Radioactive Material Dispersion Modeling using Physics Informed Neural Network

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1. Introduction

The atmospheric dispersion of radioactive materials should be evaluated for the assessment of environmental impact by radiation in the event of an accident and level 3 Probabilistic Safety Assessment (PSA) which are performed for obtaining construction permits and operating licenses in South Korea respectively. The governing equation of the air dispersion can be derived by the law of conservation of mass and it has a second-order partial differential equation form. [1] Currently, most of the computer code for level 3 PSA uses the Gaussian plume or Gaussian puff model, which are analytic solutions, as an air dispersion model. [2] Obtaining the analytic solution requires assumptions, so it may not be enough to understand the actual phenomenon. There are various methods to obtain the solution of the partial differential equation such as the Finite Difference Method (FDM), Computational Fluid Dynamics (CFD) model, and spectral analysis, in addition to the analytic solution. [3] In this paper, we present a method for solving the air dispersion equation by using the recently published Physics Informed Neural Network (PINN) method. [4] The PINN is a method to approximate a physical model by assuming the latent solution as a deep neural network and optimizing it. Unlike the analytic solution, it rarely needs assumptions and therefore, it can obtain a solution without transformation of the original equation. In this paper, we review the air dispersion model and demonstrate the procedure of obtaining the solution of it by using the PINN.

2. Air dispersion model

The concentration of a contaminant such as the radioactive material at the location (x, y, z) and time $t \geq 0$ can be derived by the law of conservation of mass as follows:

$$\frac{\partial C}{\partial t} + \nabla \cdot \vec{J} = S \qquad (1)$$

where, $C(x, y, z, t)$ $[kg/m^3]$ is a concentration of a contaminant, $\vec{J}(x, y, z, t)$ $[kg/m^2s]$ is a mass flux, and $S(x, y, z, t)$ means a source or sink term.

For the air dispersion, mass flux $\vec{J}$ is formed by diffusion and advection effect, therefore it can be written as follows:

$$\vec{J} = \vec{J}_D + \vec{J}_A \qquad (2)$$
$$\vec{J}_D = -K\nabla C$$
$$\vec{J}_A = C\vec{u}$$

where, $K = diag(K_x, K_y, K_z)$ $[m^2/s]$ is a diffusion coefficient, $\vec{u} = (u_x, u_y, u_z)$ $[m/s]$ is a wind vector.

By substitution of the equation (2) into the equation (1), the equation (1) can be rewritten as follows:

$$\frac{\partial C}{\partial t} + \nabla \cdot (C\vec{u}) = \nabla \cdot (K\nabla C) + S \qquad (3)$$

The equation (4) shows the Gaussian plume model which is used for MACCS code for level 3 PSA. It is an analytic solution of the equation (3) that can be derived with the assumptions as follows: [1]

- The contaminant is emitted with a constant rate from a single point source.
- The wind velocity and direction (x-direction) are constant.
- The solution is steady state.
- The wind velocity is sufficiently large that the diffusion in the x-direction is much smaller than advection.

$$\bar{C}(x, y, z) = \frac{Q}{2\pi\sigma_y\sigma_z\bar{u}} \exp\left(\frac{-y^2}{2\sigma_y^2}\right) \times \left(\exp\left(\frac{-(z-h)^2}{2\sigma_z^2}\right) + \exp\left(\frac{-(z+h)^2}{2\sigma_z^2}\right)\right) \qquad (4)$$

where, $\bar{C}(x, y, z)$ is a time-averaged concentration, Q is an emission rate, $\bar{u}$ is a time-averaged wind speed at the height of the release h, and σ_y and σ_z are a horizontal and vertical diffusion parameter.

The Gaussian plume model estimates time-averaged concentration distribution with a long-term time scale. Therefore, it is not possible to simulate the variation of the concentration distribution over time, and the reflection of the parameters such as wind and diffusion coefficient is restricted.

3. Physics informed Neural Network (PINN)

The PINN is a method to approximate a PDE by assuming the latent solution as a deep neural network and optimizing it by using an initial and boundary condition. It uses an original equation without assumption, so it is possible to estimate time-dependent air dispersion behavior and reflect various conditions of wind and diffusion coefficient parameters. In this section, we present the procedure of solving the air dispersion equation using the PINN. For the convenience of

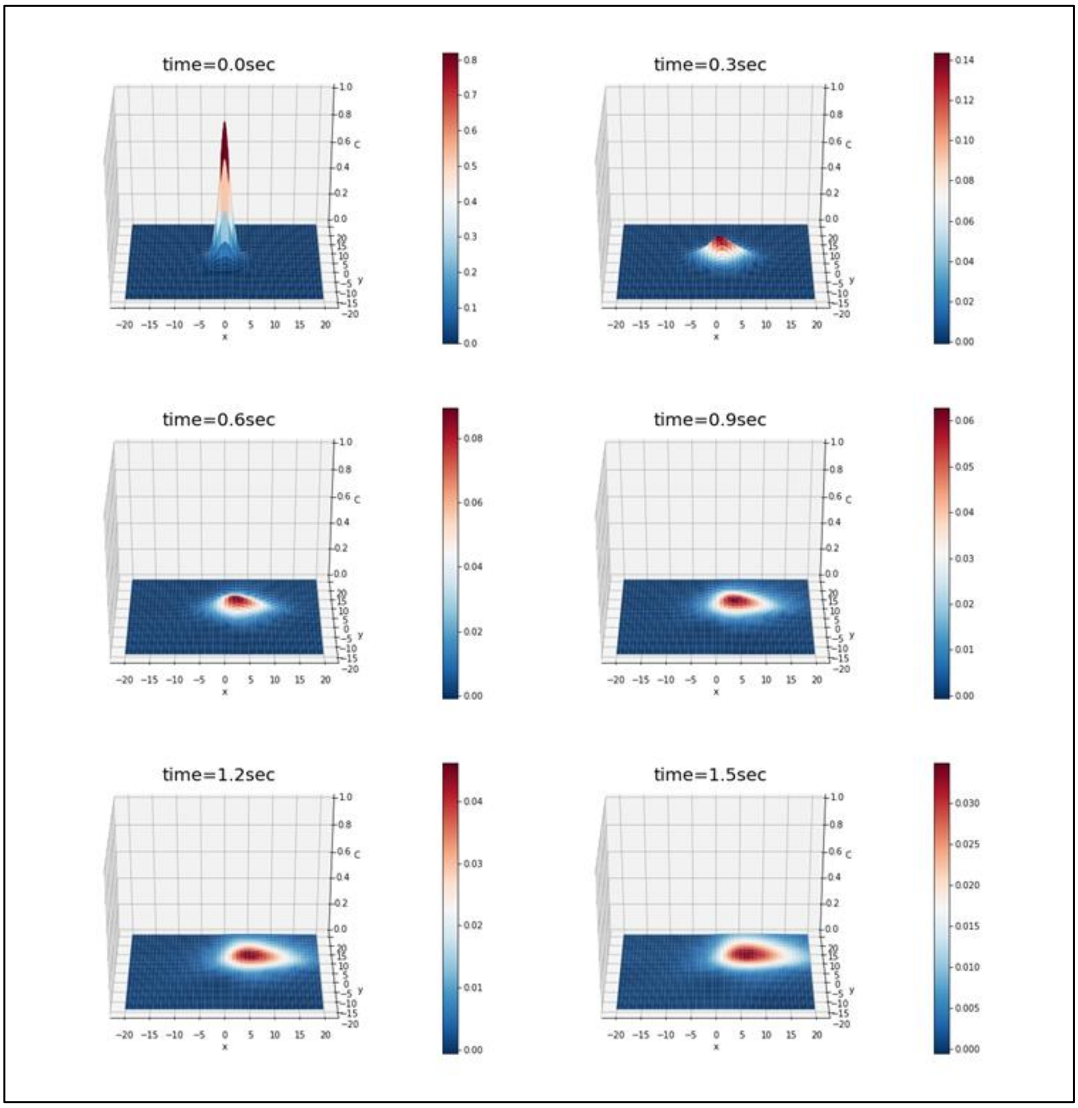

Fig. 1. The results of air dispersion simulation using PINN

explanation, let us consider a 1-dimensional air dispersion equation without source term as follows:

$$\frac{\partial C}{\partial t} + \frac{\partial}{\partial x}(C\vec{u}) - \frac{\partial}{\partial x}\left(K\frac{\partial}{\partial x}C\right) = 0 \quad (5)$$
$$C(-\infty, t) = 0$$
$$C(\infty, t) = 0$$

The second and third equation of the equation (5) present the boundary conditions. Then, let us define the left-hand side of the equation (5) as $f(x,t)$.

$$f = \frac{\partial C}{\partial t} + \frac{\partial}{\partial x}(C\vec{u}) - \frac{\partial}{\partial x}\left(K\frac{\partial}{\partial x}C\right) \quad (6)$$

and proceed by assuming the latent solution $C(x,t)$ as a deep neural network which has x and t as inputs and concentration C as an output.

$$C = NN_C(x,t) \quad (7)$$

The assumed network is optimized by minimizing the mean squared error loss defined as follows:

$$MSE = MSE_C + MSE_f \quad (8)$$
$$MSE_C = \frac{1}{N_C}\sum_{i=1}^{N_C}\left(NN_C\left(x_C^i, t_C^i\right) - C^i\right)^2$$
$$MSE_f = \frac{1}{N_f}\sum_{i=1}^{N_f} f\left(x_f^i, t_f^i\right)^2$$

where, $\{x_C^i, t_C^i, C^i\}$ $(i = 1,2,3,\ldots,N_C)$ is a training data set of the initial and boundary condition, and $\{x_f^i, t_f^i\}$ $(i = 1,2,3,\ldots,N_f)$ is randomly sampled data set. We implemented the PINN method by using the Python programming language and the Tensorflow 2.0 library. In this study, the assumed deep neural network consists of nine layers, excluding input and output layers, and each layer has 64 nodes. The nodes of the input layer consist of the position and time t values. The output layer returns the concentration corresponding to the input position and time. The developed code for this study is available at https://github.com/gibeom92/PINN_dispersion.

4. Results

In this study, we solved the 2-dimensional air dispersion equation using the PINN. The simulation was performed mainly focusing on presenting the change of the distribution over time, therefore we note that the results do not mean the exact amount of a particular radioactive material.

The simulation area is set as $20m \times 20m$ $(-20 < x < 20, -20 < y < 20)$. The wind vector is assumed as $(u_x, u_y) = (5, 5)[m/s]$. The diffusion coefficient is assumed that it increases linearly over distance according to [5]. The initial distribution is assumed as $1/\cosh(\sqrt{x^2 + y^2})$.

Fig. 1 shows the results of the simulation. It is shown that the center of the distribution moves according to the wind vector. Because the diffusion coefficient increases over the distance, the distribution changes asymmetrically.

5. Conclusions

Currently, for the air dispersion model, most of the computer code for calculating the dispersion of radioactive materials uses the Gaussian plume or Gaussian puff model that are analytic solutions. In the procedure of derivation, the analytic solution needs the assumptions that restrict the parameters such as the wind and diffusion coefficient. To compensate for the limitations, we suggested the PINN method for solving the air dispersion equation and presented the procedure of simulating radioactive material dispersion with a simple example. For further study, we plan to introduce this method into the real-time simulation framework of a radiological emergency that contains an analysis of evacuation and radioactive material dispersion and the effect of infrastructures.

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