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Analysis of Hyperbolic Models a comparison with Parabolic Diffusion Models for Contaminant Dispersion

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Abstract: The following article is about the analysis of Pollutant Dispersion Models based on Gaussian and Parabolic Models and a comparison with Hyperbolic Models, looking at some of their properties and applications, an introduction to the study of Diffusion in these Models and their results is made.

Keywords: Diffusion Equation, Diffusion and Advection Equation, Gaussian Models, Operator Separation Method, Hyperbolic Model

Introduction

Linear parabolic diffusion theories based on Fourier's or Fick's laws predict disturbances that can propagate at infinite speed. However, linear parabolic diffusion theories based on Fick's Law or Fourier's laws (in the case of mass transport or heat conduction, respectively) predict an infinite propagation velocity, their amplitudes decaying exponentially. For this reason, in some applications and the use of linear parabolic models may be accurate enough for purposes.

The theory of hyperbolic diffusion was pioneered in 1958 by Cattaneo who proposed a generalization of Fourier and Fick's Law. The study of hyperbolic diffusion has been limited mainly to pure diffusion problems up to now. The authors have recently proposed a generalization of the hyperbolic diffusion equation that can also be used in cases of convection. From a numerical point of view, the simulation of the hyperbolic diffusion equation has been limited mainly to 1D problems.

The theory of hyperbolic diffusion is derived by substituting in Fick's Law for a more general equation due to Cattaneo, viz.

$$\boldsymbol{q} + \boldsymbol{\tau}\frac{\partial \emptyset}{\partial t} = -\boldsymbol{K}\nabla\emptyset$$

In the equation, τ is the so-called relaxation tensor that has dimensions of time. So, the theory of hyperbolic diffusion is defined by the following set of equations the previous and now

$$\frac{\partial \emptyset}{\partial t} + \nabla.\boldsymbol{q} = \boldsymbol{f}$$

We observe that when $\tau = 0$ we recover the parabolic theory. Also, in the steady state, both theories are equivalent. even for $\tau = 0$. Assume isotropic and homogeneous medium, with $k > 0$, $\tau > 0$. We don't consider source terms, we obtain the so-called hyperbolic diffusion equation. Equation (1) is hyperbolic and, as a consequence, we can define a velocity finite for the transport of contaminants.

$$\frac{\partial \emptyset}{\partial t} + \boldsymbol{\tau}\frac{\partial^2 \emptyset}{\partial t^2} - \nabla^2\emptyset = 0 \qquad \textbf{(1)}$$

To compare the solution of the classical formulation with the solution of the hyperbolic theory we solve the hyperbolic one. Now, we need two initial conditions. because (1) involves second-order derivatives with respect to time. Points to consider is that in most applications the relaxation time is very small. Since Cattaneo's and Fick's laws are equivalent in the steady state, we would only see differences on the smaller time scales.

A notable fact is that the hyperbolic convection-diffusion theory is not equivalent to the parabolic convection-diffusion theory in the steady state. This implies that, for non-zero relaxation, both theories would predict different results on all time scales. Within the atmosphere we have the following possible examples which can be modeled under the previous premise of the parabolic model.

Now the analytical and numerical solutions have their advantages and disadvantages, as the analytical solutions that we will see below are accurate and provide a deep theoretical understanding of the physical problem, but they are available for specific and simplified problems, the numerical ones can be applied to a wide range of problems, except that they require more calculation time and have a loss of precision, as we can see the Parabolic Models where the mass transport is slower compared to the diffusion, the hyperbolic models are apparently the opposite where the transport is fast and the diffusion is slow or very small

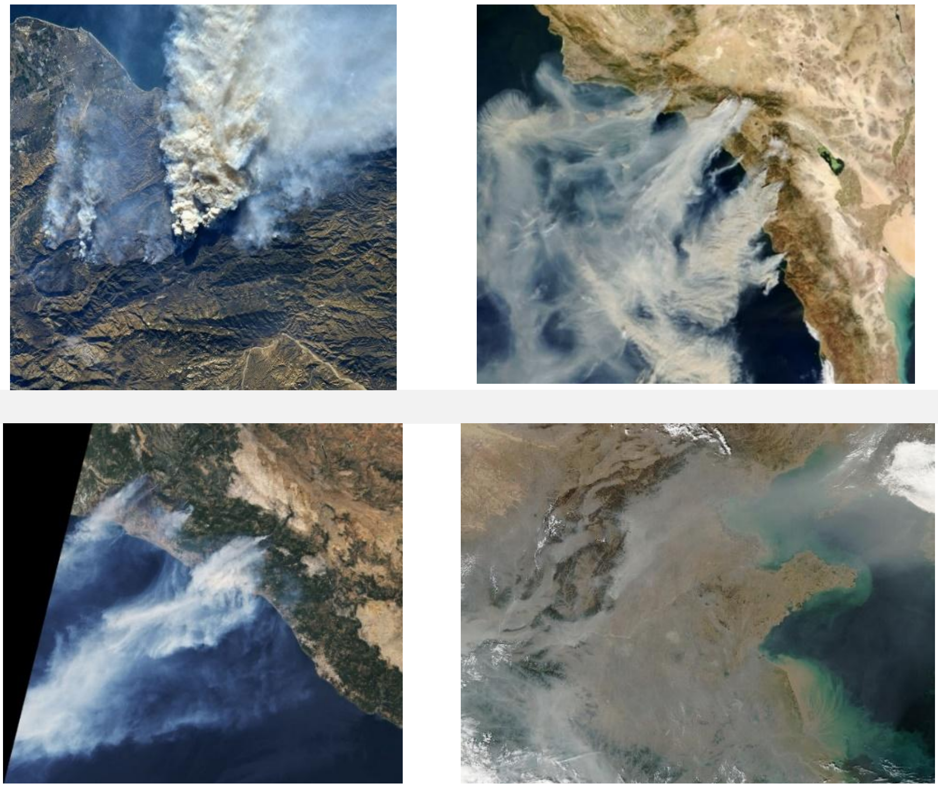


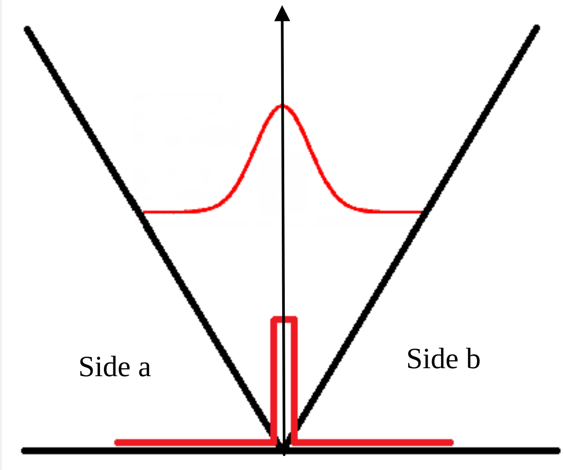
Figure 1. Contaminant Plumes and Contaminant Dispersion we can see the shape of the plume which goes in the direction of the wind and turbulence, the geometric shape of this plume can be seen and is well known (sources of images on the internet and magazines)

Figure2. Contaminant Plumes and Dispersion of Contaminants we can see the shape of the plume which goes in the direction of the wind and turbulence (sources of the images on the internet)

Let's see a brief analysis of stability and mass balance if we handle the addition of the diffusive term in the temporal part having the hyperbolic diffusion equation. Let's see the shape of the Gaussian plume a description in the following figure

Polluting Feathers

Description



$-\Delta x x_0 \Delta x$
$-\Delta\sigma \mu_0 \Delta\sigma$

Now let's see the approximation based on the probability of leaving on one negative side the same as on the other, it is seen that it makes the Gaussian form so let's see that average which would be that of the Gaussian distribution.

Figure 3 sources of the images on the internet of forest fires

Obtaining the mean or Gaussian expectation, with a change of variable$u = \frac{x-\mu}{\sigma}$

$$E(X) = \frac{1}{\sigma\sqrt{2\pi}}\int_{-\infty}^{\infty} x e^{-\frac{(x-\mu)^2}{2\sigma^2}} dx = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty}(u\sigma+\mu)e^{-\frac{u^2}{2}}du = \frac{1}{\sqrt{2\pi}}\left[\int_{-\infty}^{\infty}(u\sigma)e^{-\frac{u^2}{2}}du + \int_{-\infty}^{\infty}(\mu)e^{-\frac{u^2}{2}}du\right]$$
$$= \mu\sqrt{2\pi} = \mu$$

The normal distribution has the property that all the measures of its central tendency, such as the mean, but also the median and the mode, are equal and since we are saying that it has the same probability of going to the left or to the right, we obtain the arithmetic average$\mu = \frac{\sum_{i=1}^{n} x_i}{n}$, thus, being a and b the probabilities, this is how you have$a + b = 1$ and$a \geq \frac{1}{2} and b \leq \frac{1}{2}$ of mean.

$$\emptyset(x_0 \pm \Delta x, t) = a * \emptyset(x_0 - \Delta x, t) + b * \emptyset(x_0 + \Delta x, t) =$$
$$= \frac{\emptyset(x_0 - \Delta x, t)}{2} + \frac{\emptyset(x_0 + \Delta x, t)}{2} = \emptyset(x_0, t)$$

Thus we then have the Taylor Series approximations as

$$\emptyset(x_0, t) = \emptyset(x_0, t) + \frac{\partial\emptyset(x_0,t)}{\partial t}\Delta t + \frac{1}{2}\frac{\partial^2\emptyset(x_0,t)}{\partial t^2}\Delta t^2 + \cdots$$
$$a * \emptyset(x_0 - \Delta x, t) = a * \emptyset(x_0, t) - a\frac{\partial\emptyset(x_0,t)}{\partial x}\Delta x + \frac{a}{2}\frac{\partial^2\emptyset(x_0,t)}{\partial x^2}\Delta x^2 -$$
$$b * \emptyset(x_0 + \Delta x, t) = b * \emptyset(x_0, t) + b\frac{\partial\emptyset(x_0,t)}{\partial x}\Delta x + \frac{b}{2}\frac{\partial^2\emptyset(x_0,t)}{\partial x^2}\Delta x^2 -$$

Adding we have

$$\emptyset(x_0, t) + \frac{\partial\emptyset(x_0,t)}{\partial t}\Delta t + \frac{1}{2}\frac{\partial^2\emptyset(x_0,t)}{\partial t^2}\Delta t^2 + \cdots$$
$$= (a+b)\emptyset(x_0, t) + (b-a)\frac{\partial\emptyset(x_0,t)}{\partial x}\Delta x + \left(\frac{a+b}{2}\right)\frac{\partial^2\emptyset(x_0,t)}{\partial x^2}\Delta x^2 -$$

Parabolic form

$$\frac{\partial \emptyset(x_0,t)}{\partial t} = \frac{((a+b)-1)}{\Delta t}\emptyset(x_0,t) + (b-a)\frac{\Delta x}{\Delta t}\frac{\partial \emptyset(x_0,t)}{\partial x} + \left(\frac{a+b}{2}\right)\frac{\Delta x^2}{\Delta t}\frac{\partial^2 \emptyset(x_0,t)}{\partial x^2}$$

$$\frac{\partial \emptyset(x_0,t)}{\partial t} = (b-a)\frac{\Delta x}{\Delta t}\frac{\partial \emptyset(x_0,t)}{\partial x} + \left(\frac{1}{2}\right)\frac{\Delta x^2}{\Delta t}\frac{\partial^2 \emptyset(x_0,t)}{\partial x^2}$$

You can see the nature of the wind speed and diffusion coefficients

Now the Hyperbolic form

$$\frac{\partial \emptyset(x_0,t)}{\partial t} + \frac{\Delta t}{2}\frac{\partial^2 \emptyset(x_0,t)}{\partial t^2} = (b-a)\frac{\Delta x}{\Delta t}\frac{\partial \emptyset(x_0,t)}{\partial x} + \left(\frac{1}{2}\right)\frac{\Delta x^2}{\Delta t}\frac{\partial^2 \emptyset(x_0,t)}{\partial x^2}$$

And the Eddy Diffusion coefficient is y in terms of the standard deviation

$$K = \left(\frac{1}{2}\right)\frac{\Delta x^2}{\Delta t} = \left(\frac{1}{2}\right)\frac{\Delta \sigma^2}{\Delta t}$$

The wind coefficient or wind speed depends on the probability that it varies from one side to another

$$U = (b-a)\frac{\Delta x}{\Delta t}$$

And this term is Tao, if we can approximate it in this way

$$T = \frac{\Delta t}{2}$$

We have the parabolic equation according to [Skiba – Parra Book page 83 see References] in 2D form and with the elimination of some terms we have the following.

$$\frac{\partial \emptyset}{\partial t} + U \cdot \nabla\emptyset - \nabla \cdot \mu\nabla\emptyset = f(r,t)$$

$$f(r,t) = \sum_{i=1}^{n} Q_i\delta(r,t)$$

With

$$\mu\frac{\partial \emptyset}{\partial n} - U\emptyset = 0 in S^-$$

$$\mu\frac{\partial \emptyset}{\partial n} = 0 out S^+$$

$$\nabla \cdot U = 0$$

$$\emptyset(r,0) = 0$$

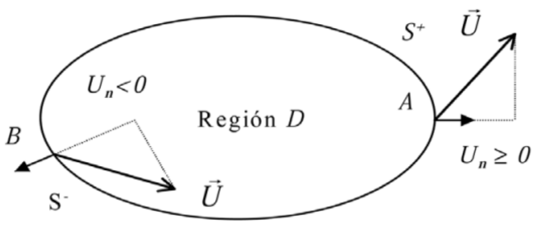


Figure 3. Schematic region D with S boundaries for the Transport Equation (Skiba – Parra Book see References)

Having the expression as

$$\frac{\partial}{\partial t}\int_D \emptyset dr = \sum_{i=1}^{N} Q_i(t) - \int_{s^+ \cup S^-} U\emptyset ds$$

This equation indicates that the rate of change of the total mass of the kth pollutant species in domain D is equal to the sum of the rates with which said substance is emitted, minus the rate of mass loss of the pollutant that escapes. from domain D through the open boundary, the latter due to advection. Now completing the term where tao intervenes in the Equation we have the following

$$\frac{\partial \emptyset}{\partial t} + \tau\frac{\partial^2 \emptyset}{\partial t^2} + U \cdot \nabla\emptyset - \nabla \cdot \mu\nabla\emptyset = f(r,t)$$

With the following Boundary conditions, we can maintain them and now having a starting time derivative

$$\mu\frac{\partial \emptyset}{\partial x} - u\emptyset = 0 in S^-$$

$$\mu\frac{\partial\emptyset}{\partial x} = 0 out S^{+}$$
$$\nabla\cdot U = 0$$
$$\emptyset(x,0) = 0 \frac{\partial\emptyset(x,0)}{\partial t} = 0$$

Now let's see the following with $\emptyset(r,t) and U$ **vector of Wind Velocity**

$$\frac{\partial}{\partial t}\int_D \emptyset dr + \tau^*\frac{\partial}{\partial t}\int_D \frac{\partial\emptyset}{\partial\tau} d\tau dr = \sum_{i=1}^{N} Q_i(t) - \int_{s^+\cup S^-} U\emptyset ds$$
$$\frac{1}{\tau^*}\frac{\partial}{\partial t}\int_D \emptyset dr + \frac{\partial}{\partial t}\int_D \frac{\partial\emptyset}{\partial\tau} d\tau dr = \frac{1}{\tau^*}\int_0^t\int_0^l f(r,\tau) dr d\tau - \frac{1}{\tau^*\mu}\int_0^t\int_0^l U\emptyset(r,\tau) dr d\tau$$

We can see the loss of concentration due to both the relaxation factor τ* and diffusion, it can be seen that the product of tao and diffusion mu, will cause the transport to change and decrease a lot if these factors increase, now let's see the analysis of instability according to [Skiba – Parra Book see Reference page 88] book with the parabolic model

$$A = a\frac{\partial}{\partial x} + b\frac{\partial^2}{\partial x^2}$$

With

$$\frac{\partial\emptyset}{\partial t} + A\emptyset = f(r,t)$$
$$\emptyset(0) = \emptyset^0$$

From the previous result, we have the following for the Parabolic model. Multiplying by ∅ the previous Equation we have

$$\left(\frac{\partial\emptyset}{\partial t},\emptyset\right) = (f,\emptyset) - (A\emptyset,\emptyset)$$

Now using the Schwarz inequality

$$\left(\emptyset,\frac{\partial\emptyset}{\partial t}\right) \le \|f\|\|\emptyset\|$$
$$\int_D \frac{\partial\emptyset}{\partial t}\emptyset dt = \frac{\partial}{\partial t}\int_D (\emptyset,\emptyset) dt = \frac{\partial}{\partial t}\int_D \|\emptyset\|^2 dt$$

Thus

$$\frac{\partial}{\partial t}\|\emptyset\|^2 \le \|f\|\|\emptyset\|$$
$$\frac{\partial}{\partial t}\|\emptyset\| \le \|f\|$$

Integrating

$$\|\emptyset\| \le \int_0^t \|f\| d\tau$$
$$\|\emptyset\| \le \|f(r,t)\| - \|f(r,0)\|$$
$$\|\emptyset\| \le \int_0^t \|f\| d\tau + \|\emptyset^0\|$$

In a definite time, one has

$$\|\emptyset\| \le Tmax\|f(r,t)\| + \|\emptyset^0\|$$

Now according to the Hyperbolic model. If we arrange the Equation in the following way

$$\frac{\partial\emptyset}{\partial t} + \tau\frac{\partial^2\emptyset}{\partial t^2} + A\emptyset = f(r,t)$$
$$\emptyset(0) = \emptyset^0$$
$$\frac{\partial\emptyset(0)}{\partial t} = \emptyset^0$$

In a very similar way we have with the second derivative in time

$$\left(\frac{\partial\emptyset}{\partial t},\emptyset\right)+\left(\tau\frac{\partial^2\emptyset}{\partial t^2},\emptyset\right)=(f,\emptyset)-(A\emptyset,\emptyset)$$

$$\left(\emptyset,\frac{\partial^2\emptyset}{\partial t^2}\right)\leq\|f\|\|\emptyset\|$$

You finally have

$$\|\emptyset\|\leq\left(\frac{1}{\tau^*}+\frac{1}{2}\right)Tmax\|f(r,t)\|+\frac{1}{2}\|\emptyset^0\|+\frac{1}{2\tau^*}\int_0^t\|\emptyset^0\|d\tau$$

But since we have 0 in the initial conditions

$$\|\emptyset\|\leq\left(\frac{1}{\tau^*}+\frac{1}{2}\right)Tmax\|f(r,t)\|$$

Now we will start with a simple model without a Diffusive and Hyperbolic boundary and not homogeneous with a tao = 1, another important point is the diffusion coefficient increases the fluid is more regular if it decreases the convective term increases and is more turbulent

Let's see the hyperbolic diffusive model with and without border and their respective initial conditions, with diffusive, advective and Source terms.

Hyperbolic model with Tao =1

$$\frac{\partial\emptyset}{\partial t}+a\frac{\partial\emptyset}{\partial x}+\frac{\partial^2\emptyset}{\partial t^2}-c^2\frac{\partial^2\emptyset}{\partial x^2}=Q$$

With CI = $\varphi(x,0)=f(x)$ and $\frac{\partial\varphi(x,0)}{\partial t}=g(x)$ now from the Z – J reduction functions we can have the reduction with

$$\emptyset(x,t)=Z(x,t)e^{\frac{1}{2}(x-t)}=Z(x,t)e^{\frac{ax}{2c^2}-\frac{t}{2}}$$

With general solution being G(x,ε,t) the Green function

$$\varphi(x,t)=\frac{\partial}{\partial t}\int_0^l f(\varepsilon)G(x,\varepsilon,t)d\varepsilon+\int_0^l g(\varepsilon)G(x,\varepsilon,t)d\varepsilon+\int_0^t\int_0^l\emptyset(\varepsilon,\tau)G(x,\varepsilon,t-\tau)d\varepsilon d\tau$$

Solution

Reduce the Equation to a Klein Gordon Equation giving the general homogeneous solution

$$\gamma>0$$

$$\begin{aligned}\varphi(x,t)=\frac{e^{-\frac{t}{2}}}{2}\left[e^{\frac{at}{2c}}f(x+ct)+e^{-\frac{at}{2c}}f(x-ct)\right]\\+\frac{e^{\frac{ax}{2c^2}-\frac{t}{2}}}{2c}\int_{x-ct}^{x+ct}e^{\frac{as}{2c^2}}(g(s)+\frac{f(s)}{2})J_0\left(\frac{\sqrt{\gamma}}{c}\sqrt{c^2t^2-(x-s)^2}\right)ds\\-\frac{e^{\frac{ax}{2c^2}-\frac{t}{2}}\sqrt{\gamma}}{2c}\int_{x-ct}^{x+ct}\frac{e^{\frac{as}{2c^2}}f(s)J_1\left(\frac{\sqrt{\gamma}}{c}\sqrt{c^2t^2-(x-s)^2}\right)}{\sqrt{c^2t^2-(x-s)^2}}ds\\+\int_0^t\int_0^l\frac{e^{-\frac{as}{2c^2}-\frac{\tau}{2}}Q}{2c}J_0\left(\frac{\gamma}{c}\sqrt{c^2\tau^2-s^2}\right)dsd\tau\end{aligned}$$

With $\gamma<0$

$$\begin{aligned}\varphi(x,t)=\frac{e^{-\frac{t}{2}}}{2}\left[e^{\frac{at}{2c}}f(x+ct)+e^{-\frac{at}{2c}}f(x-ct)\right]\\+\frac{e^{\frac{ax}{2c^2}-\frac{t}{2}}}{2c}\int_{x-ct}^{x+ct}e^{-\frac{as}{2c^2}}(g(s)+\frac{f(s)}{2})I_0\left(\frac{\sqrt{\gamma}}{c}\sqrt{c^2t^2-(x-s)^2}\right)ds\\-\frac{e^{\frac{ax}{2c^2}-\frac{t}{2}}\sqrt{\gamma}}{2c}\int_{x-ct}^{x+ct}\frac{e^{-\frac{as}{2c^2}}f(s)I_1\left(\frac{\sqrt{\gamma}}{c}\sqrt{c^2t^2-(x-s)^2}\right)}{\sqrt{c^2t^2-(x-s)^2}}ds\end{aligned}$$

$$+\int_0^t\int_0^l \frac{e^{-\frac{as}{2c^2}-\frac{\tau}{2}}Q}{2c} J_0\left(\frac{\gamma}{c}\sqrt{c^2\tau^2-s^2}\right) dsd\tau$$

Now solving the inhomogeneous system with f = g = 0 the solution is:

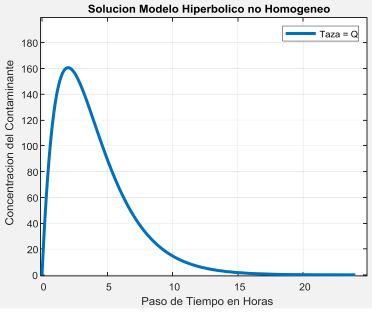
$$\varphi(x,t)=\frac{Q}{c^2}J_1\left(t\frac{\gamma}{c}\right)e^{-\beta t}\frac{\pi}{2}\left(\gamma x-\frac{\alpha x^2}{2}\right)-\frac{Q}{\beta c^2}\gamma J_1\left(t\frac{\gamma}{c}\right)\left(\gamma x-\frac{\alpha x^2}{2}\right)$$

Results

Pollution rate | **Simulation**

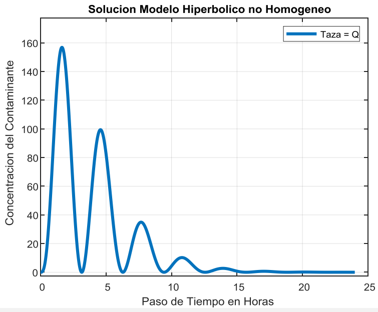
Q =100**,**where a is the wind speed and C the Diffusion coefficient is constant.

u=1.8 m/s C=0.025$\frac{m^2}{s}$



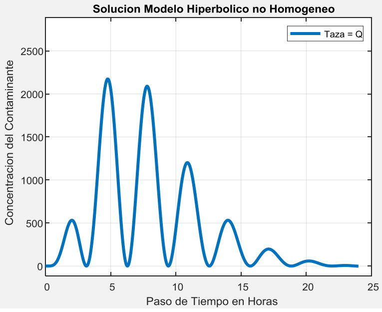
q =100, Q=q*((sin(t))^2)

u=1.8 m/s C=0.025$\frac{m^2}{s}$



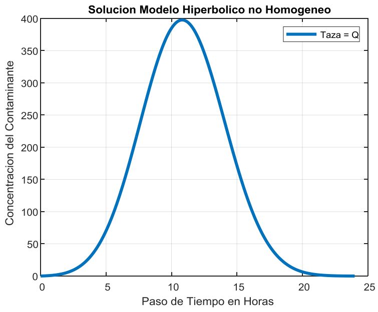
q=100,
Q =(q*(t*t)*((sin(t)).^2))

u=1.8 m/sC=0.025$\frac{m^2}{s}$



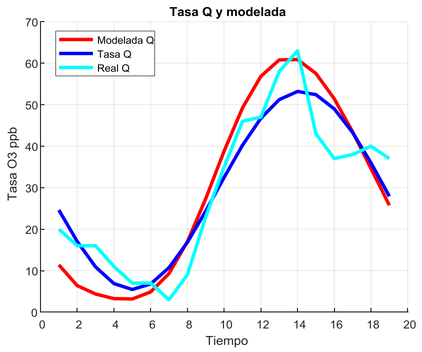
a1 =9.67195923336E+001;
b1 =1.54332964547E+001;
c1 =3.36189393472E+000;

q=100z =a1*exp((-(b1-t)^2)/(2*c1^2))
Q =q*z
u=1.8 m/sC=0.025$\frac{m^2}{s}$

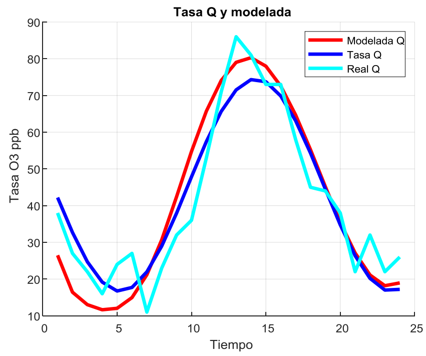


Let's now see the same Hyperbolic model with 5 days, setting a constant Rate equal to the Pollutant [O3] in time, Rate Q, with wind and diffusivity, varying against wind

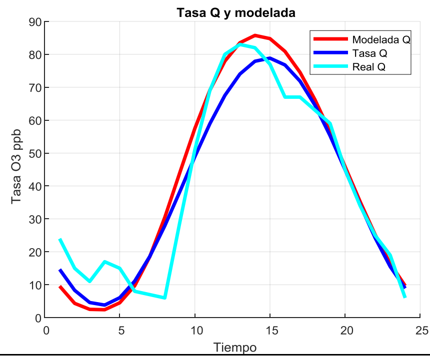
Pollution Rate 5th june 2023



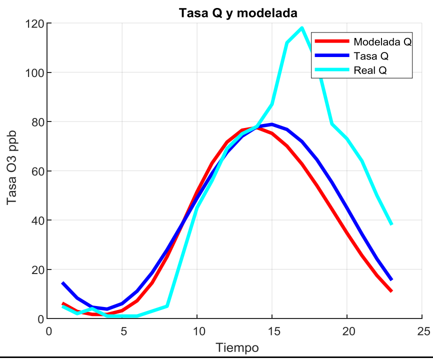
Pollution Rate 6th june 2023



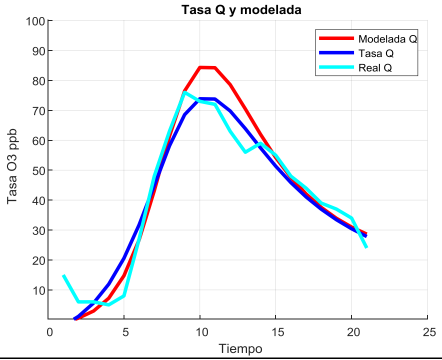
Pollution Rate 7th june 2023



Pollution Rate 8th june 2023



Pollution Rate 9th june 2023

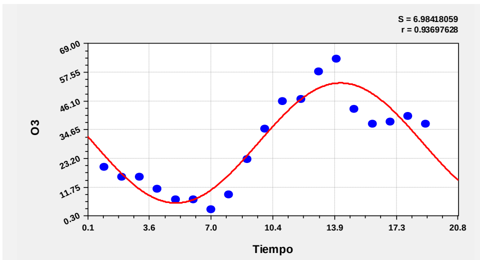


Using the Correlation Coefficient and RMSE Estimators

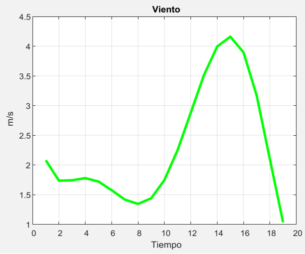
9 de Junio R = 0.9476 RMSE = 1.10
8 de Junio R = 0.9437 RMSE = 1.25
7 de Junio R = 0.9543 RMSE = 1.01
6 de Junio R = 0.9305 RMSE = 1.36
5 de Junio R = 0.9241 RMSE = 1.46

The adjustments were made taking the values of Winds of that day and the Contaminant Rate here is an example of the Adjustment of the Q Rate and the Wind in one direction

Pollution Rate of O3



Winds



Let us now see the parabolic diffusive model without boundary and its respective initial conditions, with diffusive, advective and Source terms.

Parabolic model

$$\frac{\partial \emptyset}{\partial t} + a\frac{\partial \emptyset}{\partial x} - c^2\frac{\partial^2\emptyset}{\partial x^2} = Q$$

With CI = $\varphi(x,0) = 0$ and now from the Z – J reduction functions we can have the reduction with $\alpha = \frac{a}{2c^2}\beta = \frac{a^2}{4c^2}$

$$\emptyset(x,t) = Z(x,t)e^{\alpha x-\beta t} = Z(x,t)e^{\frac{ax}{2c^2}-\frac{a^2 t}{4c^2}}$$

With general solution being G(x,ε,t) the Green function

$$\varphi(x,t)=\int_0^t\int_0^l \emptyset(\varepsilon,\tau)G(x,\varepsilon,t-\tau)d\varepsilon d\tau$$

$$\varphi(x,t)=\int_0^t\int_0^l \frac{Qe^{\alpha\varepsilon-\beta\tau}}{\sqrt{4\pi C(t-\tau)}}e^{-\frac{(x-\varepsilon)^2}{4C(t-\tau)}}d\varepsilon d\tau$$

Solution

Thus Integrating we have this first form

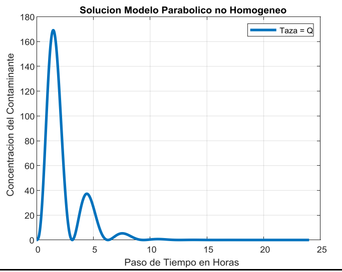
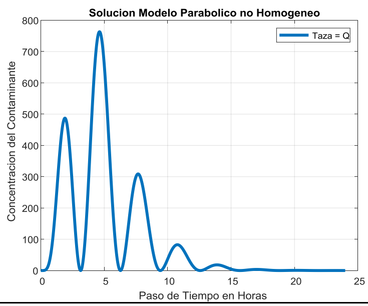
$$\varphi(x,t)=e^{-\frac{a^2t}{4c^2}-\frac{ax}{2c^2}}Q\left(\frac{erf(\frac{a}{2c^2}\sqrt{Ct})}{\frac{a^2}{2c^2}}+\sqrt{\frac{Ct}{\pi}}\frac{\frac{a}{2c^2}e^{-\frac{a^2t}{4c^2}}}{\frac{a^2}{4c^2}}\right)$$

And the second way is by deriving the previous solution with respect to t and integrating it again, thus the following expression arises satisfying the Initial Condition $\varphi(x,0) = 0$

$$\varphi(x,t)=e^{-\frac{a^2t}{4c^2}-\frac{ax}{2c^2}}Q\left(\frac{erf(\alpha\sqrt{Ct})}{2\beta}+\frac{\alpha\beta\sqrt{C}}{2\beta^{\frac{5}{2}}}erf(\sqrt{\beta t})-\frac{\alpha\sqrt{C}\,erf(\sqrt{\beta t})}{2\beta^{\frac{3}{2}}}-2\sqrt{\frac{\beta t}{\pi}}\frac{e^{-\beta t}\sqrt{C\alpha}}{2\beta^{\frac{3}{2}}}\right)$$

$$\alpha=\frac{ax}{2C^2}\beta=\frac{a^2}{4C^2}$$

Results

Pollution Rate	Simulation
q=100Q=q*((sin(t))^2) **u=1.8 m/s; C=0.8$\frac{m^2}{s}$**	
q=100Q = (q*(t*t)*((sin(t))^2)) **u=1.8 m/s C=0.8$\frac{m^2}{s}$**	

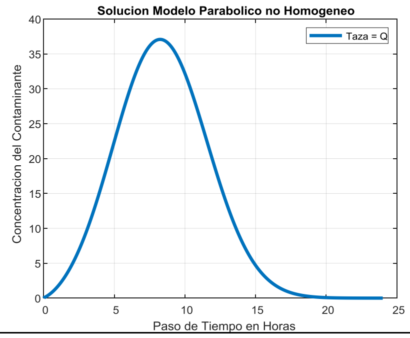
<table>
<tr>
<td>

a1 =9.67195923336E+001;
b1 =1.54332964547E+001;
c1 =3.36189393472E+000;

q=100, z=a1*exp((-(b1-t) ^2) /(2*c1^2)) Q= q*z

u=1.8 m/s $C=0.8\frac{m^2}{s}$

</td>
<td>



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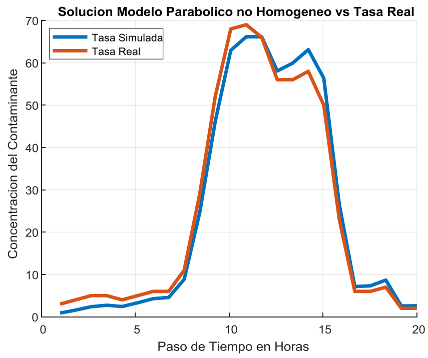
<tr>
<td>

u=[5.400,4.320,5.040,5.040, 4.680,4.320,5.040,5.040,5.400, 3.960,5.760,5.760,7.920,1.3320, 1.1160,1.1880,9.000,6.120, 7.560,4.680,4.680,7.200,4.680 ,4.680] en m/s

Q=[3,4,5,5,4,5,6,6,11, 29,52,68,69,66,56,56,58, 50,23,6,6,7,2,2]

</td>
<td>



Using the Correlation Coefficient and RMSE Estimators

R = 0.9517 RMSE = 0.6325

</td>
</tr>
<tr>
<td>

R = 0.9489 RMSE = 0.7664

u=[1.700,1.200,1.200,1.700,1.500, 1.500,1.600,1.600,1.400,1.100,1.600, 1.900,2.900,4.500,5.400,6.300, 5.900,6.200,6.300,4.600,4.000, 3.100,2.800,2.000] en m/s

Q = [1,1,1,1,2,2,3,2,6,11,29,39,43,41, 44,42,38,34,21,18,21,17,19,11];

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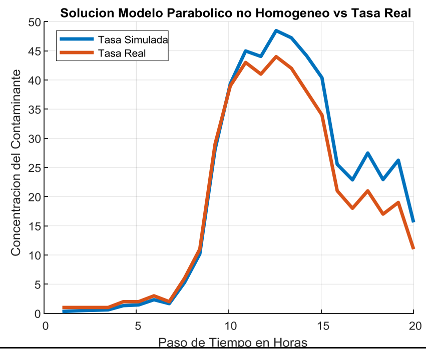
<td>



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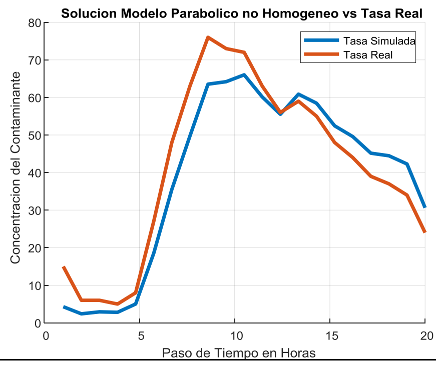
<tr>
<td>

R = 0.9083 RMSE = 1.5839

u=[1.300,1.100,1.300,1.100,1.100, 0.900,1.400,2.200,2.300,2.800,3.900 ,4.300,4.400,3.800,4.300,4.700, 4.500,4.500,3.200,1.700,1.300] en m/s

Q =[15,6,6,5,8,27,48,63,76,73,72, 63,56,59,55,48,44,39,37,34,24]

</td>
<td>



</td>
</tr>
</table>

Now the Time Series presented by the Official page of the Acolman Station, State of México, January 1 and 2, 2022, Real Concentration data (http://www.aire.cdmx.gob.mx/)

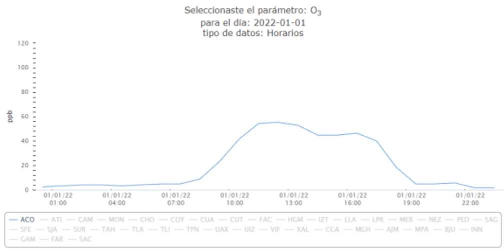


Figure 4. O3 concentration of January 1, 2022

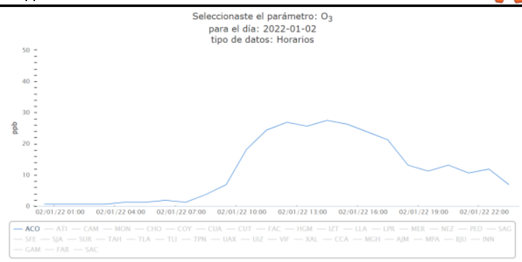
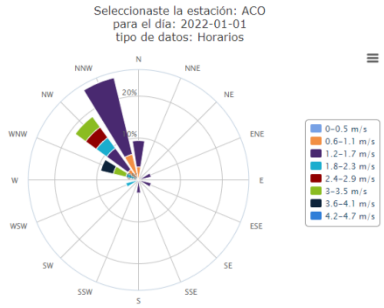
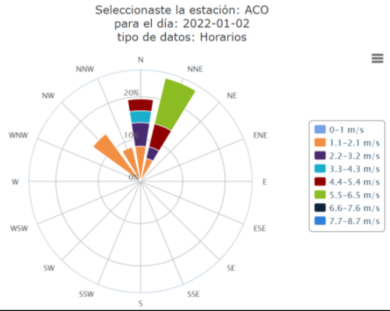


Figure 5. O3 concentration of January 2, 2022





Gaussian Parabolic Model

$$\frac{\partial \emptyset}{\partial t} + a\frac{\partial \emptyset}{\partial x} - c^2\frac{\partial^2 \emptyset}{\partial x^2} = 0$$

With CI = $\varphi(x, 0) = Q$with alfa and beta = 0 in the general solution we are left

$$\emptyset(x,t) = \int_{-\infty}^{\infty} \frac{Q}{\sqrt{4\pi C t}} e^{-\frac{(x-\varepsilon)^2}{4Ct}} d\varepsilon$$

Solution

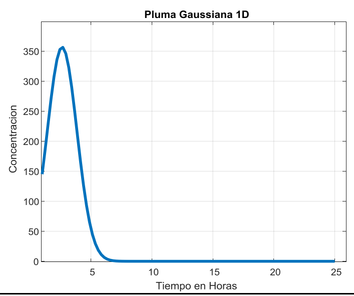
Thus Integrating we are left

$$\emptyset(x,t) = \frac{Q}{\sqrt{4\pi C t}} e^{-\frac{(x-ut)^2}{4Ct}}$$

In terms of the Error Function

$$\emptyset(x,t) = -\frac{\sqrt{\pi}}{\sqrt{\frac{1}{Dt}}} Q\left(erf\left(\frac{x-ut}{2D\sqrt{\frac{1}{Dt}t}}\right) - erf\left(\frac{x}{2D\sqrt{\frac{1}{Dt}t}}\right)\right)$$

Results

Pollution Rate	**Simulation**
Q =100D is the Diffusion coefficient and the wind speed. **D= 0.00625 $\frac{m^2}{s}$u=0.1 m/s**	

<table>
<tr>
<td>

Dx= 0.00625 $\frac{m^2}{s}$

u=[5.400,4.320,5.040,5.040,4.680,4.320,5.040,5.040,5.400,3.960,5.760,5.760,7.920,1.3320,1.1160,1.1880,9.000,6.120,7.560,4.680,4.680,7.200,4.680,4.680];

Q=[3,4,5,5,4,5,6,6,11,29,52,68,69,66,56,56,58,50,23,6,6,7,2,2];

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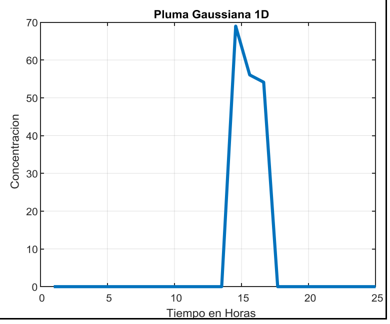

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</table>

Stationary Gaussian model and with chemical reaction

$$a\frac{\partial \emptyset}{\partial x} = cy^2\frac{\partial^2\emptyset}{\partial y^2} + cz^2\frac{\partial^2\emptyset}{\partial z^2} + \sigma\emptyset$$

With CI $\boldsymbol{a\varphi(x,0) = Q\delta(z - z0)}$with$\boldsymbol{\frac{\partial\emptyset(x,y,z)}{\partial z} = 0 \;\; z = 0 \; \frac{\partial\emptyset(x,y,z)}{\partial z} = 0 \;\; z = h}$

put the conditions of a > C

Solution

$$\emptyset(x,y,z) = \left[\frac{Q}{a}\sum_{n=|1}^{\infty} cos(\lambda_n y)e^{-\int_0^{x}\frac{\lambda_n^2 Ky}{a}dx} + \sum_{n=1}^{\infty}\frac{2Q}{ah}cos(\lambda_n y)cos(\lambda_n z)cos(\lambda_n z0)e^{e^{\int_0^x \frac{\sigma}{a}dx} - \int_0^x\frac{\lambda_n^2Ky+\lambda_n^2Kz}{a}dx}\right]$$

Ky=0, y=0 and Kz=Kx and thus$\boldsymbol{\sigma = 0}$

Results Same conditions as the previous example of this rate.

<table>
<tr><th>Pollution Rate</th><th>Simulation</th></tr>
<tr>
<td>

u=[5400,4320,5040,5040,4680,4320,5040,5040,5400,3960,5760,5760,7920,13320,11160,11880,9000,6120,7560,4680,4680,7200,4680,4680] m/s
x0=1; h=300;

R = 0.9353 RMSE = 2.3350

Q=[3,4,5,5,4,5,6,6,11,29,52,68,69,66,56,56,58,50,23,6,6,7,2,2]

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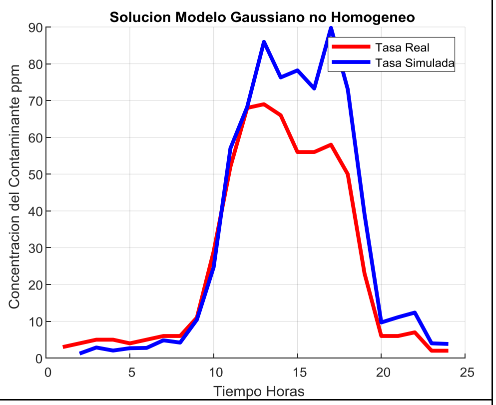

</td>
</tr>
<tr>
<td>

u=[1700,1200,1200,1700,1500,1500,1600,1600,1400,1100,1600,1900,2900,4500,5400,6300,5900,6200,6300,4600,4000,3100,2800,2000] m/s

R = 0.9208 RMSE = 2.1291

Q =[1,1,1,1,2,2,3,2,6,11,29,39,43,41,44,42,38,34,21,18,21,17,19,11]

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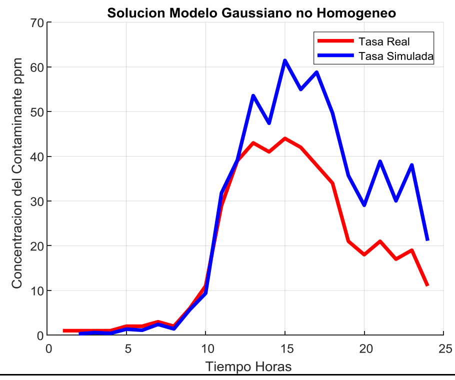

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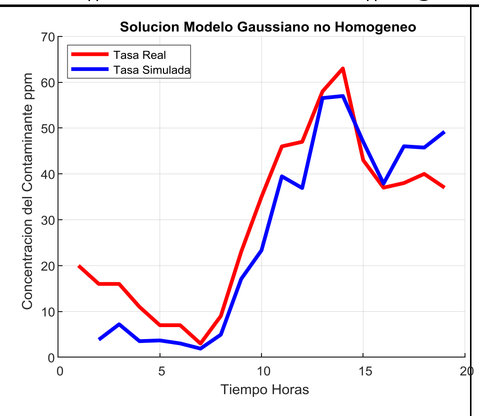
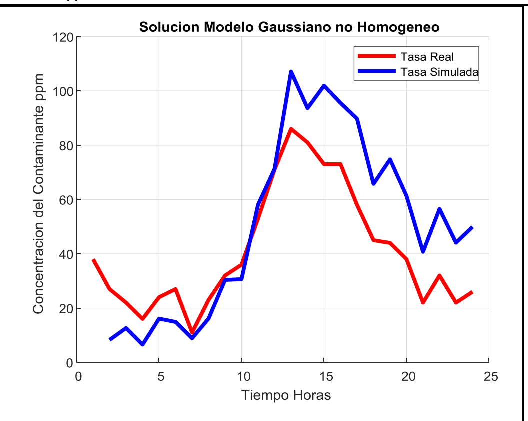
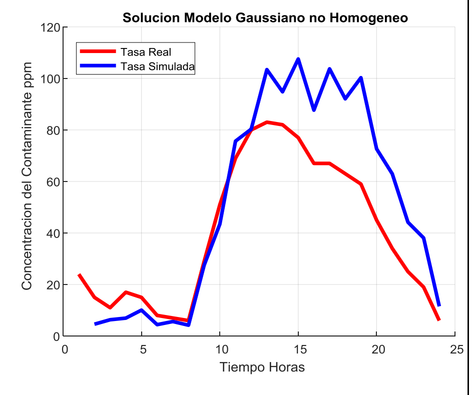
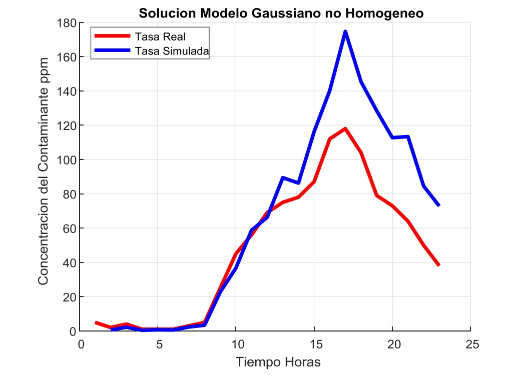
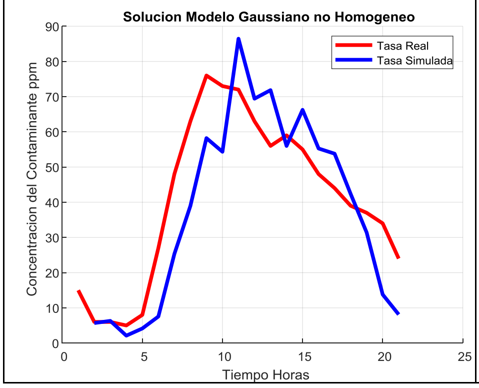
</tr>
</table>

Model of days withx0=1 h=300

Pollution Rate 5th june 2023	Pollution Rate 6th june 2023

	
Pollution Rate 7th june 2023	**Pollution Rate 8th june 2023**
	
Pollution Rate 9th june 2023	
	Using the Correlation Coefficient and RMSE Estimators 9th June R = 0.8262 RMSE = 2.66 8th June R = 0.9244 RMSE = 5.46 7th June R = 0.8940 RMSE = 3.97 6th June R = 0.8325 RMSE = 3.97 5th June R = 0.8889 RMSE = 1.90

Parabolic Model with Chemical Reaction

$$\frac{\partial \varphi}{\partial t} + a\frac{\partial \varphi}{\partial x} - c\frac{\partial^2 \varphi}{\partial x^2} + \sigma\varphi = Q(t)\delta(x - x0)$$

$$\varphi(x,0) = 0 \quad 0 < x < l$$

$$c\frac{\partial \varphi(l,t)}{\partial x} = 0 \qquad t > 0$$

$$c\frac{\partial \varphi(0,t)}{\partial x} - c\varphi(0,t) = 0 \qquad \sigma > 0$$

Solution

$$\varphi(x,t)=\sum_{n=m}^{k}\left[\cos(x\lambda)-\frac{r}{\lambda}\operatorname{sen}(x\lambda)\right]e^{-(\mu\lambda^2+s)t+r(x-x0)}\int_0^t d_k e^{(\mu\lambda^2+s)\tau}Q(\tau)d\tau$$

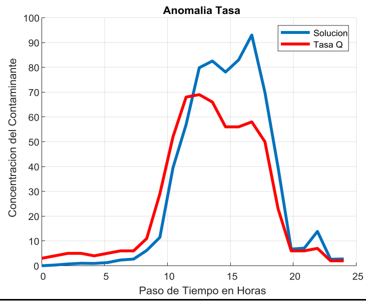
Coefficients with the Delta Modified the part of the Sinus

$$dk=\left[-\frac{0.5+\cos(x0\lambda)\left(\frac{\sin(\lambda)^2}{2\lambda}\right)+\sin(x0\lambda)\left(0.5\left(1-\frac{\sin(2\lambda)}{2\lambda}\right)\right)}{\frac{r}{2\lambda}\left(1-\frac{\sin(2\lambda)}{2\lambda}\right)}\right]$$

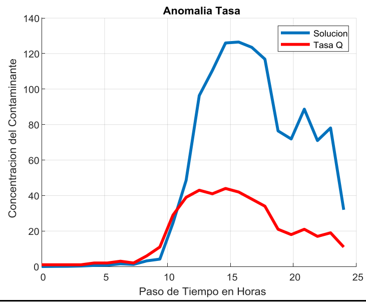
Results Same conditions as the previous example of this rate.

<table>
<tr><th>Pollution Rate</th><th>Simulation</th></tr>
<tr><td>u=[5.400,4.320,5.040,5.040,4.680,4.320, 5.040,5.040,5.400,3.960,5.760,5.760,7.920, 13.320,11.160,11.880,9.000,6.120,7.560, 4.680,4.680,7.200,4.680,4.680] m/s

Q =[3,4,5,5,4,5,6,6,11,29,52,68,69,66, 56,56,58,50,23,6,6,7,2,2]

R = 0.9037 RMSE = 2.7240</td><td>
</td></tr>
<tr><td>u=[1.700,1.200,1.200,1.700,1.500,1.500 ,1.600,1.600,1.400,1.100,1.600,1.900, 2.900,4.500,5.400,6.300,5.900,6.200, 6.300,4.600,4.000,3.100,2.800,2.000] m/s

Q =[1,1,1,1,2,2,3,2,6,11,29,39,43,41, 44,42,38,34,21,18,21,17,19,11]

R =0.8491 RMSE = 9.6192</td><td>
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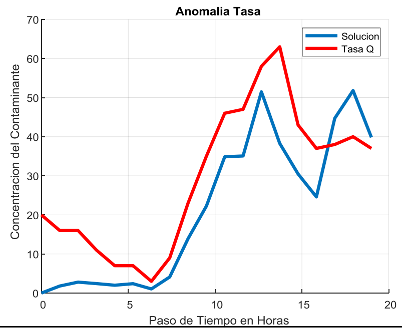
</table>

Model ofDays

<table>
<tr><th>Pollution Rate 5th june 2023</th><th>Simulation</th></tr>
<tr><td>R = 0.8432 RMSE = 2.6599</td><td>
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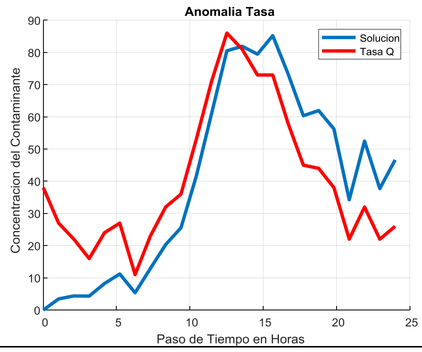
<tr><th>Pollution Rate 6th june 2023</th><th>Simulation</th></tr>
<tr><td>R = 0.7215 RMSE = 7.1252</td><td>
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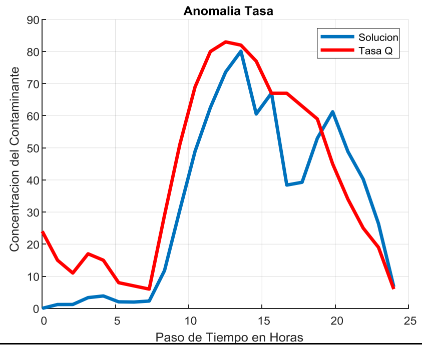
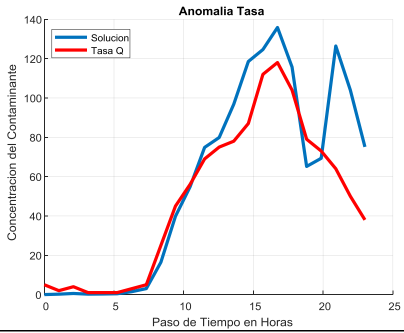
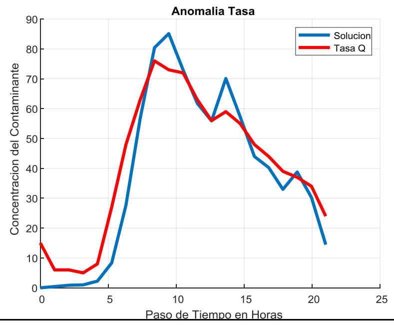
<table>
<tr><th>Pollution Rate 7th june 2023</th><th>Simulation</th></tr>
<tr><td>R = 0.8583 RMSE = 5.1621</td><td>
</td></tr>
<tr><th>Pollution Rate 8th june 2023</th><th>Simulation</th></tr>
<tr><td>R = 0.8870 RMSE = 4.6507</td><td>
</td></tr>
<tr><th>Pollution Rate 9th june 2023</th><th>Simulation</th></tr>
<tr><td>R = 0.8979 RMSE = 5.9000</td><td>
</td></tr>
</table>

Parabolic Model only Diffusion

$$\frac{\partial \varphi}{\partial t} - c\frac{\partial^2 \varphi}{\partial x^2} = Q(t)\delta(x - x0)$$

$$\varphi(x, 0) = 0 \quad 0 < x < l$$

$$c\frac{\partial \varphi(0, t)}{\partial x} = 0 \qquad t > 0$$

$$c\frac{\partial \varphi(l, t)}{\partial x} + \varsigma\varphi(l, t) = 0$$

Solution

$$\varphi(x, t) = \sum_{n=m}^{k} [\cos(x\lambda)] \int_0^t d_k e^{-\mu\lambda^2(t-\tau)} Q(\tau) d\tau$$

Coefficients with Modified Delta

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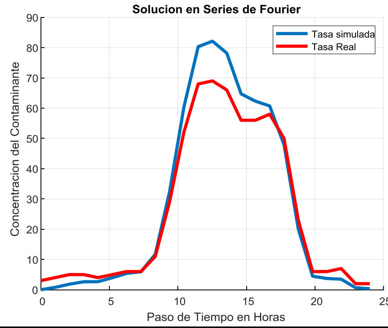
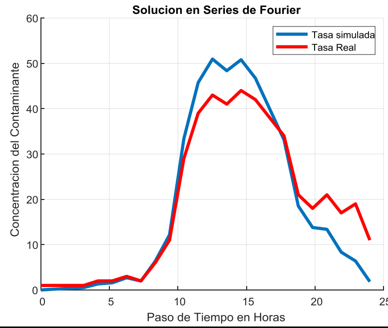
www.ijlret.com || Volume 09 - Issue 08 || August 2023 || PP. 16-36

$$dk = \left[\frac{0.5 + \cos(x0\lambda)\left(0.5\left(1+\frac{\sin(2\lambda)}{2\lambda}\right)\right) + \sin(x0\lambda)\left(\frac{\sin(\lambda)^2}{2\lambda}\right)}{0.5\left(1+\frac{\sin(2\lambda)}{2\lambda}\right)}\right]$$

Results Same conditions as the previous example of this rate.

Pollution Rate	Simulation
u=[5400,4320,5040,5040,4680,4320, 5040,5040,5400,3960,5760,5760,7920, 13320,11160,11880,9000,6120,7560, 4680,4680,7200,4680,4680] m/s **Q =[3,4,5,5,4,5,6,6,11,29,52,68,69,66, 56,56,58,50,23,6,6,7,2,2]** **R = 0.9547RMSE = 204.270**	
u=[1700,1200,1200,1700,1500,1500 ,1600,1600,1400,1100,1600,1900, 2900,4500,5400,6300,5900,6200, 6300,4600,4000,3100,2800,2000] m/s **Q =[1,1,1,1,2,2,3,2,6,11,29,39,43,41, 44,42,38,34,21,18,21,17,19,11]** **R =0.9300 RMSE = 133.8**	

Let's see the diffusive Hyperbolic model with boundary and its respective initial conditions and without Source

Hyperbolic model

$$k\frac{\partial \emptyset}{\partial t} + \frac{\partial^2 \emptyset}{\partial t^2} = a^2\frac{\partial^2 \emptyset}{\partial x^2} + b\emptyset$$

$$\emptyset(x,0) = 0$$

$$\frac{\partial \emptyset(x,0)}{\partial t} = 0$$

$$\emptyset(0,t) = 0$$

$$\emptyset(l,t) = 0$$

By using the following transformation$\emptyset(x,t) = Z(x,t)e^{-kt/2}$It becomes the Klein Gordon Equation

$$\frac{\partial^2 z}{\partial t^2} = a^2\frac{\partial^2 z}{\partial x^2} + (\frac{k^2}{2} + b)z \quad \text{Con } \gamma = \frac{k^2}{2} + b$$

By Separation of Variable we have the solution

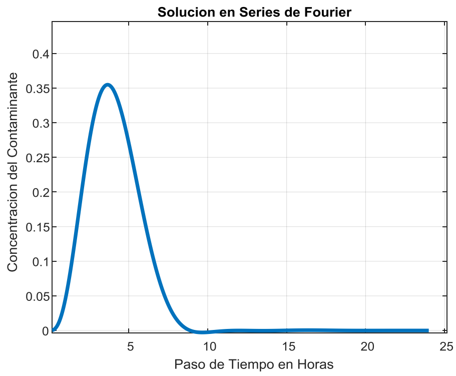
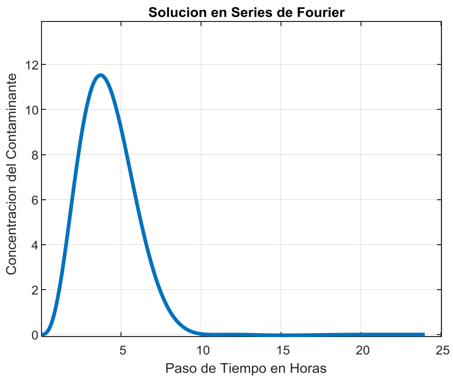
Solution

$$G(x,t) = \frac{sen\left(\sqrt{a^2{\lambda_n}^2 + b\,t}\right)}{\sqrt{a^2{\lambda_n}^2 + b}}$$

So the general solution is

$$Z(x,t)=\sum_{n\geq 1}^{n} sen\left(\frac{n\pi}{l}x\right) sen\left(\frac{m\pi}{l}x\right)\frac{sen\left(\sqrt{a^2{\lambda_n}^2+b}\; t\right)}{\sqrt{a^2{\lambda_n}^2+b}}$$

ResultsWhere C is the Diffusion Coefficient

C=0.80 $\frac{m^2}{s}$ and Wind u=0.09 m/s	C=0.025 $\frac{m^2}{s}$ u=0.09 m/s
	

Let's see the diffusive Hyperbolic model with border and its respective initial conditions, with diffusive, advective and without Source terms.

Hyperbolic model

Now we will see the behavior with and the same initial and boundary conditions.

$$k\frac{\partial\emptyset}{\partial t}+\frac{\partial^2\emptyset}{\partial t^2}=a^2\frac{\partial^2\emptyset}{\partial x^2}+b\frac{\partial\emptyset}{\partial x}$$

With the same transformation we are left with a Klein Gordon Equation, but with

$$\emptyset(x,0)=0$$

$$\frac{\partial\emptyset(x,0)}{\partial t}=0$$

$$\emptyset(0,t)=0\;\emptyset(l,t)=0$$

$$\emptyset(x,t)=Z(x,t)e^{\alpha x-\beta t}$$

$\alpha=\frac{b}{2a^2}$ *and* $\beta=-\frac{1}{2}$ y $\gamma=\frac{a^2}{4(b^2-a^2)}$

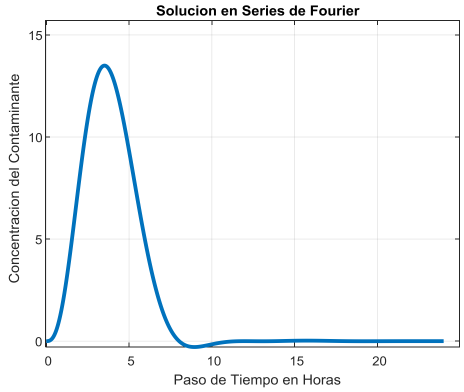
Solution

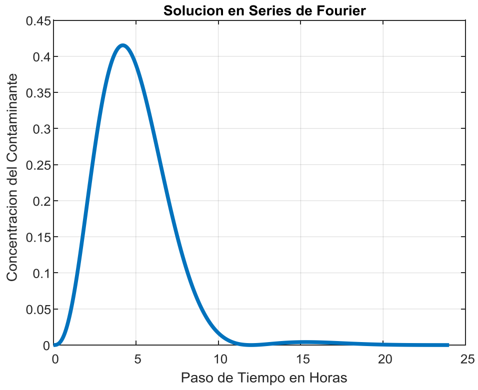
With a similar solution like this the general solution is

$$Z(x,t)=\sum_{n\geq 1}^{n} sen\left(\frac{n\pi}{l}x\right) sen\left(\frac{m\pi}{l}x\right)\frac{sen\left(\sqrt{a^2{\lambda_n}^2+\gamma}\; t\right)}{\sqrt{a^2{\lambda_n}^2+\gamma}}$$

Results

C=0.80$\frac{m^2}{s}$ and Wind u=1.2 m/s	C=0.05$\frac{m^2}{s}$, u=1.2 m/s





Now the following Hyperbolic model with tao other than 1 and less than 1

Model

$$\frac{\partial \emptyset}{\partial t} + \tau \frac{\partial^2 \emptyset}{\partial t^2} + \left(\sigma + \frac{ua^2}{V}\right)\emptyset = Q(t)$$

CI = $\varphi(x,0) = 0$ **and** $\frac{\partial \varphi(x,0)}{\partial t} = 0$

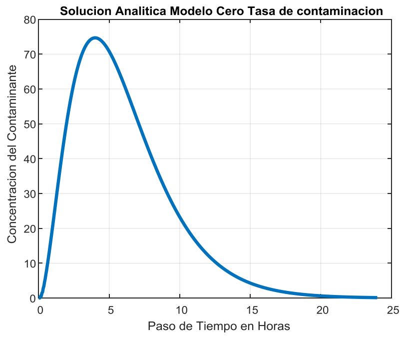
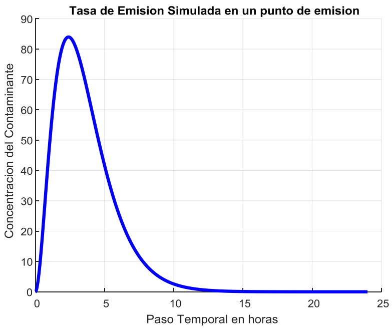
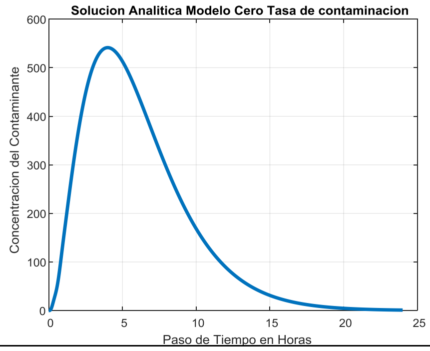
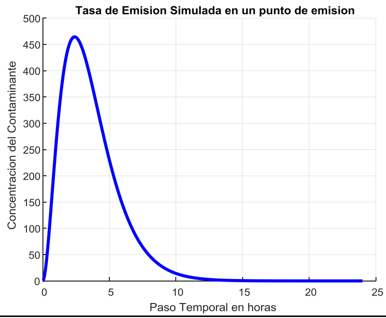
Analytical Solution

$$\varphi(t) = -\left(\frac{Q(t)}{\tau(a+b)}\right)\left[e^{-(a-ib)t} + (a - ibe^{-at})t - 1\right]$$

Con a= $\frac{1}{2\tau}$ **and b =** $\left[\frac{\sigma}{\tau} + \frac{ua^2}{\tau V} - \frac{1}{4\tau^2}\right]$

V is Volume in the Box model

Resultsvelocity pf wind u on m/s

<table>
<tr><td>Analytical Solution
Q=100*(t*t).*exp(-0.5*t);</td><td>Numerical Solution with Separation of Operators</td></tr>
<tr><td>u=1.5 rho=0.1;q=100a=1;V=1;tao= 0.05;

</td><td>sigma=0.1;u=1.5tao1=0.05V=1;a=1;

</td></tr>
<tr><td>Tao= 0.1

</td><td>sigma=0.1;u=1.5;L=1.0;tao1=0.1; V=1; a=1;

</td></tr>
</table>

Results2

Analytical Solution	**Numerical Solution with Separation of Operators**
u=1.5;rho=0.1;q=100;a=1;V=1;**tao= 0.5; y Q=100**	sigma=0.1;u=1.5;tao1=0.5; V=1;a=1;

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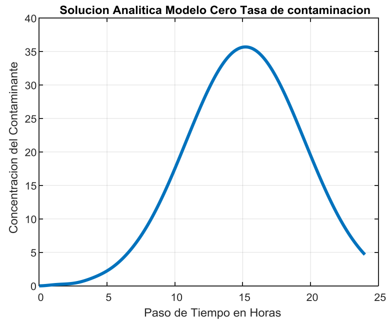
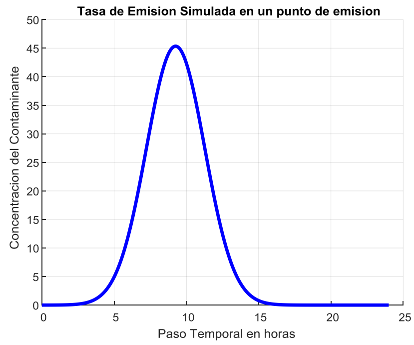
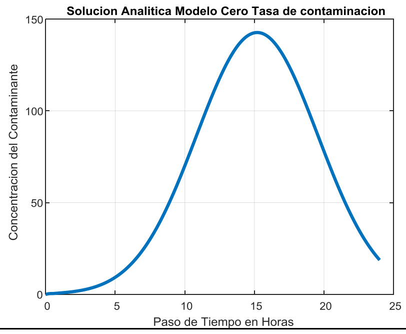
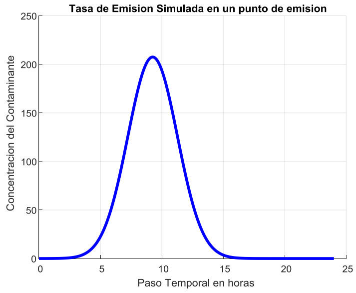
<table>
<tr><td>
</td><td>
</td></tr>
<tr><td>Tao= 0.1; y Q=1

</td><td>sigma=0.1;u=1.5;L=1.0;tao1=0.1; V=1; a=1;

</td></tr>
</table>

Model

$$\frac{\partial\emptyset}{\partial t}+\tau\frac{\partial^2\emptyset}{\partial t^2}-\mu\frac{\partial^2\emptyset}{\partial x^2}=Q(t)\delta(x-x0)$$

$$\frac{\partial\emptyset(0,t)}{\partial x}=0$$

$$\mu\frac{\partial\emptyset(1,t)}{\partial x}+\varsigma\emptyset(1,t)=0$$

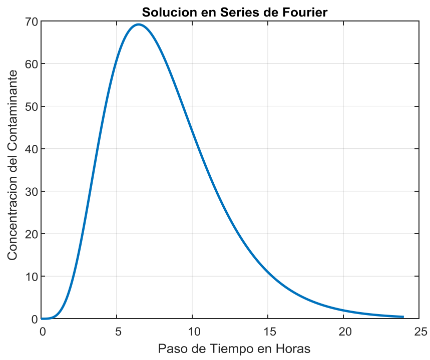
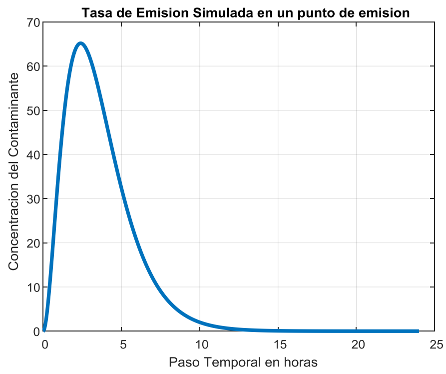
CI = $\varphi(x,0)=0\ \frac{\partial\varphi(x,0)}{\partial t}=0$

Analytical Solution

$$\varphi(x,t)=\sum_{n=1}^{k}\frac{cos(\lambda x)}{ab}\left[1-e^{-(a+i\sqrt{b})t}-(a+i\sqrt{b})t\right]Q(t)d_k$$

With a= $\frac{1}{2\tau}$ **and** **b =** $\left[\frac{\mu\lambda^2}{\tau}-\frac{1}{4\tau^2}\right]$

Results

<table>
<tr><td>Analytical Solution
Q=100*(t*t).*exp(-0.5*t);</td><td>Numerical Solution with Separation of Operators</td></tr>
<tr><td>zeta=5.0; miu=0.05; x0=0.3; R=0.8;T=20 q=100; tao=0.5;

</td><td>miu=0.05; zeta=5.0; tao1=0.5;x0=0.3;R=0.8;

</td></tr>
<tr><td></td><td></td></tr>
</table>

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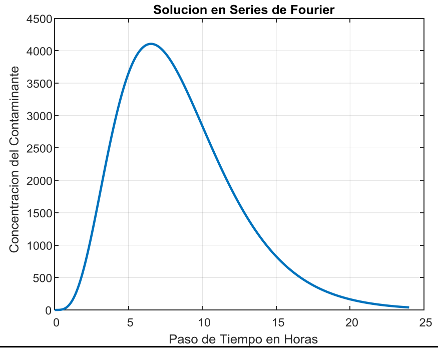
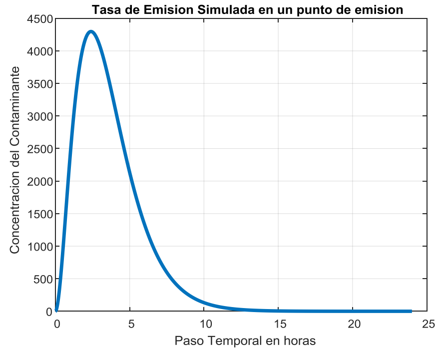
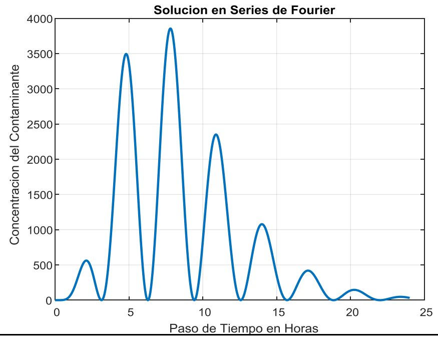
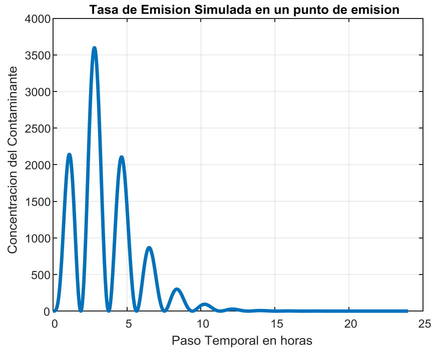
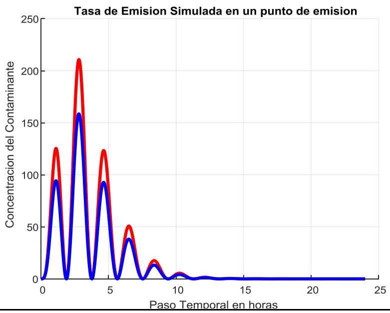
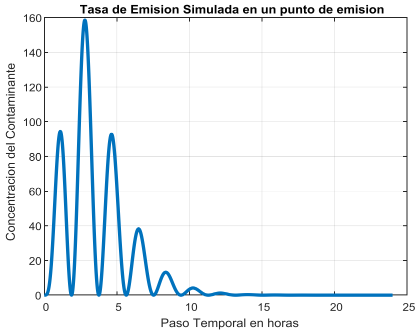
Tao= 0.6 	

Results 2

Analytical Solution	**Numerical Solution with Separation of Operators**
zeta=5.0; miu=0.05; x0=0.3; R=0.8;T=20 q=100; **tao=0.1;** 	miu=0.05; zeta=5.0; tao1=0.1;x0=0.3;R=0.8; 
Tao= 0.5 	

Operator Separation Method see references

For the first Model

$$A = \left(\sigma + \frac{ua^2}{V}\right)$$
$$T = \left(1 + \frac{\tau}{\Delta t} + \frac{\Delta t}{2}A\right)$$
$$\emptyset_{i+1} = [T]^{-1}\Delta t * f(x,t)$$

For the second Model

$$A = (\emptyset_{i-1} - 2\emptyset_i + \emptyset_{i+1})$$
$$T = \left(I + \frac{\tau}{\Delta t} - \frac{\mu\Delta t}{2\Delta x^2}A\right)$$
$$\emptyset_{i+1} = [T]^{-1}\left(\Delta t - \frac{\tau}{\Delta t}\right) * f(x,t)$$

Using the R and RMSE Correlation Coefficient Estimators

$$R = \frac{Mean(O_i - media(O_i)) * Mean(O_p - media(O_p))}{std(O_p) * std(O_o)}$$

$$RMSE = \sqrt{\frac{(O_i - O_P)^2}{N}}$$

Where O_i is observed data and the O_p is the predicted and N the number of data

Conclusions

Within the Hyperbolic models we can see that they are very susceptible to the relaxation term and including the Diffusion coefficient where it will become stable by having a value of 0.5 which can be equated with the Parabolic Model and also with the initial conditions, without the initial condition are both the same and without the relaxation term tao the parabolic model is obtained.

$$\|\emptyset\| \leq \left(\frac{1}{\tau^*}+\frac{1}{2}\right) T\, max\|f(r,t)\| + \frac{1}{2}\|\emptyset^0\| + \frac{1}{2\tau^*}\int_0^t \|\emptyset^0\| d\tau$$

$$\|\emptyset\| \leq T\, max\|f(r,t)\| + \|\emptyset^0\|$$

The hyperbolic model is good and adaptable, but under certain conditions of stability in tao and turbulence with respect to the transport of the material, in the Parabolic Models the Peclet number was used, which helps to have the expected shape in the solution and scaling. That same result, we also see how it changes in a way when having the Diffusion coefficient constant or varying with respect to the wind direction, the Eddy diffusion coefficients are taken as, where the rho is the standard deviation of the vertical wind speed

$$K_x = C_x = \alpha u x = \frac{{\sigma_v}^2}{u} x$$

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