AN ANALYTICAL NON-STATIONARY DISPERSION-DEPOSITION MODEL

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Abstract: In this work an atmospheric dispersion-deposition model to describe the radionuclides concentration after a hypothetical nuclear accident is presented. The developed model has two parts. The first one describes the concentration due to the material released after an arbitrary period from a given source. The second one describes the concentration change during the current period due to the dispersion of the material that is in the atmosphere. Here the solution for the first part is presented.

A non-stationary analytical solution is obtained from the atmospheric diffusion equation. The model solves the transport (convection-diffusion) equation in which the contaminant settling is explicitly incorporated. Regarding the boundary conditions, it is assumed a null diffusion through the mixed layer top and an albedo at the ground level. From the general solution obtained for the contaminant concentration the Gaussian plume formula is derived as a particular case when it is assumed a stationary point source, v_d =0 (total reflection) and v_s=0 (without settling). Assuming $v_d \neq 0$ and v_s= 0, is compared with the Source Depletion Model (SoDM) and with the Surface Depletion Model (SuDM). The agreement is excellent when comparing with the SuDM, which is the exact solution for the diffusion equation when the settling is modeled only in the boundary condition. Two additional cases are presented, the former is the steady state solution: $v_d \neq 0$ and $v_s \neq 0$, and the last one is a non-stationary simulation with a transport time of 3600 s with $v_d \neq 0$ and $v_s \neq 0$. For the last case, two *Erf* functions appear in the solution as result of time integration that model the plume front traveling in the atmosphere.

This new contaminant transport model describes the concentration evolution in a more realistic way, representing the plume falling. This is an improvement respect to the known dispersion-deposition models (SoDM, SuDM).

Key words: *Atmospheric Dispersion-Deposition model, Analytical solution of atmospheric diffusion equation.*

1. INTRODUCTION

There are many codes for the atmospheric dispersion calculations, like AERMOD (Cimorelli et al, 1998), HPDM (Hanna and Chang, 1993), in the nuclear industry can be consider PCCOSYMA (Brown and Ehrhardt, 1995) and MACCS2(Jow, 1990). Each of these codes uses different models to calculate the atmospheric dispersion, based on analytical solutions of the atmospheric diffusion equation (Seinfeld, 1998). A comparative analysis of some of them can be found at Caputo 2003 et al.

Regarding to the dispersion-deposition models, the most common used formulations are:

- The **So**urce **D**epletion **M**odel (**SoDM**): assumes that the downwind pollutant concentration comes from a source whose emission rate change as a function of the distance from the source. This variation is the amount of material deposited on the floor (Pal Arya, 1999), this means that the model assumes that the material is lost at the source rather than on the surface where it is deposited.
- The **Su**rface **D**epletion **M**odel (**SuDM**) assumes a sink at ground that removes the material, which is deposited on the floor. In this case the concentration of material is calculated as the difference between the dispersal from the original source and dispersion from the sink (Pal Arya, 1999), (Horst, 1977).

Murphy and Nelson, 1983, used the SoDM in a Lagrangian model for describing the particle deposition. The decrease from the source in this case is modeled as an exponential function of the emission height, the turbulent diffusivity in the z direction and the deposition velocity. These authors consider the sedimentation rate as a contour condition at the ground level. Other codes that used the SoDM are the ISC3 and AERMOD. The SuDM is not longer used, because the implementation in the atmospheric dispersion codes is difficult despites it provides the exact solution.

This paper presents a **S**ettling **D**ispersion **D**eposition **M**odel (SDDM) for calculating the atmospheric dispersion-deposition of pollutants under non-stationary conditions. This is an analytical solution for the atmospheric dispersion equation, with partial reflection on the floor and total at the top of the mixed layer. The contaminant settling is considered explicitly as a vertical transport term in the differential equation. So the sedimentation and dispersion of the contaminant is described in a more realistic approach, because it incorporates the settling throughout the considered domain. The current models consider that only the material that is near the ground is deposited, no settling in the plume bulk is modeled. Moreover, the computational program implemented to evaluate the SDDM model is simple and fast, prepared to respond in an accidental situation, allowing an effective management of an accidental situation.

2. ANALYTICAL DISPERSION-DEPOSITION MODEL

The main issues of the proposed model are: (1) solves the equation of atmospheric diffusion for non steady state conditions. (2) the dispersion in the wind direction is considered, because depending on the value of diffusivity, the contribution may be important, as will be shown later in this work, and (3) models the settling of pollutant in the term of vertical convective transport. This last is an important point, in the case of particles or dense gases, because it increases the concentration in the neighborhood of the source, mainly at the ground. Assuming that the wind speed and turbulent diffusivity are constant, the atmospheric diffusion equation for a single pollutant species is:

$$\frac{\partial C}{\partial t}+u\frac{\partial C}{\partial x}+v_s\frac{\partial C}{\partial z}-K_x\frac{\partial^2 C}{\partial x^2}-K_y\frac{\partial^2 C}{\partial y^2}-K_z\frac{\partial^2 C}{\partial z^2}=S\left(x,y,z,t\right) \tag{1}$$

Where C is the pollutant concentration dependent *(x,y,z,t)*, u is the wind speed, v_s is the settling velocity and K_i is the turbulent diffusivity in the *i,* direction this three parameters constant at least until the observation time *t, S(x,y,z,t)* is the emission source.

The initial and boundary conditions are:

$$C\left(x,y,z,0\right)=0 \qquad C\left(x,y,z,t\right)\to 0 \ \text{ for } \ \left(x,y\right)\to\infty \qquad \left.\frac{\partial C}{\partial z}\right|_{z=H}=0 \qquad K_z\left.\frac{\partial C}{\partial z}\right|_{z=0}+v_s\left.C\right|_{z=0}=-v_d\left.C\right|_{z=0} \tag{2}$$

v_d is the deposition velocity, which depends on the chemical and physical properties of pollutant and floor.

Solution development

To solve the Equation (1) with the initial and boundary conditions shown in (2) the separation of variables method will be used, similar to that used by Seinfeld, 1998, so *C(x,y,z,t)=A(x,y,t) B(z).* Therefore the Equation (1) results:

$$B\left(\frac{\partial A}{\partial t}+u\frac{\partial A}{\partial x}-K_x\frac{\partial^2 A}{\partial x^2}-K_y\frac{\partial^2 A}{\partial y^2}\right)+A\left(v_s\frac{dB}{dz}-K_z\frac{d^2B}{dz^2}\right)=S(x,y,z,t) \tag{3}$$

From Equation (3), *B(z)* must meet the following homogeneous differential equation and the corresponding initial and boundary conditions:

$$K_z\frac{d^2B}{dz^2}-v_s\frac{dB}{dz}+\lambda B=0 \qquad \left.\frac{dB}{dz}\right|_{z=H}=0 \qquad -K_z\left.\frac{dB}{dz}\right|_{z=0}+v_s\left.B\right|_{z=0}=-v_d\left.B\right|_{z=0} \tag{4}$$

If the solution *B(z) = exp(rz)* is assumed, the characteristic curves of the differential Equation (4) are given by the roots of $K_z r^2-v_s r+\lambda=0$. From the solution assumed, the roots should be imaginary, therefore $v_s^2/4K_z<\lambda$. Then $r=\alpha\pm i\beta$, with α and β given by:

$$\alpha=v_s/2K_z \qquad \beta=\sqrt{\lambda/K_z-\left(v_s/2K_z\right)^2} \tag{5}$$

So, Equation (4) has two possible solutions: $\varphi_1(z)=exp(\alpha z)cos(\beta z)$ and $\varphi_2(z)=exp(\alpha z)sin(\beta z)$. Therefore the general solution is $B(z)=B_c\ _1(z)+B_s\ _2(z)$ with B_c, B_s and β obtained from the boundary conditions. There are infinite solutions for β , therefore the solution for the Equation (4) is:

$$B_m(z)=B_{cm}e^{\alpha z}\left[\cos(\beta_m z)+\frac{\left(\frac{v_d}{K_z}-\alpha\right)}{\beta_m}\sin(\beta_m z)\right] \tag{6}$$

From the ortho-normalization conditions B_{cm} are:

$$B_{cm}^{-2}=\frac{H}{2}+\frac{\sin(2H\beta_m)}{4\beta_m}-(v_d-\frac{v_s}{2})\frac{(\sin(H\beta_m))^2}{K_z\beta_m^2}+\left(v_d-\frac{v_s}{2}\right)^2\left[\frac{H}{2K_z^2\beta_m^2}-\frac{\sin(2H\beta_m)}{4K_z^2\beta_m^3}\right] \tag{7}$$

Due to the series solution for the z direction eq. (3) can be express as:

$$\sum_{m=0}^{\infty}B_m\left(\frac{\partial A_m}{\partial t}+u\frac{\partial A_m}{\partial x}-K_x\frac{\partial^2 A_m}{\partial x^2}-K_y\frac{\partial^2 A_m}{\partial y^2}\right)+\sum_{m=0}^{\infty}A_m\left(v_s\frac{dB_m}{dz}-K_z\frac{d^2B_m}{dz^2}\right)=S(x,y,z,t) \tag{8}$$

Using the variable separation method:

$$\sum_{m=0}^{\infty}B_m\left(\frac{\partial A_m}{\partial t}+u\frac{\partial A_m}{\partial x}-K_x\frac{\partial^2 A_m}{\partial x^2}-K_y\frac{\partial^2 A_m}{\partial y^2}+A_m\lambda_m\right)=S(x,y,z,t) \tag{9}$$

Due to the ortho-normality of $B_m(z)$

$$\frac{\partial A_n}{\partial t}+u\frac{\partial A_n}{\partial x}-K_x\frac{\partial^2 A_n}{\partial x^2}-K_y\frac{\partial^2 A_n}{\partial y^2}+A_n\lambda_n=\int_0^H S(x,y,\hat{z},t)B_n(\hat{z})e^{-2\alpha\hat{z}}\,d\hat{z} \tag{10}$$

Using the Fourier transform on this equation:

$$\frac{\partial\tilde{A}_n}{\partial t}+\tilde{A}_n\left(iu\omega_x+K_x\omega_x^2+K_y\omega_y^2+\lambda_n\right)=\tilde{S}_n\left(\omega_x,\omega_y,t\right) \tag{11}$$

With

$$\tilde{S}_n(\omega_x,\omega_y,t)) = \int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\left[\int_0^H S(\hat{x},\hat{y},\hat{z},t)B_n(\hat{z})e^{-2\alpha\hat{z}}d\hat{z}\right]e^{-\iota(\hat{x}\omega_x+\hat{y}\omega_y)}d\hat{x}d\hat{y} \quad (12)$$

The complete solution for the Equation (8) is:

$$A_n(x,y,t) = \left(\frac{1}{2\pi}\right)^2 \iint_{-\infty}^{\infty} e^{\iota(\omega_x x+\omega_y y)} \left\{\tilde{S}_n(\omega_x,\omega_y,\tau)\left[\iint_{-\infty}^{\infty}\int_0^H S(\hat{x},\hat{y},\hat{z},t)\,B_n(\hat{z})e^{-2\alpha\hat{z}}d\hat{z}\; e^{-\iota(\hat{x}\omega_x+\hat{y}\omega_y)}\,d\hat{x}\,d\hat{y}\right] e^{\gamma(\tau-t)}d\tau\right\} d\omega_x\, d\omega_y \quad (13)$$

The whole solution for the eq. (3) is:

$$C(x,y,z,t) = \frac{1}{4\pi}\sqrt{\frac{1}{K_xK_y}}\int_0^t\iint_{-\infty}^{\infty}\left[\sum_{n=1}^{\infty}B_n(z)\frac{e^{-\lambda_n(t-\tau)}}{(t-\tau)}\int_0^H S(\hat{x},\hat{y},\hat{z},t)B_n(\hat{z})\,e^{-2\alpha\hat{z}}d\hat{z}\right] \exp\left[-\frac{\left[x-\hat{x}-u(t-\tau)\right]^2}{4K_x(t-\tau)}\right]\exp\left[-\frac{(y-\hat{y})^2}{4K_y(t-\tau)}\right] d\hat{x}\,d\hat{y}\,d\tau \quad (14)$$

With $B_n(z)$ given by Equation(6). The above equation is the solution for the pollutant concentration in the receptor position (x,y,z) at time t, considering the source $S(x,y,z,t)$, and K_i, u, v_d and v_s, constants. The solution consists of five terms, which represents: (1) The source integration throughout the domain and up to the time t. (2) The change of concentration due to the time elapsed since the pollutant was release. (3) The dispersion in the z direction. (4) The dispersion and transport in the wind direction. (5) The dispersion in the y direction.

3. RESULTS

To evaluate the general solution eq. (14) first of all must be calculated the β_m values. For this purpose two algorithms are executed in sequential order. The former is the procedure of Van Wijngaarden-Brent Dekker-which combines the methods of the bisection, the bracketing and quadratic reverse interpolation (Press et al 1992). The second one is the bisection algorithms (Press et al., 1992).

While the model is not restrictive with regard to the source, in the presented cases it is used a point source. The results are separated in cases, some of them for different settling and deposition velocities values, and other case for model verification:

1. Comparison, in steady-state condition for v_d =0 (total reflection) and v_s=0 (without settling), of analytical results from solution derived the with the literature from the Equation (14).
2. Comparison between SDDM and SuDM SoDM. For this comparison a stationary and homogeneous source is considered. The evaluation time $t > x/u$ is considered, being x the distance travelled by the plume in one hour and u the wind speed. With regard to v_d and v_s the following conditions are considered:
   a. $v_d \neq 0$ and v_s= 0: this case is directly comparable with SuDM and the SoDM, This comparison is presented because when v_s is equal to zero the three formulation results should be the same.
   b. $v_d \neq 0$ and v_s, 0: this case presents the first difference between the SDDM and SuDM and SoDM. This is because the differential equation that is solved with the SDDM includes the convective transport in the z direction through the settling velocity.
3. Simulation of the dispersion-deposition in a non-stationary condition. For this case 3600 s is considered for the evaluation time. The settling and deposition velocities used are the values for the case 2b.

For all the simulations the coordinate system origin is located at the source, the x direction is aligned with the wind direction; the z axis is the height and the y direction is perpendicular to both previous ones. The values of the settling and deposition velocities used are between 0.0 and 0.010 ms^{-1}. A parametric study is done varying K_x, for the non stationary simulations. The diffusion coefficients values vary within the expected ranges for different weather situations, between 1.0 and 100.0 $m^2\,s^{-1}$.

In all cases the integral of the pollutant concentration in the air was calculated, to corroborate the conservation of mass in the modeling domain. This integral used a 3D integration algorithm.

Analytical solution for a stationary point source v_d =0 and v_s=0

Considering a point source of height h and release rate q the integration of the whole solution shown in Equation (14) is:

$$C(x,y,z,t) = \frac{qe^{-2\alpha h}}{4\pi}\sqrt{\frac{1}{K_xK_y}}\int_0^t\left[\sum_{n=1}^{\infty}B_n(h)B_n(z)\frac{e^{-\lambda_n(t-\tau)}}{(t-\tau)}\right]\exp\left[-\frac{\left[x-u(t-\tau)\right]^2}{4K_x(t-\tau)}\right]\exp\left[-\frac{y^2}{4K_y(t-\tau)}\right]d\tau \quad (15)$$

Due to the boundary conditions is easy to show that $B_n(h)=H^{1/2}\cos(n\pi/Hh)$. If a lineal relation between σ_i^2 and $K_i\,\tau_i$ is assumed, shown in (Senfield, 1998) and the integration for τ is done, the obtained result is:

$$C(x,y,z,t)=\frac{q}{2\sqrt{2\pi u\sigma_y}H}\left[Erf\left(\frac{x}{\sqrt{2}\,\sigma_x}\right)-Erf\left(\frac{x-t\,u}{\sqrt{2}\,\sigma_x}\right)\right] \qquad (16)$$
$$\exp\left[-\frac{y^2}{2\sigma_y^2}\right]\left\{1+\sum_{n=1}^{\infty}\cos\left(\tfrac{n\pi}{H}z\right)\cos\left(\tfrac{n\pi}{H}h\right)\exp\left[\left(\tfrac{n\pi}{H}\right)^2\left(\frac{\sigma_z}{\sqrt{2}}\right)^2\right]\right\}$$

The last equation is the non stationary solution for a punctual source with $v_d=0$ and $v_s=0$. If large time and slender plume approximation is considered, the steady state Gaussian plume model is obtained:

$$C(x,y,z,t)=\frac{q}{\sqrt{2\pi u\sigma_y}H}\exp\left[-\frac{y^2}{2\sigma_y^2}\right]\left\{1+\sum_{n=1}^{\infty}\cos\left(\tfrac{n\pi}{H}z\right)\cos\left(\tfrac{n\pi}{H}h\right)\exp\left[\left(\tfrac{n\pi}{H}\right)^2\left(\frac{\sigma_z}{\sqrt{2}}\right)^2\right]\right\} \qquad (17)$$

Finally, Equation (17) is the same that the one presented by Seinfeld, 1998 for steady state Gaussian plume model with a point and uniform source with total reflection on the ground.

Comparison between SDDM and SuDM SoDM

Case 2a: In this case v_d =-0.010 ms^{-1} and v_s=0.0 ms^{-1} are considered. In Figure 1 shows the Cross Integrated Concentration (CIC) at the ground level for SDDM, SuDM and SoDM. The results obtained with the first two models are quite similar because the settling velocity is null, while the third is significantly different to the previous ones. It is important to mention that the difference observed between SDDM and SuDM is because the former is an approximation through a series to the exact solution of the problem, while the SuDM is the exact solution to the Gaussian stationary model with deposition on the ground.

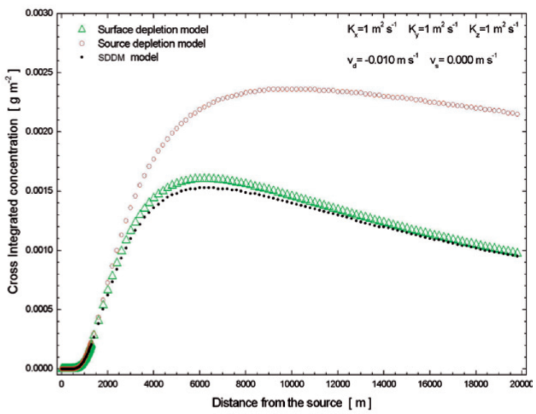

Figure 1. CIC at a ground level for the three models with v_d =-0.010 ms^{-1} and v_s=0.0 ms^{-1}

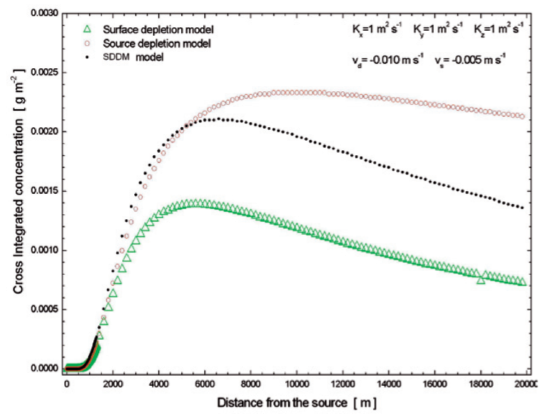

Figure 2. CIC at a ground level for the three models with v_d =-0.010 ms^{-1} and v_s=-0.005 ms^{-1}

Case 2b: In this case v_d =-0.010 ms^{-1} and v_s=-0.005 ms^{-1} are considered. The result of SuDM will differ significantly from those of SDDM. This is because the former considers a fictitious deposition velocity, that is the sum of settling and deposition velocity at ground level and is therefore considered in the boundary condition. Due to this, the pollutant removal becomes effective when it approaches to the ground. The SDDM model predicts that the concentration (Fig. 2) near the source is greater than that predicted by SuDM, because pollutant coming from the upper layers of the atmosphere due to the explicit modeling of settling.

4. NON-STATIONARY CASE

In this case v_d =-0.010 ms^{-1} and v_s=-0.005 ms^{-1} are considered. The SDDM model can predict the plume front movement because it is a time dependent formulation. The time considered for the concentration evaluation is at 3600s, that is the typical averaging time for meteorological data.

To compare the spread in the wind direction, three values for K_x are used 1, 10 and 100 m^2 s^{-1}, which correspond to stable atmosphere, neutral and unstable atmospheric stability conditions (Seinfeld, 1998). The wind speed considered is 2 m s^{-1}.

Figure 3 shows the ground level concentration in the wind direction for different values of K_x. This figure shows that the contaminated area is grater if K_x increases. The upper right picture of the same figure shows the ground level concentration in the *(x,y)* plane, predicted by the SDDM model. The lower right picture of the same figure shows a section in a *(x,z)* direction at the plume center line, where the plume falls due to the settling and deposition velocities.

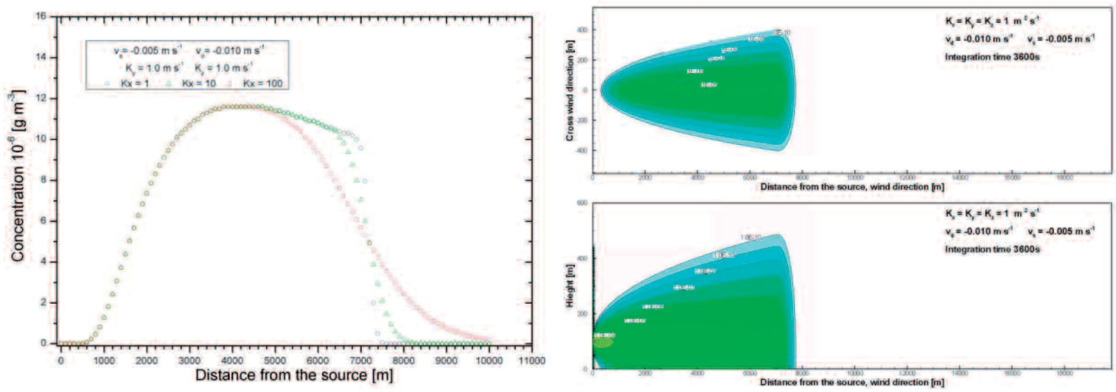

Figure 3. Left: ground level concentration above the plume center line for different K_x. Right-upper: ground level concentration. Right-lower *(x,z)* at the plume center line direction.

5. CONCLUDING REMARKS

This paper presents a new model based on a non-stationary analytical solution of the atmospheric diffusion equation which includes the settling velocity in the differential equation. The main characteristics are:

- The settling velocity is modeled as a convective term in the differential equation, which, in the case of particles or dense gases, is an important topic.
- The diffusion in the wind direction, because depending on the value of diffusivity, the contribution may be important, as is demonstrated above.
- The diffusion coefficients, wind speed and the sedimentation and deposition velocities are constant during the transport time; this means that the atmospheric condition remains constant during this period.
- Partial reflection of the pollutant on the floor and total reflection at the top of the mixed layer.
- The initial concentration of pollutants in the air is zero.
- There are no restrictions about the source type.

With the aforementioned assumptions a formulation obtained shows satisfactory comparisons with the widely used models as the SuDM and the SoDM as seen in figures presented in the preceding paragraphs. Differences between SuDM and SDDM, when v_d is different from zero and v_s, zero is because the first is the exact solution to this problem while the latter is an approximation. Nevertheless this difference does not exceed in any case 5%.

Regarding the status of non-stationary, the model predicts the progress of the plume considering the wind transport and the diffusion in the wind direction, a situation that is not considered on stationary models.

New developments are being implemented to model wind changes using as source the previous hour plumes.

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