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Methodology to Estimating Aquatic Dispersion of Effluents from Accidental and Routine Releases

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1 ABSTRACT

This paper presents a methodology to analysis of dispersion of radioactive materials in an aquatic environment, specifically for estuaries, based on the Regulatory Guide 1.113. The objective is to present an adaptation of methodology for computational user, that it is possible by means of the use of numerical approximations techniques.
The methodology to be present consist in a numerical approximation of the Navier-Stokes Equation applied in a finite medium with known transport mechanisms, such as Coriolis Effect, floor drag, diffusion, salinity, temperature difference and adhesion per water molecule. The basis of methodology is substantiated in a transport diffusive-convection equation, which has similarity with the Partial Differential Burgues' Equation for one dimension and with the Kardar-Parisi-Zhang Equation for multidimensional cases.

1. INTRODUCTION

The Liquid Waste Management System (LWMS) is designed to ensure that liquids and liquid wastes produced during normal operation, including anticipated operational occurrences (AOOs), are handled, processed, stored, and released or routed to their final destination in accordance with the relevant regulations [1]. In the case of Brazil, these regulations come from *Comissão Nacional de Energia Nuclear* (CNEN).

In order to comply with the relevant regulations, NRC suggests the Regulatory Guide (RG) 1.113 [2] as an acceptable methodology for the analysis of radioactive material dispersion from nuclear reactors to unrestricted areas [1]. The result of the analysis should be satisfactory if the dose values for any individual in an unrestricted area, considering all routes of exposure to the radioactive material, do not exceed the dose limits determined in CNEN 3.01 [3] .

1.1 Scope

Understanding the relevance and wide application of the methodology on dispersion of liquid radioactive materials, addressed in RG 1.113, this paper proposes to carry out the following activities:

- An approach on the methodology of radioactive materials dispersion analysis for estuaries, as well as its applications;
- Discourse about accidents of release of liquid radioactive material and acceptable premises for application of the methodology;
- Approach on phenomena involved in the dispersion analysis of liquid radioactive material;
- Present solution methods for the dispersion analysis; and
- To approach methods of numerical solution for the computational treatment of the phenomenon of dispersion.

2 METHODOLOGY OF RADIACTIVE MATERIALS DISPERSION ANALYSIS

RG 1.113 presents application cases for dispersion analysis; however, this paper will be based on estuaries. For this case, the methodology addressed by the Regulatory Guide consists of the Burgers' Equation. This equation is one of the most celebrated examples of nonlinear diffusion equation. It arose (Burger, 1948) as a simplified form of the Navier-Stokes equation, in an attempt to study some aspects of turbulence. It appears also in gas dynamics, in the theory of sound waves and in traffic flow modelling and it constitutes a basic example of competition between dissipation (due to linear diffusion) and steepening (shock formation due to the nonlinear transport term) [4]. The Non-Linear Burgers' Equation that has the following form [5]:

$$\frac{\partial u}{\partial t} + u\,\frac{\partial u}{\partial x} = \beta\,\frac{\partial^2 u}{\partial x^2} \tag{1}$$

This equation approaches the methodology indicated by RG 1.113 for the analysis of dispersion of liquid radioactive material in estuaries, however due to the fact that the material is radioactive, the Burgers' Equation in this format is incomplete. For the consideration of the radioactivity present in the material, the Burgers' Equation must be adapted. This adaptation consists of the consideration of a term known as space-time noise. By the addition of this term, the Burgers' Equation takes the following form:

$$\frac{\partial u}{\partial t} + u\,\frac{\partial u}{\partial x} = \beta\,\frac{\partial^2 u}{\partial x^2} - \lambda\,\frac{\partial u}{\partial t} \tag{2}$$

This stochastic partial differential equation, is equivalent to the Kardar–Parisi–Zhang equation in a field $h(x,t)$ upon substituting $u(x,t) = -\lambda\,\partial h/\partial x$. The Burgers' Equation only applies in one spatial dimension, whereas the Kardar–Parisi–Zhang equation applies to multiple dimensions.

For the case of the dispersion, the concentration of the radioactive element by volume of analysis is considered as the main variable. For this, the modified Burgers' Equation must be written as:

$$\frac{1}{A}\frac{\partial(AC)}{\partial t}+\frac{1}{A}\frac{\partial(AUC)}{\partial x}=\frac{1}{A}\frac{\partial(AE\frac{\partial C}{\partial x})}{\partial x}-\lambda C \quad (3)$$

Where:

- A (x,t) is the cross-sectional area of material flow;
- E(x) is the sectionally averaged, one-dimensional longitudinal dispersion coefficient;
- U(x,t) is the sectionally averaged longitudinal velocity;
- λ is the decay constant;
- t is the analysis time; and
- C is the concentration in terms of radioactive activity and cross-sectional area.

The Burguer's Equation presented (Eq. 3) is the Linear Burguer's Equation, transformed by Hopf-Cole Transformation Method, modified for dispersion analysis with radioactive material. The transformation was necessary for the determination of an analytical solution and to determine the stability conditions of the numerical approximation presented during the paper. With the application of the Hopf-Cole Method, the Burger's Equation results in a parabolic equation that has known conditions for the application of numerical methods.

The simplified model by Eq. 3 generates results whose graph has the following format:

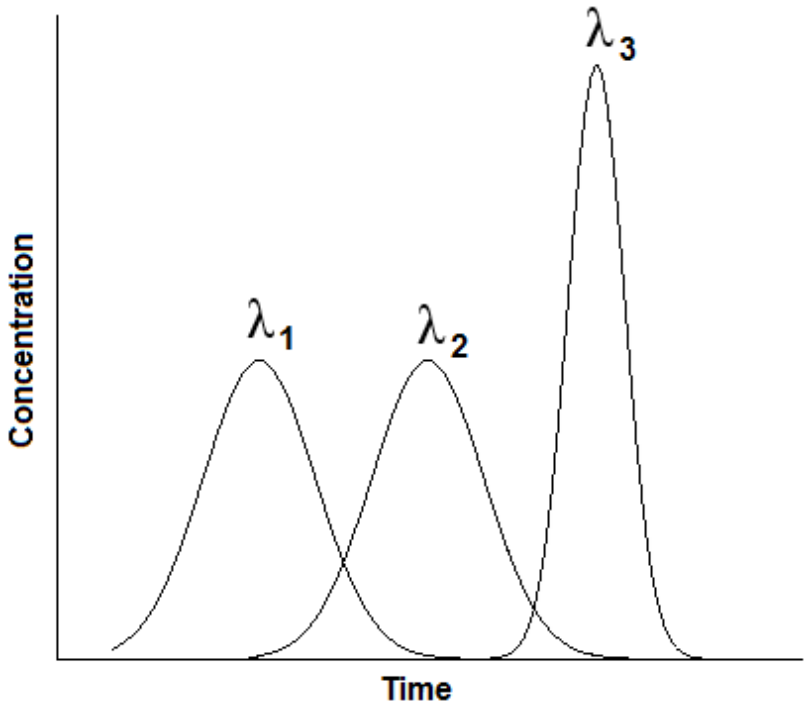

Figure 1: Shape of Concentration by Time

The Fig. 1 represents the concentration for three different radioactive materials for a distance, analysis time and assumptions defined.

2.1 Use of the Methodology for Analysis of Liquid Radioactive Release in Estuaries

There are simple and complex methods for the solution of the dispersion model. The simplest models depend on the "tidally averaged" approximation, in which the tidal oscillations are not included explicitly, but are considered to be responsible for large-scale longitudinal diffusion. The more elaborate "real-time" models consider the actual tidal flow to be advective, with longitudinal diffusion occurring through motions having time scales considerably shorter than a tidal cycle [2].

Regulatory Guide 1.113 presents two cases of solution one for stationary states and another one for short releases. For the stationary states, the guide presents the following simplification of the model [2]:

$$E\frac{d^2C}{dx^2} - U\frac{dC}{dx} - \lambda C = 0 \tag{4}$$

The model is based on a steady state under conditions in which the variables velocity, longitudinal diffusion coefficient and cross-sectional area are constants. For this, the analytical solution is given by [2]:

$$C = \frac{W}{AU\sqrt{1+\frac{4\lambda E}{U}}}\, e^{\left(\frac{U}{2E}\left[1\pm\sqrt{1+\frac{4\lambda E}{U}}\right]x\right)} \tag{5}$$

Where W is the amount of activity introduced and x is the release point distance.

For short releases, the RG 1.113 presents the following simplification of the model (given by equation 3):

$$E - \frac{dC}{dt} + U\frac{dC}{dx} = \frac{d^2C}{dx^2} - \lambda C \tag{6}$$

The model considers the variables velocity, longitudinal diffusion coefficient and cross-sectional area are constants. For this, the analytical solution is given by [2]:

$$C = \frac{M}{A\sqrt{4\pi Et}}\, e^{\left(\frac{(x-ut)^2}{4Et} - \lambda t\right)} \tag{7}$$

Where M is the release rate and x is the release point distance.

2.1.1 Acceptable premises for application of the methodology

A premise for applying the methodology for dispersion analysis of liquid radioactive material in estuaries is the extreme case consideration. For this, the analysis can be considered for a hypothetical case in which the radioactive material travels from a point of release to the point of analysis, which should be short and inside of the installation site, solely by the diffusion mechanism. By means of this premise, all radioactive material is considered in the dose analysis before it is directed to a point beyond the analysis. If the dose values are below the limit, values in the unrestricted area will comply with the established dose limits.

Another acceptable premise is to consider the point of analysis at the center of the volume of dispersed material at the site of the installation and to consider the diffusion mechanism as the only means of moving the material. If the dose limits for the analysis time are less than the established limits, the facility is acceptable as determined by current regulations.

Through the assumptions discussed, the methodology for short duration can be used and simplified so as not to consider the velocity of the medium. Only the diffusion mechanism is considered, which leads to a processing gain during the analysis of the dispersion phenomenon and ease in the treatment of the model.

2.2 Dispersion Mechanisms

In addition to diffusion, several other mechanisms may affect the dispersion of a material in a liquid medium. Among them:

- Difference in salinity;
- It differs from temperature;
- Coriolis effect;
- Adhesion to water molecule;
- Floor drag effect; and
- Drag caused by wind.

The consideration of these mechanisms results in more real but more demanding results of processing power. Most of these variables are represented by variable vectors in space and time, thus constituting large matrices with dynamic cells, that is the values oscillate for different times of analysis.

Without the use of computational processing, the processing for dispersion analysis of radioactive material becomes impractical. The use of computational processing nevertheless becomes effective using techniques of numerical methods for the evolution steps of the analysis computational.

2.3 Application of the Methodology for Dispersion Analysis of Liquid Radioactive Material

The application of the presented methodology is vast and can be used for analysis of concentrations in diverse situations, such as:

- Analysis of passage of radioactive material in pipes;
- Analysis of accidents with release of radioactive material in liquid media;
- Control of material in chemical and volumetric control systems; and
- Analysis with non-radioactive materials, which will depend on the correct adoption of the initial and boundary conditions.

In addition to the nuclear sector, with correct considerations the methodology can be used in several research sectors, which draws attention to methodologies that describe material dispersion phenomena.

3 PROPOSAL OF NUMERICAL SOLUTION FOR THE DISPERSION OF LIQUID RADIOACTIVE MATERIAL IN ESTUARIES

Using numerical methods, a more detailed analysis of each point of interest of the dispersion phenomena is possible. In addition, possible problems of analytical solutions can be intermediated by the use of numerical methods. The use of numerical modeling allows a more efficient treatment for the consideration of variables that have complexity in size and processing. Thus, this paper proposes the use of concepts involved with finite differences for the elaboration of an equation capable of nodalizing a region for solution study and comparison with the analytical solution for the dispersion methodology presented in RG 1.113, which should be evaluated, discussed and tested for its accuracy.

3.1 Approximation Mechanisms for Derivative Solutions

The proposed numerical solution that this paper proposes involves the combination of operators of finite differences, such as:

- Centered Difference Operators;
- Retrograde Difference Operators; and
- Advanced Differential Operators.

The obtaining of this operator to be given by means of the expansion of Taylor's Series. This series have the following format:

$$f(x) = f(x_0) + f'(x_0)(x - x_0) + \frac{f''(x_0)}{2!}(x - x_0)^2 + \cdots + \sum_{n=0}^{\infty} \frac{f^{(n)}(x_0)}{n!}(x - x_0)^n \quad (8)$$

Taylor's Theorem gives quantitative estimates on the error introduced by the use of such an approximation. The polynomial formed by taking some initial terms of the Taylor's series is called a Taylor's polynomial. By manipulating the Taylor's Series it is possible to determine approximations of derivatives with their respective approximation errors O (h^n). Thus, the operators are given by:

Be $\frac{\partial y}{\partial x}$ the derivative to be approximated. For such [6]:

$$\Delta y(x_j) = \Delta y_j \equiv y(x_j + h) - y(x_j) = y_{j+1} - y_j \quad (9)$$

is the Advanced Differential Operator;

$$\nabla y(x_j) = \nabla y_j \equiv y(x_j) - y(x_j - h) - = y_j - y_{j-1} \quad (10)$$

is the Retrograde Difference Operator; and

$$\delta y(x_j) = \delta y_j \equiv y\left(x_j + \frac{h}{2}\right) - y\left(x_j - \frac{h}{2}\right) = y_{j+\frac{1}{2}} - y_{j-\frac{1}{2}} \quad (11)$$

is the Centered Difference Operator.

For second-order derivatives $\left(\frac{\partial^2 y}{\partial x^2}\right)$ the approximation is given by:

Be $\frac{\partial^2 y}{\partial x^2}$ the derivative to be approximated. For such, the approximation is represented by the following combination of Centered Difference Operator:

$$\frac{\partial^2 y}{\partial x^2} = \frac{1}{\Delta x^2}(y_{j+1} - 2y_j + y_{j-1}) \quad (12)$$

3.2 Approximation of the Methodology of Liquid Radioactive Material Dispersion Analysis

Considering the methodology presented in RG 1.113 for estuaries (Eq. 3), the differential equation can be reduced to:

$$E\,\frac{\partial^2 C}{\partial x^2} = \frac{\partial C}{\partial t} + \Psi\frac{\partial C}{\partial x} + \Phi C \quad (13)$$

Where:

- $\Psi = U - \frac{1}{A}\frac{\partial AE}{\partial x}$; and

- $\Phi = \frac{1}{A}\frac{\partial AU}{\partial x} + \lambda.$

After the differential equation, it is possible to apply the finite difference operators to obtain:

$$\frac{C_{j,K+1} - C_{j,k}}{\Delta t} = \frac{E}{\Delta x^2}\left(C_{j+1,k} - 2C_{j,k} + C_{j-1,k}\right) - \frac{\Psi}{2\Delta x}\left(C_{j+1,k} - C_{j-1,k}\right) - \Phi C_{j,k} \qquad (14)$$

Simplifying the approximation, it is possible to obtain the following expression:

$$C_{j,K+1} = C_{j,k} + A\left(C_{j+1,k} - 2C_{j,k} + C_{j-1,k}\right) - B\left(C_{j+1,k} - C_{j-1,k}\right) - \Phi C_{j,k} \qquad (15)$$

Where:

- $A = \frac{E\Delta t}{\Delta x^2}$; and
- $B = \frac{\Psi \Delta t}{2\Delta x}$.

The approximation obtained is progressive in time and centered in space. This scheme is of first order of accuracy in time and of second order in space. The term advective can generate instability due to the appearance of the numerical diffusion, however, it is possible to obtain a stabilization by adding the actual diffusion, provided that the time step is smaller than the diffusive stability limit. The stepping stencil for the approach is shown in Fig. 2.

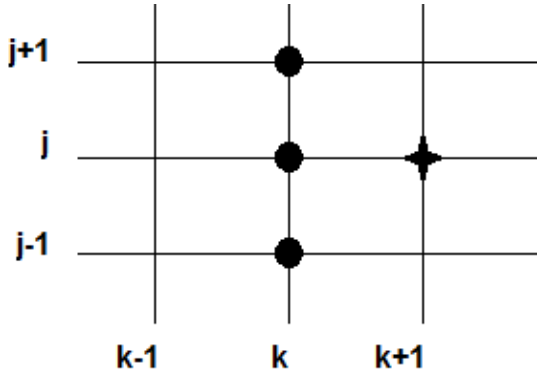

Figure 2: Stencil of Approximation Method

In Fig. 2 it is possible to observe that with three points of entry (j,k, j-1,k and j+1,k) a point in j,k+1 is obtained. However, the method should have its stability controlled through pre-stabilized conditions. For the stability control, the proposal is to use the Von Neumann's Method. This method is a procedure used to check the stability of finite difference schemes as applied to linear partial differential equations. The analysis of the method is based on the Fourier decomposition of numerical error. Applying the Von Neumann's Method it is possible to obtain the following stability conditions:

$$-4A - \Phi + 1 \leq 1 \qquad (16)$$

$$-2A - 2B - \Phi + 1 \leq 1 \quad (17)$$

$$-\Phi + 1 \leq 1 \quad (18)$$

$$-4\mathrm{A} - \Phi + 1 \leq 1 \quad (19)$$

3.2.1 Comments about the Approach

One of the difficulties with the approach is give by determining the point j+1,k possible due to the lack of this information, which comes down to a boundary problem. Due to the characteristics of the phenomenon of the dispersion and the radioactive activity of the material to be dispersed, it is possible to determine conditions for the aforementioned point to be known. From the radioactivity bias, it is possible to know the quantity of material in a control volume (domain of the analysis) by means of the following formula:

$$A = A_0 e^{-\lambda t} \quad (20)$$

Known as the Law of Exponential Decay, (Eq. 20) can be used to determine boundary conditions associated with the dispersion analysis of a radioactive material. In contrast, the bias of the mass transport phenomenon is known that

$$C = 0 \; for \; x \to \infty \quad (21)$$

Where x represents a point that distances to the infinity of the release site.

For the determination of initial values, it is necessary to know the radioactive concentration of the analysis material, that is, activity of the material by volume of the sample, which can be easily determined by the applicant of the methodology.

Another important consideration to be made is the precision of the solution. It is not the scope of the paper to present comparisons between the approach and the analytical solution of the methodology. This paper sums up an approach to a dispersion analysis methodology presented by a recognized international body and how it can be adapted for the use of computational processing. However, it is of interest that the approach is eventually applied and tested for its stability and accuracy, which should be sufficient to determine their limitations and use versatility.

3. CONCLUSIONS

The methodology presented in RG 1.113 has a wide application, which is disseminated by several research sectors. A more realistic analysis with the use of the methodology requires consideration of variables that require a considerable amount of processing power. In order to mediate this drawback, it is possible to use numerical solution methods for these variables to be processed computationally.

Using numerical methods, a more detailed analysis of each point of interest of the dispersion phenomena is possible. In relation to the boundary conditions (initial and boundary conditions) involved in the application of the dispersion analysis, the use of the Exponential Decay Law (Eq. 20) may reveal important information for the appropriate treatment of the numerical approximation.

The numerical approximation obtained is of the first order of accuracy in time and of second order in space. However, it should be applied and tested in relation to its accuracy, stability and assumptions considered in the analysis. In the event of problems in the application of the approximation, due to the appearance of the numerical diffusion, it can be worked with other operators of finite differences in order to obtain an approximation of greater accuracy and greater stability.

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