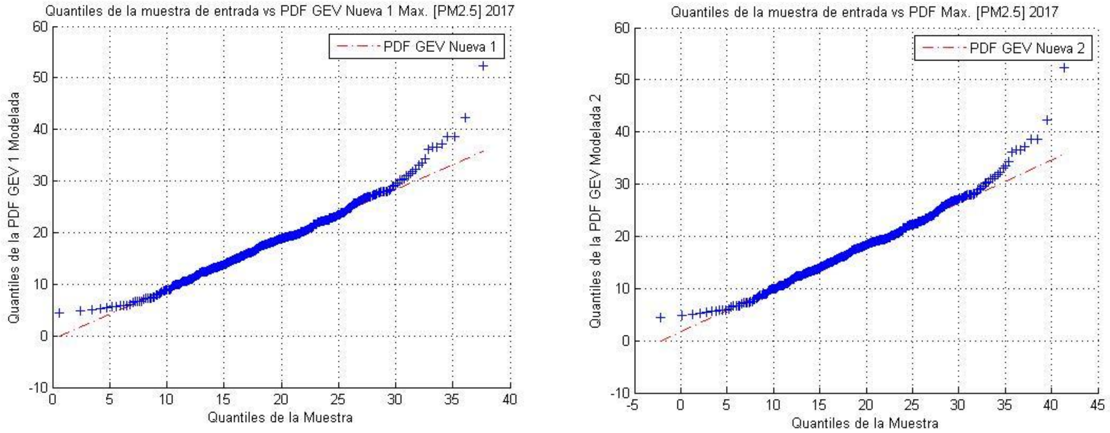


Figure 8.Graph of the QQ plot adjustment of the GEV and Gama model Concentration of PM2.5 in **μ**gr/m^3 and its CDF, Mexico City 2017.

In these screen shoots with the Fit Distribution tool program in Matlab we can see that the data of Maximum Daily of PM2.5 the pdf GEV is very similar to the New GEV found, which we can make a comparison between the improvement of the New GEV.

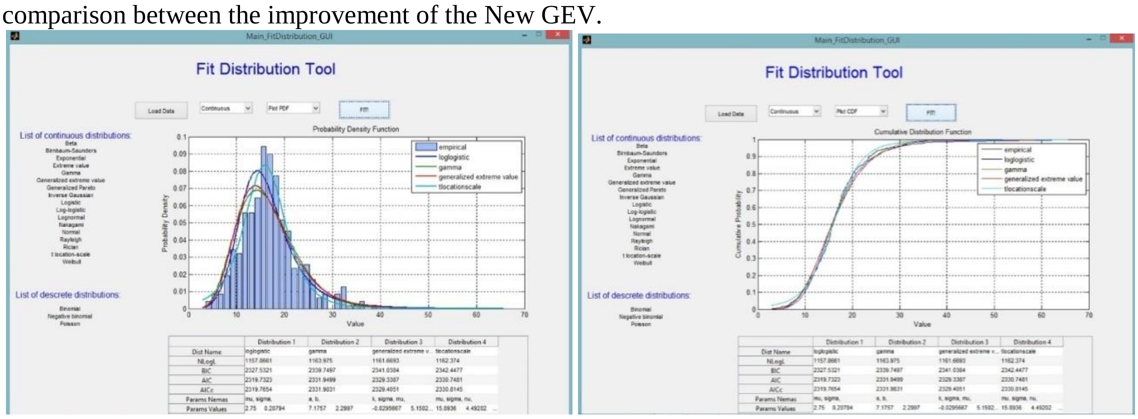


Figure 9. Graph of the adjustment of the GEV model (Red) of the Concentration of PM2.5 Maximos daily in **μ**gr/m^3 and its CDF, Mexico City of 2018

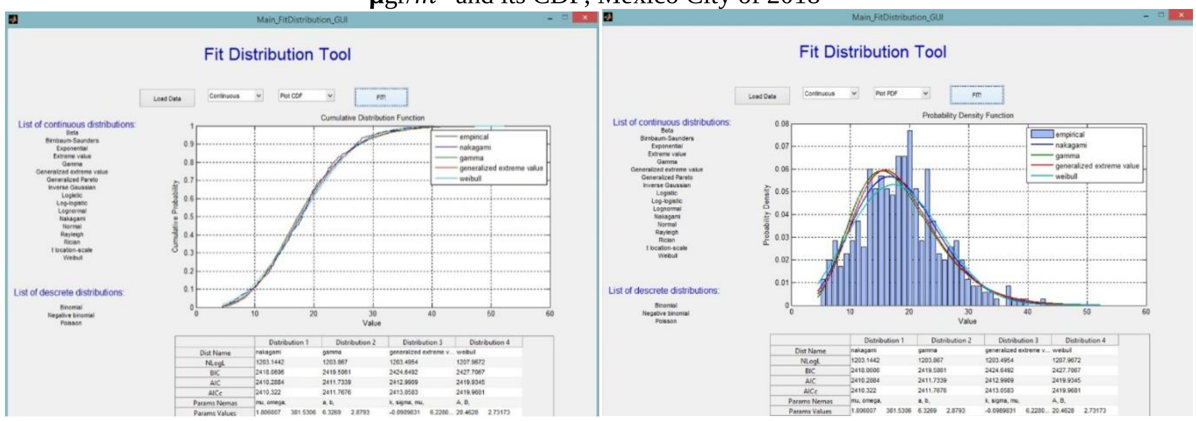


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Figure 10.Graphic of the adjustment of the GEV model (Red) of the PM2.5 Concentration Maximos daily in **μ**gr/m^3 and its CDF, Mexico City of 2017.

We also compared the result against the Bayesian Model for a mean and standard deviation unknown, using the Gamma Inverse pdf [19] as a forecast to observe the new Means of the Maximum daily of PM2.5, use the Gibbs Sampling within the algorithm, with very optimal results, thus corroborating the method approach [18] for the New GEV which both gave good approximation that were found for these almost Gaussian data, both techniques were satisfactory, although the GEV follow the trend of the modeled data and the pdf of the Gamma Inverse forecasts the parameters that we want to obtain.

Year	PDF IGamma
2010	Alfa = 2.02 Beta =13.38
2011	Alfa = 2.03Beta =15.75
2012	Alfa = 2.04Beta =20.79
2013	Alfa = 2.03Beta =23.21
2014	Alfa = 2.04Beta =19.89
2015	Alfa = 2.03Beta =20.10
2016	Alfa = 2.02 Beta =19.10
2017	Alfa = 2.03Beta =18.89
2018	Alfa = 2.03Beta =17.10

Comparando la Tendencia con el Grafico de la pagina Oficial de la Ciudad de Mexico

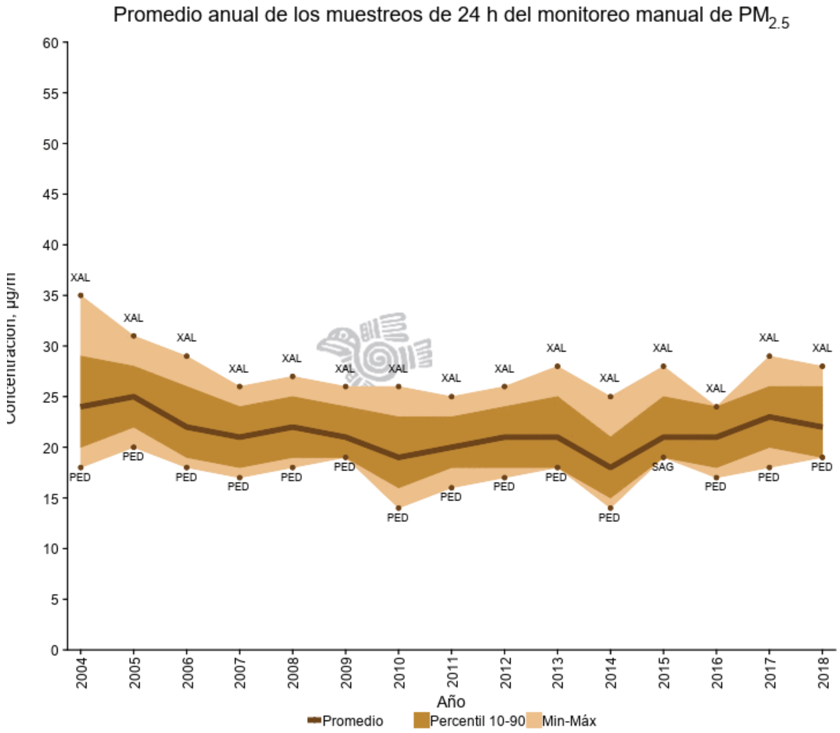

Figure 8. Graph of Concentration of PM2.5 (Source: **http://www.aire.cdmx.gob.mx)**

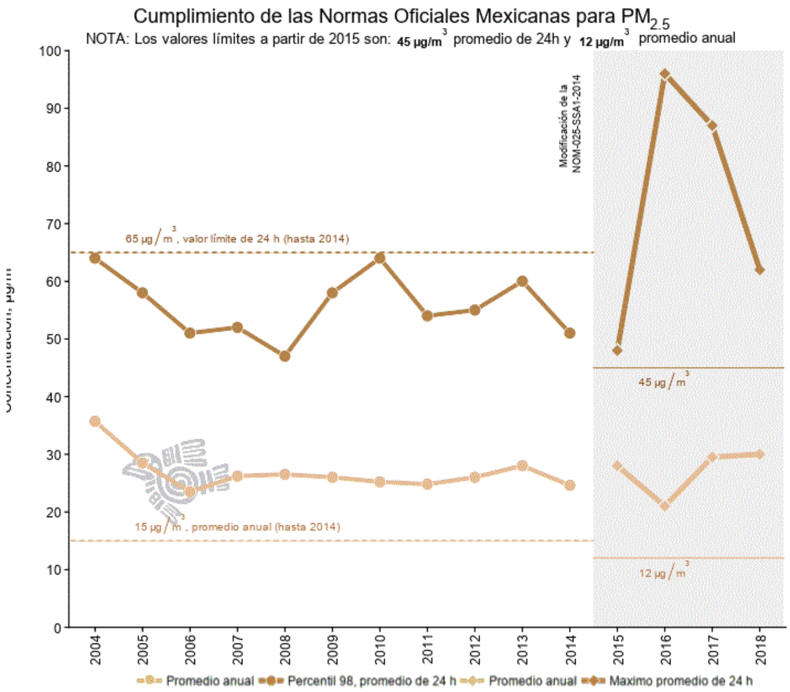

Figure 9. Graph of Concentration of PM2.5 (Source: http://www.aire.cdmx.gob.mx)

Table 7.Means for the Daily Maximum of PM2.5 of Mexico City found and compared to the annual averages of the 24-hour samplings, we also find that the annual average of 12 **µgr/m^3** is exceeded. http://www.aire.cdmx.gob.mx

PDF Gaussian 2010 in µgr/m^3	**New GEV µgr/m^3**	**Average PM2.5 µgr/m^3 aprox.**	**New GEV 2 in µgr/m^3**	**IGamma Model MeanForecast**
Mean=13.05 sdt=6.10	Mean =13.80	18	Mean =16.53	Mean= 13.054
PDF Gaussian 2011 in µgr/m^3	New GEV			
Mean=15.22 sdt=6.02	Mean =15.95	20	Mean=19.00	Mean= 15.22
PDF Gaussian 2012 in µgr/m^3	New GEV			
Mean=19.82 sdt=6.64	Mean = 20.598	21	Mean=22.06	Mean= 19.82
PDF Gaussian 2013 in µgr/m^3	New GEV			
Mean=22.40 sdt=8.74	Mean = 23.1987	23	Mean=25.25	Mean= 22.40
PDF Gaussian 2014 in µgr/m^3	New GEV			
Mean=19.12 sdt=7.07	Mean =19.8991	18	Mean=21.99	Mean= 19.12
PDF Gaussian 2015 in µgr/m^3	New GEV			
Media=19.50 sdt=8.27	Mean =20.047	22	Mean=27.03	Mean= 19.50
PDF Gaussian	New GEV			

2016 in µgr/m^3				
Mean=18.59 sdt=8.27	Mean =19.23	22	Mean=25.19	Mean= 18.59
PDF Gaussian 2017 in µgr/m^3	New GEV			
Mean=18.21 sdt=7.05	Mean =19.0804	22	Mean=19.65	Mean= 18.21
PDF Gaussian 2018 in µgr/m^3	New GEV			
Mean=16.50 sdt=6.38	Mean =16.59	22	Mean=19.50	Mean= 16.50

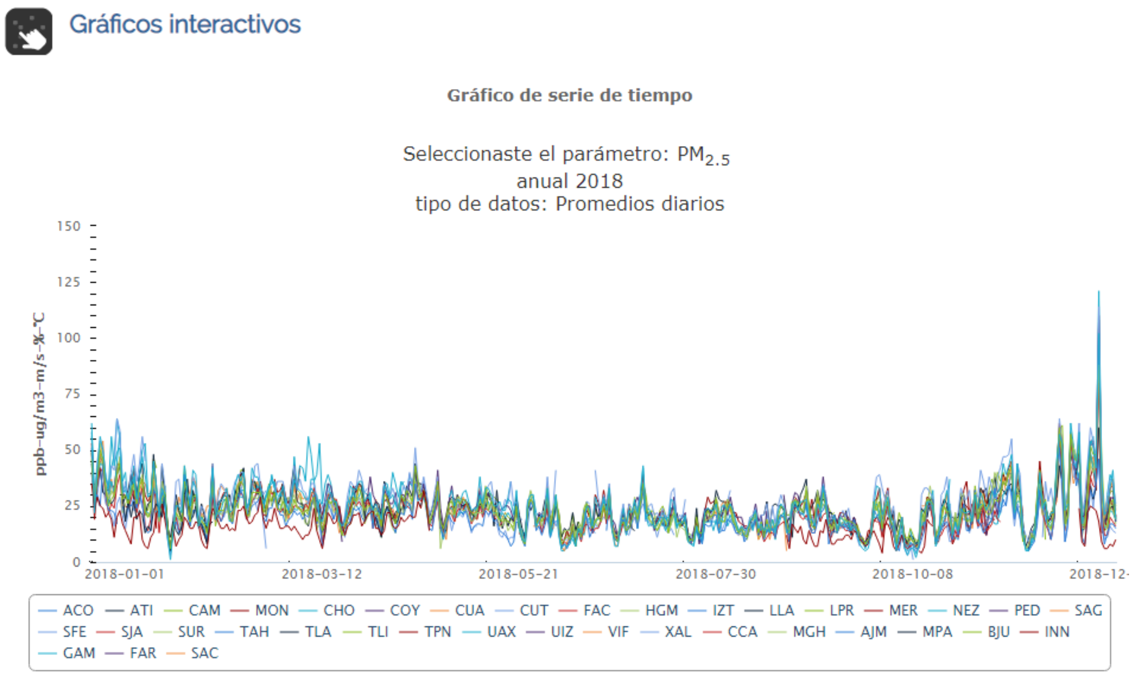

Figure 10. Consultation of daily averages of PM2.5 2018 of Mexico City(Source: http://www.aire.cdmx.gob.mx/)

Conclusions

With this study it was verified which type of probability distribution function was the most adequate for the behavior of daily data of PM2.5 which were with the best adjustment the pdf GEV and the pdf Gama, is comparative with the adjustment given by the official page of the Mexico City, these functions of distribution are part of the Theory of Extreme Value, for events of this nature.

With the trend analysis we used the methodology proposed in [18], for data with Gaussian behavior, which for maximum ozone data is perfectly coupled, in this case it was used for the maximum data of PM2.5 which also adjusted but in a biased way, almost Gaussian data up to a certain point, if the maximum data are adjusted and give a good obtaining of the data that we want to look for as the average for the generated functions, both normal and the GEV, giving us approximate results and comparative with the graph of the page of the mexico city. We can also see in the QQ plot graphs that the new pdfs New GEV and New GEV 2 adjust to more extreme concentrations, can see the histogram next to the adjusted pdf as it touches those points while the GEV does not always touch them, this makes each one have a different variance giving us good approximations of each.

It was also found that the tendency of the concentration of PM2.5 is above the annual average, that is not good according to the standards of the established norms of the air quality in the city, but the tendency of the concentration goes downward.

The New Air Quality Standard for Mexico City is also given, in the following link: NADF-009-AIRE-2017 (http://www.aire.cdmx.gob.mx/default.php?ref=Z2Q=)

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