

## A NOVEL PSEUDO-STATIONARY MODELING OF POLLUTANT MEASUREMENT PREDICTION FROM INDUSTRIAL EMISSIONS

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**Abstract:** Pollutant measurement prediction is a topic of great interest in the area of environmental measurements and health protection. Stationary description of pollutants is an approach in which the amount of pollutant per time unit is considered constant. But in many circumstances, this quantity is subject to a flow delay. In this paper we introduce a novel pseudo-stationary modeling based on Delay Differential Equations (DDE) that can better reflect forced and spontaneous emissions of pollutants from industrial plants and natural processes respectively. Emissions of Volatile Organic Compound (VOC) from industrial plants and leakage of decayed radioactive wastes are respectively a concrete example. The concentration of VOC that are present in the atmosphere can be predicted by using mathematical models. Among the deterministic models that utilize an Eulerian approach, the Gaussian model can be interpreted as a simple solution to the problem. However, the variables that are present in such model, and which are subjected to simplifying assumptions, may not objectively represent reality. The purpose of this work is to utilize a delay logistic equation for the modeling of the data regarding VOC emissions, and to demonstrate its efficiency through a comparison with the classical Gaussian Plume Model.

**Keywords:** Air monitoring, VOC, Delay Logistic Equation, Gaussian Model, Environmental Measurements.

### 1. INTRODUCTION

The U.S. Environmental Protection Agency (EPA) defines VOC as any compound of carbon, excluding carbon monoxide, carbon dioxide, carbonic acid, metallic carbides or carbonates, and ammonium carbonate, which participates in atmospheric photochemical reactions [1]. Moreover, other particular organic compounds are excluded, given their negligible photochemical reactivity. VOC are further defined by the Directive 2004/42/CE, which defines a Volatile Organic Compound as any organic compound having an initial boiling point less than or equal to 250°C measured at a standard pressure of 101,3 kPa [2]. The VOCs' implication in the process of formation of ozone and their negative effect on human health renders necessary the implementation of severe and unrelenting measures of

control on the evolution process of these compounds in the air. The National Emission Inventory (NEI) is in charge of gathering data from several sources, such as governments, local agencies, and factories, and owns a database containing data from the U.S.A., D.C., U.S. Territories of Puerto Rico and Virgin Islands, dating as early as 1990. However, each source has the ability to gather data utilizing different methods. One of the most common is the method 25/25A, provided by the EPA, and is characterized by a static gathering of data, which is not reliable in terms of accuracy and is not able to provide precise estimates. To solve these problems, there are many alternative methods and provisional models that utilize innovative mathematical instruments, such as DDE [3][4].

### 2. PURPOSE

Examining a point source that emits pollutants at a constant rate  $q$ , the total quantity emitted in a time interval of  $dt$  length is  $dQ = qdt$ . The idea consists in determining the VOC emission from a fixed punctual source through the delay logistic equation and in introducing the result into the formula of the pollutant concentration present on the soil of the multiple reflections model with soil-only reflections.

### 3. AIR POLLUTION MODEL WITH DDE

#### 3.1 Delay Differential Equation

To define a general form that represent a DDE we consider a function  $x$  on the space of continuous functions  $C$  defined by:

$$C = C([-σ - r, σ + a], \mathbb{R}^n) \quad \text{with } \sigma \in \mathbb{R}, a \geq 0, r \geq 0$$

and a function  $f: \mathbb{R} \times C \rightarrow \mathbb{R}^n$ ; using the Shimanov notation [10], is defined:

$$x_t(\theta) = x(t + \theta) \quad \forall t \in [\sigma, \sigma + a], \theta \in [-r, 0].$$

Then, a general DDE is given by the relation:

$$\dot{x}(t) = f(t, x_t) \quad (1)$$

where  $\dot{x}$  denote the right hand derivative.

Using the notations in [11], given  $\phi \in C$ , if  $f(t, \phi)$  is continuous with respect to  $t$  and  $\phi$ , a solution of the DDE trough  $(\sigma, \phi) \in \mathbb{R} \times C$  is given by the solution of the integral equation:

$$\begin{cases} x(t) = \phi(0) + \int_{\sigma}^t f(s, x_s) ds, & \forall t \geq \sigma \\ x_{\sigma} = \phi \end{cases}$$

### 3.2 The Model

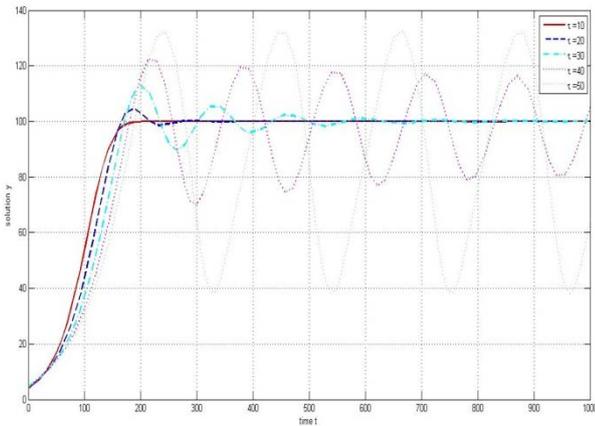
In pollution phenomena, the data collected on the emissions of pollutants in the air can be interpreted as the discretization of a continuous flux of observations, represented by a DDE. This kind of equation illustrates that the diffusion process has past memory. Assuming  $n = 1$ ,  $\theta = -\tau$  and  $\sigma = 0$  the equation (1) becomes:

$$\frac{dx(t)}{dt} = f(t, x(t), x(t-\tau)), \quad \tau \in [0, r] \quad (2)$$

in which  $x(t)$  is the state variable (emission of the VOC) at the time  $t$  and  $\tau$  is the delay of the argument, supposed to be constant. To model data,  $f$  is chosen as a variation of the logistic equation of Verhulst, utilized by Schuster-Schuster [5] for the description of the number of tumoral cells in the Ehrlich Ascites Tumor, of which equation is given by:

$$\frac{dx(t)}{dt} = rx(t-\tau) \left[ 1 - \frac{x(t-\tau)}{K} \right] \quad (3)$$

According to our studies,  $r$  is the emission rate and  $K$  is the maximum concentration of pollutants that the environment is able to sustain (determined by the law which is in force in the state where environmental surveys are performed). To solve the equation, we use as initial function  $\phi$ , the solution of the ordinary Verhulst Logistic Equation on the  $[0, \tau]$  interval, with initial point  $\phi(0) = \phi_0$ :



**Figure 1.** Delay Logistic Equation at the variation of  $\tau$  delay with  $K = 100$ ,  $r = 0.04$  and initial point  $\phi_0 = 4$ .

$$\phi(t) = \frac{K}{1 + Pe^{-rt}} \quad \text{with} \quad P = \frac{K - \phi_0}{\phi_0}.$$

The function  $f$  considered in (3) is continuous and Lipschitzian in  $\phi$ , therefore exists a unique solution [12].

## 4. DDE-GAUSSIAN COMPARISON

The Gaussian model takes in consideration a specific source of pollution placed at the origin of a point of reference ( $O_{xyz}$ ). This emission is constantly equal to  $q$  and it is contained in an atmospheric volume delimited by a closing surface. This model presupposes the presence of a vector wind with average velocity  $u$  and directional axis of the abscissa, and defines that the temporal variation of pollutant amounts  $C$ , is equal to the sum of pollutant quantity produced, plus the net quantity of pollutant that flows through the contour surface [6]:

$$\frac{\partial C}{\partial t} + u \cdot \nabla C = -\nabla^2 C + E + R \quad (4)$$

In (4)  $E$  is the instantaneous emission and  $R$  represents the chemical reaction of the pollution in the atmosphere. With a series of reductions and considerations (see [7] for more details), equation (4) can be simplified to:

$$\frac{\partial C}{\partial t} = \frac{\partial C}{\partial x} \left( k_{xx} \frac{\partial C}{\partial x} \right) + \frac{\partial C}{\partial y} \left( k_{yy} \frac{\partial C}{\partial y} \right) + \frac{\partial C}{\partial z} \left( k_{zz} \frac{\partial C}{\partial z} \right) \quad (5)$$

(where  $[k_{ji}]$  is the tensor of scattering coefficient) and solved, obtaining the formula for the concentration:

$$C = \frac{Q}{2\pi\sigma_y\sigma_z\bar{u}} \exp\left(-\frac{1}{2}\left(\frac{y_r}{\sigma_y}\right)^2\right) \exp\left(-\frac{1}{2}\left(\frac{h_e - z_r}{\sigma_z}\right)^2\right) \quad (6)$$

$Q$  is the total pollution emitted from a source placed at height  $h_e$ , and  $\sigma_y$ ,  $\sigma_z$  are respectively lateral and vertical dispersion coefficients.

The pollutant emission, called plume, is subject to a convective transport in the initial phase of the route, in which its centre of gravity settles at height  $h_m$ . Successively we have a transport phase without soil interaction and finally, at a certain distance from the emission center, the plume is diffused so much that it interacts with the soil and with the top part of the atmosphere and is reflected from itself (a reflection that is considered total for simplicity). Supposing that the reflections in the top part of the atmosphere are negligible and calculating the concentration at a height equal to zero ( $z = 0$ ) we obtain the formula of the model of multiple reflections only on soil:

$$C = \frac{Q}{\pi\sigma_y\sigma_z\bar{u}} \exp\left(-\frac{1}{2}\left(\frac{y_r}{\sigma_y}\right)^2\right) \exp\left(-\frac{1}{2}\left(\frac{h_m}{\sigma_z}\right)^2\right) \quad (7)$$

The stationarity of  $Q$  is a simplistic assumption of the stationary Gaussian model. If the quantity emitted by the source varies with time, we can suppose that such variation is described by an ordinary Verhulst logistic equation. However keep in mind that between the beginning of the pollutant production till the emission into the atmosphere there is a certain time lapse. Such value is considered in the equation as  $\tau$  delay, obtaining (3). In (7), substituting the solution of (3) in place of  $Q$  that which is obtained is a pseudo-stationary model with multiple soil-only reflections. of the pollutant concentration at the soil.

The parameter estimate of dispersion has been calculated following the work of Draxler [8]:

$$\begin{aligned} \sigma_y &= \sigma_\theta x \left(1 + 0.0308x^{0.4548}\right)^{-1}, & x \leq 10^3 \\ \sigma_z &= \sigma_\phi x \left[1 + 0.945(t/T_0)^{0.8}\right]^1, & z \geq 50m \end{aligned} \tag{8}$$

with  $\sigma_\theta = 1.95 \pm 0.5$  and  $\sigma_\phi = 1.25 \pm 0.03$  called standard deviation of the azimuth and elevation angles, respectively, and  $x$  is the downwind distance .

Another estimate has been calculated using the relations of Green with the constants in function of the atmospheric stability classes:

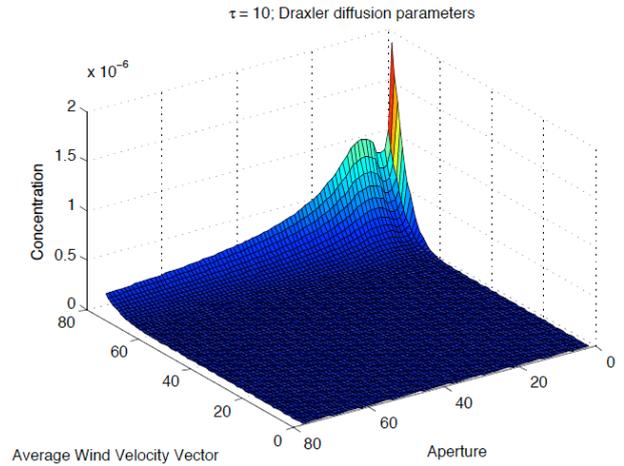
$$\begin{aligned} \sigma_y &= k_1 x \left(1 + x/k_2\right)^{-k_3}, \\ \sigma_z &= k_4 x \left[1 + x/k_2\right]^{-k_5}, \end{aligned} \tag{9}$$

with:

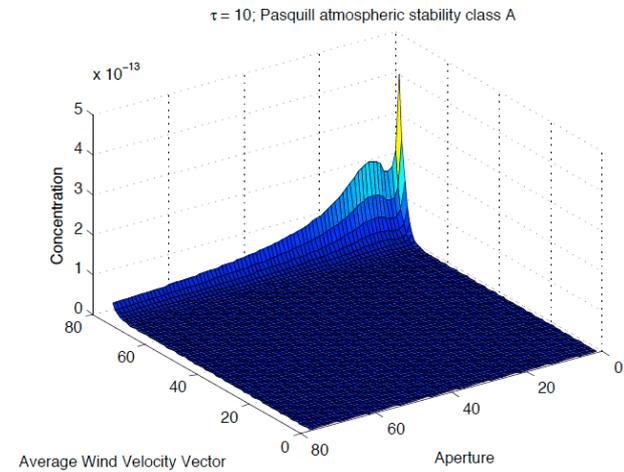
| Stability Class | $k_1$  | $k_2$ | $k_3$ | $k_4$  | $k_5$  |
|-----------------|--------|-------|-------|--------|--------|
| A               | 0.2500 | 927   | 0.189 | 0.1020 | -1.918 |
| B               | 0.2020 | 370   | 0.162 | 0.0962 | -0.101 |
| C               | 0.1340 | 283   | 0.134 | 0.0722 | 0.102  |
| D               | 0.0787 | 707   | 0.135 | 0.0475 | 0.465  |
| E               | 0.0566 | 1070  | 0.137 | 0.0335 | 0.624  |
| F               | 0.0370 | 1170  | 0.134 | 0.0220 | 0.700  |

**Tables 1.** Green’s constants for each Pasquill class of atmospheric stability.

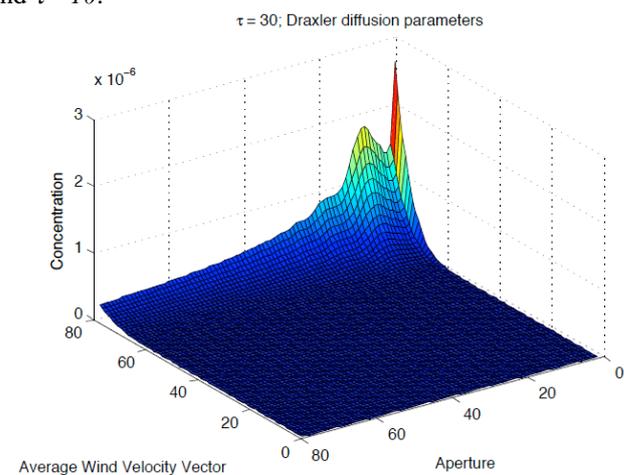
The results obtained are represented in the successive plots where the concentration  $C$  ( $z$ -axis) is represented, if Average Wind Velocity Vector  $u$  ( $x$ -axis) and Aperture ( $y$ -axis) vary. This representation is similar to those display by common scientific literature; but the true difference consists in a reliable representation that takes into account the delay, hence creates actual conditions.



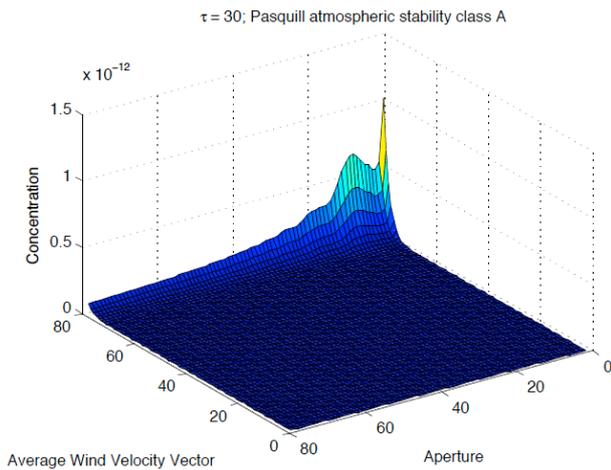
**Figure 2.** Spatial distribution of concentration with Draxler diffusion parameters and  $\tau = 10$ .



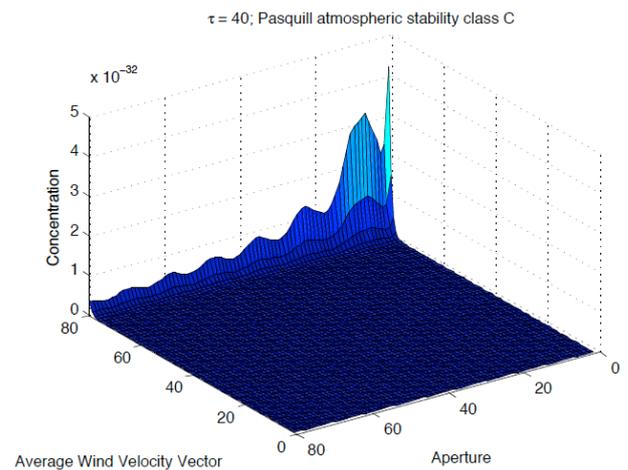
**Figure 3.** Spatial distribution of concentration with Green diffusion parameters, Pasquill atmospheric stability class A and  $\tau = 10$ .



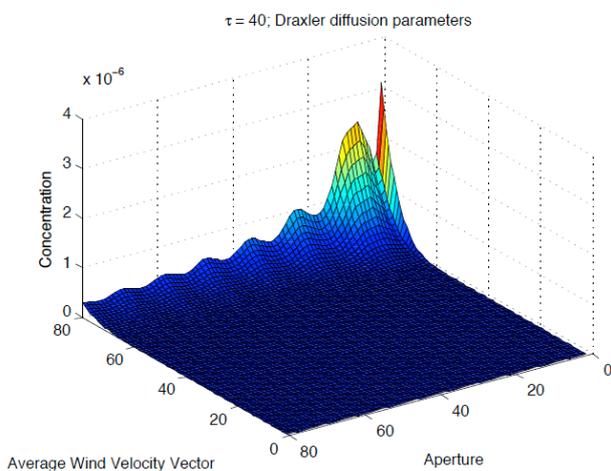
**Figure 4.** Spatial distribution of concentration with Draxler diffusion parameters and  $\tau = 30$ .



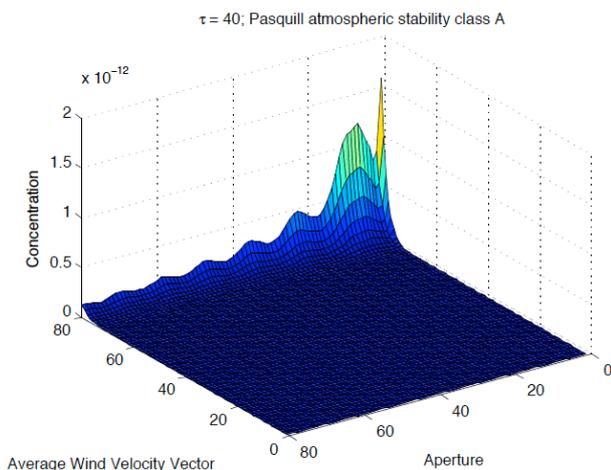
**Figure 5.** Spatial distribution of concentration with Green diffusion parameters, Pasquill atmospheric stability class A and  $\tau=30$ .



**Figure 8.** Spatial distribution of concentration with Green diffusion parameters, Pasquill atmospheric stability class C and  $\tau=40$ .



**Figure 6.** Spatial distribution of concentration with Draxler diffusion parameters and  $\tau=40$ .



**Figure 7.** Spatial distribution of concentration with Green diffusion parameters, Pasquill atmospheric stability class A and  $\tau=40$ .

## 5. CONCLUSION

The results displayed in the previous section testify the novelty introduced in this paper. First of all we have considered the total pollution as a delayed function so that we can describe and model the behavior of the pollution emitted from the plant as a force emission and from other sources as spontaneous emission.

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