18th World IMACS / MODSIM Congress, Cairns, Australia 13-17 July 2009
http://mssanz.org.au/modsim09

Asynchronous Evolutionary Modeling for PM_{10} Spatial Characterization

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Abstract: One of the main questions, describing the behavior of a pollutant in the atmosphere, is determining its concentration in some point within a study area, where we come across areas that are difficult to access and where it is impossible to carry out measuring campaigns, or where it is not known with certainty how and in which form the discharge of a pollutant from a source occurs. This without counting, that there is little information, that a group of *m_monitoring* stations, which monitor the quality of the air, provides about the spatial behavior of the phenomenon. To overcome these problems in an integral way, this article proposes and analyzes a computational model, based on the principles of *evolutionary computation* (EC), in order to determine the behavior in terms of space and time of the concentration of the particulate matter PM_{10} within a defined area. The model consists of a solution structure or individual with two *submodels* or *genetic substructures* that in turn determines two evolutionary submodels that evolve in an asynchronous manner: an estimate *submodel* which permits to know the emissions in *n_sources* based on the principles of a *BGPT* model (*Backward Gaussian puff Tracking*) from *m_monitoring* stations in an inverse way, and a spatial interpolation submodel of the type *Takagi Sugeno NUPFS* (*Non Uniform puffs Functions*) in order to determine the spatiotemporal behavior in terms of the analytic representation that defines each one of the puffs emitted from each one of the considered *n_sources*. In accordance with this structure, the asynchronous evolution mechanism is given mainly by the dependence that the *interpolation submodel* presents with respect to the *estimate submodel*, as this fixes and defines the base functions or *NUPFS* that serve as a base for the interpolator. The proposed evolutionary model was validated using for the estimate a series of concentration measurements for PM_{10}, which were taken starting from a group of *m_monitoring* stations, which monitor the quality of the air, and starting from a series of *n_selected* spatial sources within the study area. For the case of the spatial validation, a series of analytic surfaces of concentration for PM10 were obtained from the interpolation model. Each of these surfaces was duly validated by using the CALMET/CALPUFF model and it was validated for each measurement campaign. In this way, the proposed evolutionary model allowed to determine the spatial behavior of the concentration for PM_{10} in a dynamic way over time, mainly due to the construction which the estimate model uses of the *NUPFS* base functions applied by the interpolator with reference to the phenomenon.

Keywords: *BGPT (Backward Gaussian puff Tracking), Evolutionary Computation (EC), Lagrangian puff Model (LGP), Environmental Modeling, Takagi Sugeno (TKS), macropuffs (Non Uniform puff Functions - NPFS)*

1. INTRODUCTION

One of the main concerns when it comes to mitigating the effects of concentration for PM10 particulate material in a study area is to determine their spatial distribution over time. In order to determine this behavior, a series of mathematical and physical constraints are presented, which from a physical point of view, are determined by the quantity of available monitoring stations for air quality, or by the inability to carry out massive measurements, that allow to identify the behavior of the contaminant over time, especially in areas where access is difficult. From a mathematical point of view, these constraints extend from a spatiotemporal representation of the concentration through the estimation of the emission source, the type of pollutant, and how and in which form a discharge of PM10 can affect a particular point in the area (Aceña et al., 2007), (Martin et al., 2007). To solve this problem, geostatistics and computational intelligence have developed a variety of methods of representation and interpolation, which in many cases do not adjust to the modeling of a specific phenomenon, mainly due to the size and quality of the initial sample of points that represent a phenomenon in a study area (Cruzado, 2004), which in the case of atmospheric phenomena, may cause that the set of points of concentration for PM10 suffer dynamic changes over time. That is why methods are required that conduct search, adaptation or have memory, so that they can generate a number of surfaces over time in terms of the phenomenon that enable decision-making with regard to the mitigation of the impact of this pollutant .

Having said this, different models for solving the problem of estimating emissions at the source have been developed, among them, the models proposed by (Lundquist et al., 2005) stand apart, who makes a reconstruction of the emission starting from the design of monitoring networks using the UDM model and two models proposed by Allen (Allen et al. 2007 (a)), one for optimizing variables, using genetic algorithms based on the model SCIPUFF, and a second model (Allen et al. 2007 (b)) based on genetic algorithms and a Gaussian plume model to estimate the position, the emissions and the source size plus the wind field, all this from a set of concentration values obtained from a set of theoretical monitoring stations uniformly distributed in a study area. Also the work of (Kyats et al., 2007) stands out, which uses a Bayesian inference model for the reconstruction of emissions from a set of monitoring stations. Similarly (Monache et al., 2007) proposed a model of Bayesian inference, but in this case to rebuild emissions on a continental scale. However, one can observe a significant absence of spatial models, that would allow us to determine the concentration of a pollutant in a study area analytically, incorporating elements specific to the physical phenomenon of dispersion, mathematical elements that are specific to the representation and spatial interpolation and computational elements that are specific to learning, adaptation or memory (CISTI-Symposium-2009).

In this article a computational model which is based on the principles of the Evolutionary Computation (EC) will be developed and analyzed in order to determine the spatiotemporal behavior of the concentration of the particulate matter PM10 within a research area. The integrated model consists of two sub-models that defines two genetic substructures of the solution, a first genetic substructure which permits to estimate the emissions in *n-sources* starting from *m-monitoring* stations that measure the quality of the air, accordingly to a LPG model (Martin et al., 2007) and based on the principles of a model BGPT (Israelsson et al. 2006). In this first stage the construction of a series of *macropuffs* functions or NUPFS functions (Non Uniform Rational Basis Functions) is carried out with respect to concentration of *puffs* in space. A second genetic substructure, establishes a fuzzy model of the spatial interpolation TSKN (Takagi Sugeno NUPFS) (Hernandez and Pena, 2007b), (Hernandez and Pena, 2005), (Sanchez et al., 2005) which permits to determine analytically the spatial behavior of the concentration in terms of the phenomenon (EvoStar2009).

In order to develop this model, there are a number of mathematical concepts that allow the estimation of emissions at the source in terms of a model BGPT (Israelsson et al. 2006), (Aceña et al., 2007), as well as concepts that define a fuzzy model for an adaptive interpolation (Peña and Hernández, 2007b). Subsequently, the solution structure or *individual* will be defined in accordance with each of the sub-models which in turn define two *genetic* substructures in the individual. The transformation of the solutions over time, which lasts a measurement campaign, will progress through an asynchronous evolution, mainly due to the dependency which the genetic substructure of interpolation demonstrates and due to the genetic estimation substructure, which permits the construction of the base functions of the interpolator or NUPFS. Finally, the proposed evolutionary model will be validated in two stages determined by each substructure using the model CALMET/ CALPUFF against a series of measurement campaigns carried out in a study area (EvoStar2009).

2. DEFINITION OF THE MODEL

The proposed evolutionary model will be determined by a solution structure or individual, which will have two integrated models or genetic substructures, a substructure for the estimation of emissions in each of the considered *n-sources*, and by the construction of a series of *macropuffs* or *NUPFS* functions, which allow to determine the concentration of puffs in the study area with reference to the phenomenon. A second substructure will be determined by a fuzzy TKSN model of spatial interpolation in terms of each of the base functions obtained during the estimation process. The transformation of the solutions will be given through an asynchronous evolution algorithm, due to the dependency of the interpolation representation submodel, presented with respect to the estimation submodel.

2.1. Genetic substructure of Estimated Emissions:

The general problem of estimating emissions is defined in equation (1) (Martín et al., 2007):

$$C\left(x_j, y_j, z_j, k\right) = \sum_{k=1}^{np}\sum_{i=1}^{nf} Q_i * \phi\left(x_{o,i,k}, y_{o.i.k}, x_j, y_j\right) * G\left(z_{o.i.k}, z_j\right) \tag{1}$$

Where,

$C_c\left(x_j, y_j, z_j, k\right)$: Concentration measured in the monitoring *station j*, in the instant *k* [gr/m^3].

Q_i: Quantity of pollutant contained in each of the emitted puffs [*gr*]

nf: Number of sources. *i=1,2,3,………nf*

ne: Number of monitoring stations*;* *j=1,2,3,……..ne*

np: Number of *puffs* emitted by each of the *i-sources*. *k=1,2,3,…..,np*

x_j, y_j, z_j: Location of each monitoring station within the research area indicated by the coordinates UTM_x, UTM_y, MSL (*meters sea level*) [m].

$\phi\left(x_{o,i,k}, y_{o.i.k}, x_j, y_j\right)$: Size and location of the *puffs* in each instant *k* of time.

$G\left(z_{o.i.k}, z_j\right)$: Reflections one puff with the earth surface and the inversion thermal layer

The genetic substructure for the estimation is given as follows:

Q_1	Q_2	Q_3	…………..	Q_n	K_{11}	K_{12}	K_{13}	……………	K_{1n}	K_{2n}	K_{3n}	*BDL*

Where

BDL: Height of the layer for the initial mix in the research area [m].

K_{1i}: Factor that depends on the information about the size of the source i [m^2].

K_{2i} : Multiplier which depends on the information available about the flow volume of the emitted gases for source i [m^2/s]

K_{3i} : Multiplier which depends on the quantity of pollutant emitted [gr/m^3] by source i.

$$FA = \frac{Ke}{\frac{1}{2}\left(\sum_{j=1}^{ne}\left(\sum_{i=1}^{nf}\sum_{k=1}^{np} C_{Cj}\left(xo_{i,k}, yo_{i,k}, zo_{i,k}\right)\right) - C_{Bj}\left(x_j, y_j, z_j\right)\right)^2} \tag{2}$$

Where

$C_{Bj}\left(x_{o.i.k}, y_{o.i,k}, z_{o,i,k}\right)$: Initial concentration at the monitoring station *j*, in the instant of *k* [gr/m^3].

$C_{cj}\left(x_j, y_j, z_j\right)$: Calculated Concentration (*Submodel Estimation)*- Monitoring Station *j* [gr/m^3].

FA: Fitness Function.

Ke: Constant of proportionality.

2.2. Interpolation Representation Model - *Takagi Sugeno NUPFS* Model.

According to the estimation substructure, the construction of a series of *macropuffs* or NUPFS that indicate the concentration of *puffs* in a specific area within the study area, is carried out. Each of the *macropuffs* is analytically defined as follows:

$$\Phi\left(c_{i,x}, c_{i,y}, x_j, y_j\right) = \frac{1}{(2\pi)^{3/2}\sigma_x\sigma_y} Exp\left[-\frac{1}{2}\left[\left(\frac{c_{i,x} - x_j + k_{i,x}}{\sigma_x}\right)^2 + \left(\frac{c_{i,y} - y_j + k_{i,y}}{\sigma_y}\right)^2\right]\right] \quad (3)$$

Where:

i: Indicates the number of macropuffs determined by the interpolation representation model *i=1,2,3,….,m*.

C_{ix}, C_{iy}: Spatial location of each *macropuff or NUPF(UTM_x, UTM_y)* .

x_j, y_j: Regular partition of the space in the study area, which will be evaluated against each NUPFS (m).

k_{ix}, k_{iy}: Deformation of *macropuffs* by eccentricity (m).

In this way, in order to determine the spatial temporal behavior of the concentration for PM10, the Takagi Sugeno fuzzy model, each NUPFS or *macropuff is* separated in each axis as follows:

$$\phi_x = \left[\phi_{1,x}, \phi_{2,x}, \ldots\ldots, \phi_{m,x}\right] \qquad \phi_y = \left[\phi_{1,y}, \phi_{2,y}, \ldots\ldots, \phi_{m,y}\right] \quad (4)$$

Where:

$\phi_{i,x}$: Indicates the decomposition of each *i_macropuff* on the axis *UMT_x*.

$\phi_{i,y}$: Indicates the decomposition of each *i_macropuff* on the axis *UMT_y*.

In this way, in order to determine the analytical behavior of the spatial concentration of PM10, the equation will be given as follows:

$$PM_{10,1} = \sum_{i=1}^{np}\phi_{i,x}\left(u_{i,x}PM(i,j) + \left(1-u_{i,x}\right)PM(i+1,j)\right) \Big/ \sum_{i=1}^{np}\phi_{i,x} \qquad PM_{10,2} = \sum_{i=1}^{np}\phi_{i,x}\left(u_{i,x}PM(i,j+1) + \left(1-u_{i,x}\right)PM(i+1,j+1)\right) \Big/ \sum_{i=1}^{np}\phi_{i,x} \quad (5)$$

According to the equations mentioned above, the output value of the interpolator will be given:

$$PM_{10,s} = \sum_{i=1}^{np}\phi_{i,y}\left(u_{i,y}PM_{10,1} + \left(1-u_{i,y}\right)PM_{10,2}\right) \Big/ \sum_{i=1}^{np}\phi_{i,y} \quad (6)$$

The genetic substructure of estimation is given as follows:

C1x	C2x	………	Cnx	C1y	C2y	……….	σ 1x	σ 2x	………	σ nx	σ 1y	σ 2y	……….	σ ny

Where

Cix, Ciy: Location of each *macropuff* in the study area with coordinates UTM_x, UTM_y.

σ_{ix}, σ_{iy}: Base size of each *macropuff* considered by the interpolator.

K_{ix},K_{iy}: Parameters that indicate deformation due to eccentricity for each *macropuff.*
i=1,2,…,nx: Spatial resolution representation of the concentration on *UTM_x*.
j=i, 2,….,ny: Spatial resolution representation of the concentration on *UTM_y*.

In accordance with the DEM provided by the evolutionary model, and in accordance with the DEM of concentration delivered by the CALPUFF model, the fitness function is (11):

$$FA = 1 \Big/ \sqrt{\frac{1}{n}\sum_{i=1}^{(n+1)(m+1)}\left(PM10_d(i,j) - PM10(i,j)\right)^2} \quad (7)$$

Where
FA: Inverse RMSE (*Root Mean Square Error)* of each point that constitutes the DEM.
$PM10_d$*:* DEM *of* concentration or DEM reference – CALPUFF model.
PM10: DEM calculated by the proposed evolutionary model.

2.5 Asynchronous Mechanism of Evolution

The proposed evolutionary model consists of two sub-models, that are interrelated through a series of DEM's for PM10, emitted in each instant of time of the sampling by the estimate model. Each DEM of concentration is renewed by the interpolation sub-model, which in turn begins a process of evolution which will deliver the spatiotemporal behavior of the concentration for PM10 as a result. The evolution of these two sub-models will generate a dependency with regard to the evolution, because the initial concentration values produce the patterns of transformation of the analytic surface, which the DEM of concentration represents for PM10. The evolution process is described in the following way (Coello, 2006):

1. *Initialization:* The initial population of individuals is generated for the estimate models and for the representational and spatial interpolation. For the proposed first part of the individual the evaluation of the fitness function is carried out. The initial population is generated only once, right at the beginning.
2. *Estimate Stage:* In this stage the operator of *Stochastic Universal Selection* is used with the purpose to keep alive the genetic diversity of the population, the operator of *Crossing for an arithmetic total* with the purpose to carry out a more gradual crossing of the genes, and an operator of *Mutation* which will make the fine adjustment of the genes of an individual possible. The estimate stage delivers a DEM of concentration for PM10 as a result, for each instant in time of the sampling of air quality.
3. *Stage of Representation Interpolation:* In this stage three evolution operators are used – similar to those of the previous stage - although the mutation operator has to maintain a topology structure, which depends on the location of each of the considered *macropuffs*. This indicates that the Operator of Mutation will make it possible that the *puffs* move in a gradual way within the space (Peña and Hernández, 2005), (Peña and Hernández, 2007(a)), (Peña and Hernández, 2007(b)).

3. ANALYSIS OF THE ASYNCHRONOUS EVOLUTIONARY MODEL.

In order to analyze the behavior of the concentration in terms of space and time for PM10, a series of measurement campaigns were carried out in different study areas, comprising an area of 25* 25 km^2 with a resolution of 0.5 km for the grid, for different spatial configurations of *n-sources* and *m-stations* that monitor the quality of the air. Each campaign lasts 48 hours, while the dynamics of the LGP model are given by a series of wind fields calculated at a height of 10 m. For this analysis, we proceeded estimating emissions for every hour and in each of the sources using the metrics for the concentration of PM10 taken from each of the *m-stations* as a pattern of learning and adaptation. As a result of the asynchronous evolution a number of analytical surfaces for the concentration of PM10 with respect to the concentration of *puffs* or NUPFS within the study area were obtained. Based on the estimated emissions, the measurement campaigns that were mentioned before, were carried out using the model CALMET / CALPUFF, which resulted in a series of hourly DEM's (Digital Elevation Model) of concentration for PM10, which was evaluated with respect to the analytical surface obtained from the evolution.

For the analysis eight statistic metrics were used according to the fuzzy model proposed by Ok-Hyum (Park and Seok, 2007): Fractional Bias (FB), Normalized Mean Square Error (NMSE), Geometric Mean (MG), Geometric Variance (VG), Index of Agreement (IOA), Unpaired Accuracy of Peak (UAPC2), Within a Factor of Two (FAC2), Mean Relative Error (MRE), where each of the metrics assumes a qualitative fuzzy value of Good (G), Fair (F), OverFair (OF), UnderFair (UF) and Poor (P). With respect to the performance indicator of the model, quantitative values are assigned to each quality in the following way: G (8.5), F(5.5), OF (6.0), UF (5.0) and P(2.5). According to this, the results which were obtained in order to determine the behavior for PM10 concentrations in terms of space and time are as follows:

Table 1. Interpolation Analysis Interpolation and Representation Model - Spatial behavior over time for PM10 (*20 macropuffs*), 0.5 km resolution of the grid**.**

Days	n_Sources	m_Stations	FB	NMSE	MG	VG	FAC2	IOA	UAPC2	MRE	Score	Grade
03-05	4	20	0.44319	0.48772	1.26427	1.03386	0.8725	0.82499	0.01162	0.13422	68	A
08-10	4	6	0.4763	1.04459	1.13548	1.12435	0.9425	0.65279	-0.43389	0.04745	68	A
08-10	4	10	0.4763	1.04459	1.13548	1.10488	0.9425	0.65279	-0.434	0.04745	68	A
08-10	4	15	0.28956	1.02242	1.10437	1	0.945	0.6316	-0.09792	0.02986	68	A
08-10	4	20	0.22943	0.61457	1.10225	1	0.9475	0.74391	0.1015	0.04245	68	A
32-33	4	4	0.45975	0.97824	1.26312	2.40296	0.8675	0.65331	-0.15473	0.07567	68	A
60-62	4	4	0.56669	0.96783	1.32869	2.86428	0.8575	0.68926	-0.12711	0.12158	63.92	A
91-92	4	4	0.30769	0.67503	1.11597	1.12435	0.9225	0.73782	-0.31272	0.04541	68	A
121-122	4	4	0.40397	0.66605	1.17398	1.17398	0.9	0.76205	-0.2365	0.08598	68	A
152-153	4	4	0.54585	0.91876	1.28117	1.83936	0.86	0.73979	0.1605	0.12874	68	A
169-170	4	4	0.26164	0.51027	1.06283	1.06458	0.9525	0.87339	0.371	0.03636	68	A

200-201	4	10	0.40367	0.65264	1.14673	1.14767	0.93	0.77427	0.15712	0.06338	68	A
215-216	5	5	0.35517	0.48774	1.12555	1.21708	0.9275	0.83883	0.2	0.06085	68	A
215-217	5	10	0.48474	0.80462	1.22977	1.91243	0.865	0.77214	0.21282	0.11617	68	A
215-217	5	15	0.47965	0.77726	1.25506	1.84594	0.865	0.75884	0.28742	0.12469	68	A
215-216	5	20	0.39944	0.74279	1.13849	1.14958	0.935	0.73471	0.02807	0.05042	68	A
215-216	5	25	0.49625	0.94807	1.26543	2.075	0.86	0.68471	-0.02641	0.1032	68	A
281-282	4	4	0.47754	0.74424	1.25916	5.02138	0.87	0.72551	-0.1536	0.07433	65.45	A
299-300	4	5	0.47634	0.60145	1.28413	1.06091	0.8725	0.86194	0.30155	0.17091	68	A
299-300	4	10	0.02536	0.05539	1.0158	1.0158	0.99	0.84829	0.16517	0.00858	68	A
299-300	4	15	0.37195	0.60577	1.11842	1.32463	0.9375	0.81073	0.25418	0.05026	68	A
299-300	4	20	0.29817	0.78764	1.15497	1.17662	0.9025	0.68184	0.335	0.04	68	A
335-336	4	4	0.02854	0.05869	0.97228	1.1263	0.79541	0.8547	0.19023	0.00785	68	A
			0.380747	0.70419	1.17101	1.55678	0.9026	0.75253	0.03475	0.07242	67.71	A
			G	G	G	G	G	G	G	G		

According to Table 1, we can observe that the average obtained for (FB) settled down at 38,075%, achieving qualifications of (G) and (UF), with predominance for (G) according to the fuzzy model proposed by Ok-Hyum (Park and Seok, 2007). This FB tells us that the model had a tendency to underestimate the concentration values, mainly due to the spatial location of *macropuffs* used by the interpolation evolutionary fuzzy model. It should be noted that due to the shapes that the rational base functions or *NUPFS* took and that were used for the interpolation, the model tended to round the peaks that constitute each DEM, as shown in Figure No. 1.

From Table 1 we can observe that the MRE was close to 0.07242, which indicates that the interpolated surfaces had a slight underestimation of the concentration interpolated values, which confirms the concept of rounding which predominates in the interpolation. According to the FAC2 and UAPC2, that took average values of 0.9026 and 0.03475 respectively, it turns out that the maximum concentration values obtained by each of the models only differ in a 3.3475%, while over 90% of the points obtained from the interpolation were within the interval which defines the FAC2. If you look at the metrics MG and VG, values were 1.17931 and 1.56374 respectively; this reveals that this model can be considered as good, since these values will be within a range of 95% which defines an interval of trust between 0.5 and 2.0 - similar to FAC2. In the light of the score obtained using the fuzzy model of Ok-Hyum, we can see that the performance index was close to 68 points which ranks the performance of the model in category A (Park and Seok, 2007). We can also observe that the IOA achieved values close to 75%, although this value decreases with the number of sources. This value of IOA, was fostered by the dynamics of the interpolation model, which does not depend on the quality and quantity of points that represent a phenomenon in the study area.

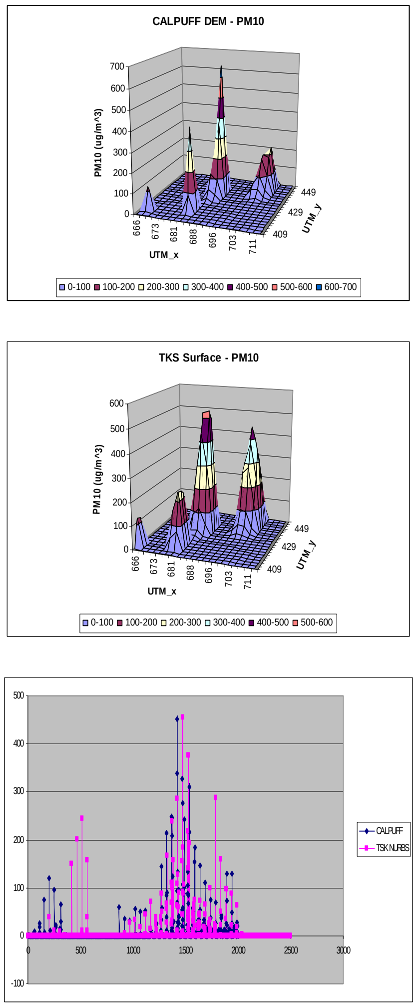

Figure 1. Surfaces Caracterization, 12 Hour Days 91-92. (a) DEM CALPUFF (b) Surface TKS (c) IOA

4. CONCLUSIONS.

The proposed evolutionary model overcame the limitations imposed by the limited spatial information which a set of *m-stations* that monitor the quality of the air provide about the spatial behavior of the phenomenon of dispersion for particulate material in a study area. However, over time these limitations imposed a series of patterns of change with respect to the form and the evolution of the surface of the concentrations that were obtained as a result of the interpolation representation process.

Unlike the models used in geostatistics and computational intelligence for representing such phenomena, which build their potential on the quantity and quality of the points obtained from the phenomenon, the proposed model was able to develop an interpolation by learning and adaptation, starting from the identification of a set of base functions, which indicate the concentration of *puffs* or pollutants in a study area. In this way, the evolutionary model uses its own elements of the dynamics of the phenomenon, which improves its performance compared to other methods used for the representation of such phenomena.

The proposed evolutionary model allowed to represent the spatial behavior of the concentration for PM_{10} over time in a more comprehensive manner, mainly due to the existent dependency between the genetic substructures of estimation and the interpolation, which joined with an initial population, generated only once at the beginning of the process of the evolution, implicates that the model only requires minor adjustments during the estimation of emissions and in the forming of the base functions with respects to the metrics of the concentrations, that is also reflected in a gradual change of surfaces that represent the spatial behavior for PM10 concentrations over time in a study area.

The model of interpolating NUPFS allows the reduction of the phenomenon of spatial dispersion, in terms of the solution structure or individual, making the spatial representation of the concentration in accordance with the TKS interpolation model easier. Similarly, the spatial mapping of genes that establishes the solution structure or individual on top of the surfaces of the concentration will permit to generate a roadmap with reference to of the genetic behavior presented by the individual during the period of a measurement campaign.

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