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THE MONTE CARLO METHOD IN NON-HOMOGENEOUS MEDIA FOR EVALUATING THE RISK OF EXPLOSION IN TANKS

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The paper presents an application of the Monte Carlo method to a model of a parallel-plane non-homogeneous medium corresponding to a parallelepiped tank. We derive the expressions for the primary and secondary statistical estimators. The network is considered rectangular, and the non-homogeneous media have the separation surface parallel to the coordinate axes. Based on these principles, we have calculated the electrostatic field at the air-gasoline separation surface and evaluated the risk of explosion based on the electric charge state of the gasoline.

1. INTRODUCTION

When an insulating liquid with electrical resistivity between 10^7 Ωm and 10^{14} Ωm passes through a pipe, it becomes electrostatically charged. The electric charge is positive if the pipe is metallic. If the pipe is made of dielectric material, the rule [1] is that the medium with higher permittivity gains positive charge. The phenomenon of electrostatic charging is more pronounced in the case of flammable liquids with superior characteristics, such as gasoline. This accumulation of charge can have dire consequences.

Thus, when loading road tankers or railway tank wagons isolated from the ground [2], their walls can reach a dangerous potential. If the electrostatic field created by the voltage between the metal walls and the ground exceeds the value of 30 kV/cm, the risk of explosion is imminent.

Another problem caused by the charging of gasoline flowing through pipes occurs when filling a tank without a floating lid. The charged liquid causes an electrostatic field to appear in the empty space above the gasoline, which, if it exceeds the critical value, can lead to an explosion, also favored by the flammable vapors present in that area. The floating lid, which has recently been equipped on tanks, solves the problem, but there can still be risks related to the appearance of foreign bodies floating on the surface of the gasoline or the deterioration of the grounding system of the movable lid. Of course, the risk of explosion only appears in the air zone of the tank; inside the gasoline, the electrostatic field can be as large as possible, but the lack of oxygen makes the appearance of a triggering spark impossible.

In this paper we will deal with the case of a rectangular tank buried in the ground, with a fixed lid. The volume density of the charge inside the gasoline will be considered constant [3]. We will work with the value of the electric charge density $\rho_v = 10^{-5}$ C/m^3 [1]. Considering the direct proportionality of the electrostatic field with the volume density of the electric charge, the interpretation of the results will be easy for other values of this density. Given the large dimensions of the parallelepiped tanks used in practice (for example, in the Port of Constanța, there are tanks with dimensions on the order of tens of meters), the problem can be considered as parallel plane.

2. A GENERAL OUTLINE OF THE PROBLEM

The tank we have analyzed is 4 meters wide, 10 meters high, 20 meters long and is filled with gasoline up to a height of 8 m. Considering the parallel plane problem, the domain will consist of a rectangle with a base OB = 4 m and height OM = 10 m, filled with gasoline up to the height OA = 8 m, as shown in Fig.1. Using conventional numerical methods in such cases [4,5] involves determining the potential (field) at each point in the domain. For example, the finite difference method with an acceptable step of 5 cm would lead to 16,000 points within the domain [6].

The Monte Carlo method has the advantage that it suffices to determine the values of the potential for points within a specific area of interest from the inside of the tank [7]. To have a basis for verifying the results obtained with the proposed method, we chose an identical model to that in [9], Fig.1, where the problem was approached with a hybrid, analytic-numerical method.

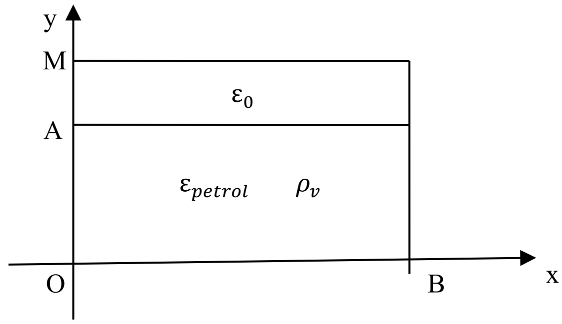

Fig. 1 – A section through the petrol tank.

We remark than on the domain occupied by air within the tank, on the height AM = 2 m the electrostatic field equations lead to a Laplace equation:

$$\frac{\partial^2 V}{\partial x^2} + \frac{\partial^2 V}{\partial y^2} = 0. \tag{1}$$

In the domain occupied by gasoline the electrostatic field equations lead to a Poisson equation:

$$\frac{\partial^2 V}{\partial x^2} + \frac{\partial^2 V}{\partial y^2} = -\frac{\rho_v}{\varepsilon}. \tag{2}$$

By applying the separation of variables method, we obtain the potential for the air region [9]:

$$V^{(1)}(x,y) = \sum_{k=1}^{\infty} F_k \,\mathrm{ch}kx \cdot \sin ky, \tag{3}$$

and for the gasoline region:

$$V^{(2)}(x,y) = \sum_{k=1}^{\infty} F_k \,\mathrm{ch}kx \cdot \sin ky - \tag{4}$$

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$$-\frac{\rho_v}{2\varepsilon}y^2 + \frac{\rho_v h}{2\varepsilon}y.$$

Here h = OA represents the height of the gasoline inside the tank. The axis Oy is the perpendicular bisector of the line segment [OB] in Fig.1

Expressions (3) and (4) were obtained in [9] after partially using the conditions of the problem. A purely analytic solution was intractable beyond the relations found, so the authors had to rely on a numerical/analytic method.

3. MATHEMATICAL FOUNDATIONS OF THE MONTE CARLO METHOD FOR NON-HOMOGENEOUS MEDIA

For a clearer presentation of the method, we will succinctly illustrate the steps leading to the general formula that characterizes the calculation of the potential in non-homogeneous environments using the Monte Carlo method.

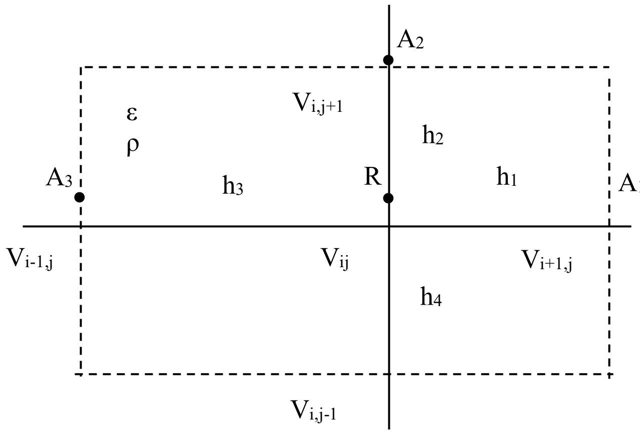

Fig. 2 – Model for Poisson numerical equation in homogeneous media.

Here the potentials of the points R, A_1, A_2, A_3 and A_4 are $V_{i,j}$, $V_{i+1,j}$, $V_{i,j+1}$, V_{i-1j} and respectively $V_{i+1,j}$, with $RA_1 = h_1$, $RA_2 = h_2$, $RA_3 = h_3$ and $RA_4 = h_4$.

We write the Taylor series expansion for each of the 4 points adjacent to (i,j), Fig.2, keeping only the first three terms. We eliminate the first derivative of the potential and then use it (2). We then obtain the numerical finite difference form of the Poisson equation with distinct discretization steps on all directions for homogeneous medium.

$$V_{i,j}\left(\frac{1}{h_1h_3} + \frac{1}{h_2h_4}\right) = \frac{V_{i+1,j}}{h_1(h_1+h_3)} + \frac{V_{i,j+1}}{h_2(h_2+h_4)} + + \frac{V_{i-1,j}}{h_3(h_1+h_3)} + \frac{V_{i,j-1}}{h_4(h_2+h_4)} + \frac{\rho}{2\varepsilon} \tag{5}$$

To transition from the formula (5) valid in a homogeneous medium to one that is valid in a non-homogeneous medium (Fig.3), an interesting trick is used [10,11]. We write a formula of type (5) for the point $(i,j+1)$ with (ε_1 and ρ_1) and then for the point $(i,j-1)$ with (ε_2 and ρ_2) if the point (i,j) lies at the same distance y from the two points considered. The distance between $(i,j+1)$ and $(i,j+2)$ is h_2 and between $(i,j-1)$ and $(i,j-2)$ it is h_4. We then make y go to 0. Then the points $(i,j+1)$ and $(i,j-1)$ turn into (i,j) the point $(i,j+2)$ becomes the new $(i,j+1)$ and the point $(i,j-2)$ becomes the new $(i,j-1)$. The points $(i-1,j+1)$ and $(i-1,j-1)$ both turn into $(i-1,j)$ and the points $(i+1,j+1)$ and $(i+1,j-1)$ turn into $(i+1,j)$.

Thus, the finite difference numerical form of Poisson's equation is obtained for a discretization grid with unequal steps, for a point located on the horizontal separation surface of a non-homogeneous medium charged with different charge densities (Fig. 3)

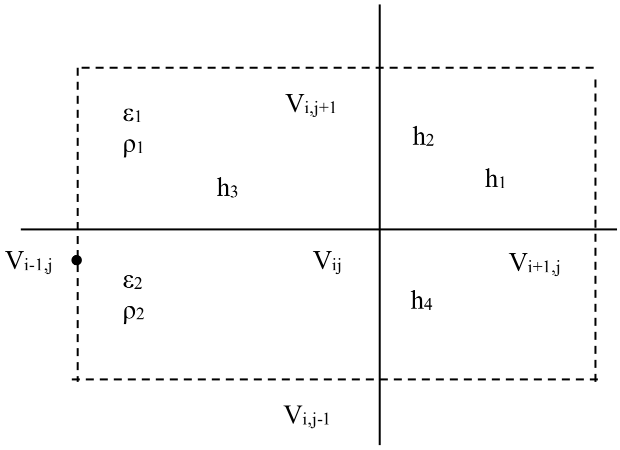

Fig. 3 – Model for Poisson numerical equation in inhomogeneous media.

$$\begin{aligned} V_{i,j}\left(\frac{\varepsilon_1 h_2 + \varepsilon_2 h_4}{h_1 h_3} + \frac{\varepsilon_1}{h_2} + \frac{\varepsilon_2}{h_4}\right) &= \frac{\varepsilon_1 h_2 + \varepsilon_2 h_4}{h_1(h_1+h_3)}V_{i+1,j} + \frac{\varepsilon_1}{h_2}V_{i,j+1} \\ &+ \frac{\epsilon\varepsilon_1 h_2 + \varepsilon_2 h_4}{h_3(h_1+h_3)}V_{i-1,j} + \frac{\varepsilon_2}{h_4}V_{i,j-1} \\ &+ \frac{\rho_1 h_2 + \rho_2 h_4}{2} \end{aligned} \tag{6}$$

If the separation surface were vertical (which is not the case in the practical situation for which we are preparing to apply the method) with the medium with ε_1 and ρ_1 on the left and the medium with ε_2 and ρ_2 on the right, the numerical form of Poisson's equation would be obtained by rotating the drawing in Fig. 3 by a right angle around the point (i,j) in a counterclockwise direction.

Consequently, in relation (6), the quantities h_1, h_2, h_3, h_4 will be replaced respectively with h_4, h_1, h_2, h_3 and the quantities $V_{i-1,j}$, $V_{i,j-1}$, $V_{i+1,j}$, $V_{i,j+1}$ will be replaced with $V_{i,j+1}$, $V_{i-1,j}$, $V_{i,j-1}$, $V_{i+1,j}$. In the case of a rectangular grid with invariant steps in the direction of the coordinate axes, we have $h_1 = h_3 = h_x$ and respectively $h_2 = h_4 = h_y$. In this case, relation (6) becomes

$$V_{i,j}\left(\frac{2}{h_x^2} + \frac{2}{h_y^2}\right) = \frac{1}{h_x^2}V_{i+1,j} + \frac{2\varepsilon_1}{\varepsilon_1+\varepsilon_2}\frac{1}{h_y^2}V_{i,j+1} + \frac{1}{h_x^2}V_{i-1,j} + + \frac{2\varepsilon_2}{\varepsilon_1+\varepsilon_2}\frac{1}{h_y^2}V_{i,j-1} + \frac{\rho_1+\rho_2}{\varepsilon_1+\varepsilon_2} \tag{7}$$

We denote:

$$m = \frac{2h_y^2}{h_x^2+h_y^2},\ n = \frac{2h_x^2}{h_x^2+h_y^2},\ p = \frac{h_x^2 h_y^2}{2(h_x^2+h_y^2)}.$$

Thus eq. (7) is written as:

$$V_{i,j} = \frac{1}{4}\left(mV_{i+1,j} + \frac{2\varepsilon_1}{\varepsilon_1+\varepsilon_2}nV_{i,j+1} + mV_{i-1,j} + + \frac{2\varepsilon_2}{\varepsilon_1+\varepsilon_2}nV_{i,j-1}\right) + p\frac{\rho_1+\rho_2}{\varepsilon_1+\varepsilon_2}. \tag{8}$$

In our application, we will consider the discretization grid to be square, *i.e.*, $h_x = h_y = h$, so in relation (8) we will take $m = n = 1$ and $p = h^2/4$.

A2

The volume density of the electric charge in medium (1), *i.e.*, in air, is obviously $\rho_1 = 0$, while the volume density of the electric charge in medium (2), i.e., in gasoline, is $\rho_2 = \rho_v = \rho$. The electric permittivity in air is $\varepsilon_1 = \varepsilon_0$, while in medium gasoline, it is $\varepsilon_2 = \varepsilon_r\varepsilon_0 = 2\varepsilon_0$, with the relative permittivity of gasoline being known, $\varepsilon_r = 2$. With these particularizations of relation (8), the finite difference expression of the potential at a point on the horizontal separation surface between medium (1), air, obviously above, and medium (2), gasoline, is:

$$V_{i,j} = \frac{1}{4}\left(V_{i+1,j} + \frac{2}{3}V_{i,j+1} + V_{i-1,j} + \frac{4}{3}V_{i,j-1}\right) + \frac{h^2}{4}\frac{\rho}{3\varepsilon_0}. \quad (9)$$

For the point (i,j) in the homogeneous medium (1), air, we get by particularizing equation (5):

$$V_{i,j} = \frac{1}{4}\left(V_{i+1,j} + V_{i,j+1} + V_{i-1,j} + V_{i,j-1}\right). \quad (10)$$

For the point (i,j) in the homogeneous medium (2), gasoline, we get by particularizing eq. (5):

$$V_{i,j} = \frac{1}{4}\left(V_{i+1,j} + V_{i,j+1} + V_{i-1,j} + V_{i,j-1}\right) + \frac{h^2}{4}\frac{\rho}{2\varepsilon_0}. \quad (11)$$

Relations (9), (10), (11) will be interpreted probabilistically in the spirit of the Monte Carlo method. A fictitious particle is considered, which starts from point (i,j) and reaches one of the adjacent points $(i+1,j)$, $(i,j+1)$, $(i-1,j)$, $(i,j-1)$ with equal probability (1/4).

Depending on the adjacent point where the fictitious particle arrives, a certain value is assigned to the potential of point (i,j), as follows:

If the fictitious particle reaches point $(i+1,j)$, *i.e.*, moves to the right

$$V_{i,j}=V_{i+1,j} + T_{i,j}. \quad (12)$$

If the fictitious particle reaches point $(i,j+1)$, *i.e.*, moves up

$$V_{i,j}=qV_{i,j+1} + T_{i,j}, \quad (13)$$

where $q = 2/3$ if point (i,j) is on the separation surface and $q = 1$ otherwise.

If the fictitious particle reaches point $(i-1,j)$, *i.e.*, moves to the left

$$V_{i,j}=V_{i-1,j} + T_{i,j}. \quad (14)$$

If the fictitious particle reaches point $(i,j-1)$, *i.e.*, moves down

$$V_{i,j}=qV_{i,j-1} + T_{i,j}, \quad (15)$$

where $q = 4/3$ if point (i,j) is on the separation surface and $q = 1$ otherwise. $T_{i,j}=0$ if the point (i,j) is in medium (1), *i.e.*, air,

$$T_{i,j} = P = \frac{h^2}{4}\frac{\rho}{3\varepsilon_0}. \quad (16)$$

If the point (i,j) is on the separation surface,

$$T_{i,j} = Q = \frac{h^2}{4}\frac{\rho}{2\varepsilon_0}. \quad (17)$$

If the point (i,j) is in medium (2), *i.e.*, gasoline.

The movement of the fictitious particle can be simulated on a computer by generating pseudo-random numbers (0,1,2,3) with the 'random 4' variant, thus commanding the direction of movement of the fictitious particle to the right, up, left, or down. The primary statistical estimator corresponding to the Monte Carlo method is determined. A square discretization grid with step h is attached to the cross-sectional surface of the parallelepiped tank represented in Fig. 1. A random path TrK is considered, starting from point (i,j) where the potential is of interest and ending at a point on the boundary Γ of the domain, which in this case is represented by the sides of the rectangle.

By successively expressing the potentials reached by the fictitious particle and successively eliminating these potentials with relations of the form (9)-(11), the starting potential $V_{i,j}$ is expressed as a function of the potential of the endpoint of the path and the sources in the domain. It is observed that since the tank is buried, the potential on the contour Γ of the domain is zero, so the potential at the starting point will depend only on the sources in the domain.

Thus in air we have $V_{i,j} = V_{i,j\pm 1}$ or $V_{i,j} = V_{i\pm 1,j}$ and in gasoline $V_{i,j} = V_{i,j\pm 1} + Q$ or $V_{i,j} = V_{i\pm 1,j} + Q$, while on the separation surface

$$V_{i,j} = V_{i\pm 1,j} + P,$$

$$V_{i,j} = \frac{2}{3}V_{i,j+1} + P \text{ and } V_{i,j} = \frac{4}{3}V_{i,j-1} + P.$$

We denote by $S_{(a,b)}$ the source corresponding to the point (a,b), so $S_{(a,b)} = 0$ in air, $S_{(a,b)} = Q$ in gasoline and $S_{(a,b)} = P$ for the separation surface.

We deduce the expression for the primary statistic estimator of the random path TrK [11]:

$$V_{i,j}^{(K)} = \sum_{(a,b)\in TrK} \left(\frac{4}{3}\right)^{\gamma(a,b)} \left(\frac{2}{3}\right)^{\delta(a,b)} S_{(a,b)} \quad (22)$$

where $\gamma(a,b)$ represents the number of transitions of the fictitious particle from the separation surface to the domain occupied by gasoline, and $\delta(a,b)$ represents the number of transitions of the fictitious particle from the separation surface to the domain occupied by air.

These transitions are counted from the moment the particle starts until the fictitious particle reaches point (a,b). The last point of the path TrK, for which the source $S(a,b)$ is still considered, is the penultimate point of the path, with the last point being on the boundary. The potential of the penultimate point on the path will be the potential of the point on the boundary, which is zero.

The improved secondary statistical estimator is the arithmetic mean of the primary statistical estimators, averaged over a very large number N of random paths.

$$V_{i,j} = \frac{1}{N}\sum_{K=1}^{N} V_{i,j}^{(K)}. \quad (23)$$

This is the value corresponding to the potential at point (i,j) using the Monte Carlo method.

4. NUMERICAL RESULTS

The Oy axis is taken as in Fig. 1, and the abscissa axis is taken right on the separation surface between gasoline and air, meaning the origin of the axes becomes the point A (Fig.1). The discretization grid step is taken as h = 5 cm on both axes. Thus, on the abscissa we will have 80 points, and on the ordinate, we will have 200 points, of which 40 are in the air.

We apply the Monte Carlo Method to find the potential $V_{1,1}$, $V_{2,1}$, $V_{3,1}$,...,$V_{40,1}$ of the points in the air immediately above the separation surface, as well as $V_{1,0}$, $V_{2,0}$, $V_{3,0}$,...$V_{40,0}$ of the points on the separation surface. We note that the symmetry of the problem has been considered and only the potentials of the points in the left half of the section have been calculated.

Each of these points will be starting points for $N = 5000$ random paths.

The electric field at the surface of separation has two components $E_{xk,0}$ and $E_{yk,0}$, so we calculate

$$E_{k,0} = \sqrt{\left(\frac{V_{k,0} - V_{k-1,0}}{h}\right)^2 + \left(\frac{V_{k,0} - V_{k,1}}{h}\right)^2} \tag{24}$$

for $k = 1,2,3...40$.

The numerical results obtained for the potential at the separation surface for the first 3 points on the separation surface and for the last three points located in the middle of the section are: $V_{1,0}$ = 16.99 kV, $V_{2,0}$ = 36.56 kV, $V_{3,0}$ = 59.89 kV, $V_{38,0}$ = 333.32 kV, $V_{39,0}$ = 365.93 kV, $V_{40,0}$ = 390.65 kV.

The calculated values of the electric field at the points on the separation surface of the section are: E_1 = 3.39 kV/cm, E_2 = 3.9, kV/cm, E_3=5.23 kV/cm, E_{39}=35.91 kV/cm, E_{40} = 37.80 kV/cm.

At these values, the dielectric strength of air at 30 kV/cm is exceeded, and an explosion occurs.

Considering the direct proportionality between the electric field and the volume density of the electric charge, we deduce that for the given configuration, the risk of explosion starts at the value of 0.79 x 10^{-5} C/m^3 of the volume density of the electric charge in the tank.

The electric fields corresponding to the points on the separation surface in the left half of the section form the following angles with the left-oriented abscissa axis: α_1 = 2.03 deg. α_2 = 11.84 deg. α_3 = 26.95 deg., α_{39} = 79.52 deg. and for reasons of symmetry α_{40} = 90 deg. It should be noted that at the coordinate point (40,0), the electric field has two components on the abscissa axis that are equal and opposite, so at this point, the electric field has only a vertical component.

For comparison, the analytic method [9] yields similar results, for example the field E_{40} = 38.92 kV/cm.

Let us recall another aspect of the Monte Carlo method. Each time the program is rerun, the results are different, but the differences do not exceed 5%. Another specific aspect of the method refers to the number of random paths. From the results obtained for $N = 5000$, $N = 10000$, $N = 50000$ and $N = 100000$ we notice that the differences are not significant, so we chose to work with $N = 5000$. The convergence of the Monte Carlo method [8] is typical for random methods.

All the data used in the paper was obtained by means of a C++ script.

The use of the Monte Carlo method, supported by the finite difference method (including the corresponding discretization grid) was preferred to other numerical methods (such as FEM) for two reasons. The first has to do with the specificity of the field of interest, while the second is of theoretical nature, considering that the Monte Carlo method for inhomogeneous media is very little known and used.

5. CONCLUSIONS

There are situations, such as the one considered in this paper, where a method that provides the solution only in a certain part of the domain is preferable to classical methods of numerical calculation of the electrostatic field. The non-homogeneous medium adds an extra layer of difficulty, particularly in the implementation of the program. Being a method derived from the finite difference method, Monte Carlo provides acceptable results, as demonstrated in this paper. For the configuration used to exemplify the method, the calculation of the maximum electric field in the air allows the determination of the charge loading from which the danger of explosion begins.

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