



PSO-based modeling particulate emission rates in nuclear accidents

Brasil^a D.R., Nicolau^b A.S., Schirru^c R., Pereira^d C. M. N. A.

^{a,b,c} Universidade Federal do Rio de Janeiro (UFRJ), Rio de Janeiro, Brazil

^a <u>brasil.docm@gmail.com</u> ^b <u>andressa@lmp.ufrj.br</u> ^c <u>schirru@lmp.ufrj.br</u> ^d Instituto de Energia Nuclear (IEN), Rio de Janeiro, Brazil ^d <u>cmnap.ien@gmail.com</u>

ABSTRACT

This paper aims to estimate the rate of particulate contaminants emitted by multiple sources, whose values are unknown, using the values identified by the receptors distributed around the sources. In a nuclear emergency with release of radionuclides into the atmosphere, in order to make the correct decision, it is necessary to identify the source term and its release rate, as well as the meteorological data, essential factors for defining the direction and size of the radioactive plume. For this purpose, a model of Particle Swarm Optimization (PSO) is applied together with a mathematical model of Gaussian dispersion, being created the program Particle Swarm Optimization Dispersion Model (PSODM).

Keywords: Source term, atmospheric dispersion, PSO, nuclear accident.



1. INTRODUCTION

Nuclear power plants are complex systems that follow the highest safety standards. Its construction, operation and decommissioning are done following protocols that guarantee the safety, prevention and mitigation of accidents. The purpose is to ensure a safe operation, the safety of the public and the environment.

In history around the world three major nuclear accidents can be mentioned: the Three Mile Island accident [1], which occurred on March 28, 1979, the Chernobyl accident [2], on April 26, 1986, and the most recent, the Fukushima Daiichi accident [3], on March 11, 2011. Each of these accidents brought lessons and revisions in the concepts, standards and safety Nuclear Power Plants procedures. Moreover, they showed the importance in the development of atmospheric dispersion models [4]: it is important to estimate the source term [3], and consequently the release rate to the atmosphere to support decision making in case of a radiological emergency.

The identification of the radioactive plume released into the atmosphere is necessary so that a more precise evacuation occurs according to the affected region after a nuclear accident. This allows for the real-time monitoring of the rate of release of the sources and the projection of the areas affected by the radiation. The projection of the radioactive plume is developed by means of a mathematical model of atmospheric dispersion, which can be approached by the Lagrangian, Eulerian, Gaussian or Gaussian puff models [5],[6].

This paper presents a methodology based on Particle Swarm (PSO) algorithm [7] and Gaussian plume dispersion calculation [8] to estimate the particulate contaminants rate emitted by multiple sources, whose values are unknown using only the identified values by receivers distributed around the sources. Here, the PSO was used to optimize (find) the release particulate contaminants values released from 4 broadcasting sources, in order to obtain a solution for the source emission rate values for a given concentrations data set measured in 9 receptors.

The results found with Particle Swarm Optimization Dispersion Model (PSODM) [9] were effective in solving the problem approached and demonstrate that the proposed methodology is a promising tool in problems of this nature.

1.1. Atmospheric dispersion models

The atmospheric dispersion model is a mathematical simulation of the physics and chemistry that govern the transport, dispersion and transformation of contaminants in the atmosphere. Also, they are a means of estimating the concentrations of atmospheric contamination in the direction of the wind, based on information about the emissions of these contaminants and the nature of the atmosphere.

These models are physical and mathematical. Physicists represent, with a given degree of simplification, the real phenomena of interest, while mathematicians describe the systems using relationships and mathematical equations.

Most modern atmospheric dispersion models are computer programs, which calculate the concentration of particulates released by a source, using the emission rate of contaminants, the characteristics of the emitting sources, weather conditions and concentrations of particulates in the environment.

Atmospheric dispersion models are simplified images of reality. These models do not contain all the characteristics of the real system, but the characteristics of interest in solving the scientific problem being studied. Models are widely used in science to make predictions and solve problems, and are often used to identify the best solutions to environmental problems [4].

Currently, the most commonly used dispersion models are based on mathematical models of Lagrangian, Eulerian, Gaussian, or Gaussian puff plumes [5],[6]. Mathematical models of atmospheric dispersion describe and interpret experimental data, analyze air quality in real time, manage accidental releases and assess risk areas, identify sources and evaluate the contribution of a single source or sources to the concentration of identified contaminants [10].

It can be said that atmospheric dispersion models calculate the concentration of radionuclides dependent on time and space. Deterministic mathematical models are widely used in atmospheric studies. Differential equations are usually employed to describe the atmospheric dispersion process, and the system is summarized in terms of the solution of these equations. Several dispersion models have been developed, which are basically classified as Lagrangian and Eulerian models.

The Gaussian plume model [5],[6] is a standard approach to study the transportation of airborne contaminants due to turbulent diffusion and wind advection. To estimate the dispersion with a Gaussian model it is necessary to follow the following sequence:

- i. Determine the cartesian coordinates of the source and receiver;
- ii. Determining the characteristics of the emitting source;
- iii. Check the atmospheric stability class, based on weather conditions;
- iv. Calculate wind speed at plume release height;
- v. Calculate the effective launch height;
- vi. Determine the value of parameters (σ_Y) and (σ_Z) , are the width and height of the radioactive plume respectively;
- vii. Calculate the concentration of contaminant in the receiver.

1.2. Particle Swarm Optimization (PSO)

In 1995, the Particle Swarm Optimization (PSO) [7] algorithm had its beginnings from the simulation of a social environment inspired basically on the behavior of a swarm birds flock and fish shoals, in its ordered movement in search of food.

The learning of PSO particles is done in function of individual learning (of a particle) and collective learning (of the group). The socio-cognitive ability is the foundation, because a particle has found a position corresponding to a solution in the search space of the problem, and can influence others in the swarm, causing them to walk towards it. There will always be the possibility of the swarm finding some better position in space, a fact that with the algorithm evolution, one can converge to better solutions.

The term particle is used to characterize the members (individuals) of a population of the PSO that seeks solutions in the search space of the problem. Each particle cannot evaluate itself if its position is good or bad, it is necessary that it refers the coordinates of a new position found, to a function that evaluates them quantitatively, providing a number as a result corresponding to that position.

The objective function or fitness [7], is a measure of fitness, that is, it will be able to say how good a position is compared to another already found. In the search for better results in the PSO, it is necessary that a new position be compared, both with the best individual position obtained by the particle itself, and with the best global position. Table 1 presents the nomenclature used in the PSO.

Bird	Particle
Flock of birds	Swarm
Area overflow	Search space
Location of the bird at the time it finds food or nest	Position
Fitness assessment	Fitness
Best known position for the bird	Pbest
Best known position by the swarm	Gbest

Table 1: PSO Nomenclature.

From observed in Figure 1, the basic PSO flowchart presents two steps. In the first stage occurs the initialization of the PSO performing the LOOP of the particles, where the random particles (p) of the speed (v_{ij}) and position (x_{ij}) vectors are initiated, then is made the evaluation of the fitness function, if fitness (p) lower than fitness (pbest) then (pbest) is replaced by particle (p).

In the second stage, the LOOP takes place up to the maximum of iterations, evaluating if fitness (pbest) is smaller than fitness (gbest), then (gbest) is replaced by (pbest), thus updating the particle's speed and position. When reaching the stop parameter (maximum iteration number), the PSO provides the best value found for (gbest), which is the best solution.



Figure 1: PSO flowchart [9].

2. METHODOLOGY

Given a nuclear accident with the radionuclides/particulates release into the atmosphere, is important to estimate the radionuclide rates released from each of these sources. A way to estimate this rates is based on data obtained by receivers (detectors) located around the sources. Knowing the positions and source emission rates, and having the atmospheric conditions well defined, it is possible to calculate the concentrations in receivers, according to their positions on the ground [11],[12].

To solve this problem, a prototype model was developed using the PSO algorithm coupled with the Gaussian plume dispersion model, called here the Particle Swarm Optimization Dispersion Model (PSODM) [9]. Applying PSODM to the studied problem, each PSO particle is a solution for the particulate emission rate into the atmosphere released by the four sources (*S1*, *S2*, *S3* and *S4*).

The output is the solution that the best represents the emission rates of these four sources, that is, it is the solution with the best fitness, which is given by the smallest error between the values measured in the real receivers (VR) and the values measured in the calculated receivers (VC) [9]. The Equation 1 represents the PSO fitness, that calculates the mean squared error between the actual data measured and those estimated by the PSO.

$$fitness = \left[\frac{1}{N}\sum_{i}^{N} (VR_{Ri} - VC_{Ri})^2\right]^{1/2}$$
(1)

Where Ri is the receiver, whose number ranges from i to N.

To evaluate the fitness function, the values of the velocity and position vectors are calculated at each iteration. The value of the new velocity is obtained by Equation 2, where the iteration t+1 is given by the vector v_{ij}^{t+1} . The new position of the particle is obtained by Equation 3, which presents x_{ij}^{t+1} as the position vector in iteration t+1.

$$v_{ij}^{t+1} = wv_{ij}^{t} + c_1 r_1^{t} (pbest_{ij} - x_{ij}^{t}) + c_2 r_2^{t} (gbest_j - x_{ij}^{t})$$
(2)

$$x_{ij}^{t+1} = x_{ij}^{t} + v_{ij}^{t+1}$$
(3)

The term $(wv_{ij})^{t}$ represents the influence of the previous velocity on the new velocity $(v_{ij})^{t+1}$. The factors $(pbest_{ij}-x_{ij})^{t}$ and $(gbest_{j}-x_{ij})^{t}$, indicate for the particle the directions of the best individual and global positions, with their attraction forces defined by the values $c_{1}r_{1}^{t}$ and $c_{2}r_{2}^{t}$, respectively. Since c_{1} and c_{2} are acceleration constants, the sum of which should not exceed four [7]. Random factors r_{1}^{t} and r_{2}^{t} , which are random variables, must belong to the interval [0,1]. The vector $(x_{ij})^{t}$ represents the influence of the previous position on the new position $(x_{ij})^{t+1}$. Figure 2 illustrates the geometric interpretation in two dimensions for what happens to a particle *i* of the swarm, when its position $(x_{ij})^{t+1}$ and velocity $(v_{ij})^{t+1}$ are updated, at each iteration. Position $(x_{ij})^{t+1}$ and velocity $(v_{ij})^{t+1}$ values do not have units because they are vector sums.



Figure 2: Geometric interpretation of the PSO [9].

The Figure 3 presents the PSODM flowchart, developed based on the standard PSO flowchart (Figure 1), that presents two steps. The first step is given by the PSODM initialization performing the particle loop, where the random particles (p) of the velocity (v_{ij}) and position (x_{ij}) vectors are initiated. Then, the *forward2* program (plume dispersion) [8] is applied to calculate the concentrations of the four sources in the nine receivers at ground level. Afterwards, the fitness function is evaluated using the mean squared error. If fitness (p) is less than fitness (pbest) then *pbest* is replaced by particle p. In the second step, the loop takes place up to the maximum of the iterations evaluating if fitness (pbest) is less than fitness (gbest), then *gbest* is replaced by *pbest*. Thus, updating the particle velocity and position. When reaching the maximum number of predefined iterations, the PSODM stops running providing the best value found for *gbest*, which is the best result found for the problem.



Figure 3: PSODM flowchart [9].

The PSO is applied to Equation 4 [10], which estimates the particulate emission rate using the values obtained in the receivers around the sources. The Equation 4 is a derivation of the Gaussian plume solution, which takes into account the deposition and sedimentation velocities in the soil. Using the linear least squares method the expected results for the emission rates of the four sources are found [8].

$$C_{(r,y,z)} = \frac{Q}{2\pi u \sigma_y \sigma_z} \exp\left(-\frac{y^2}{2\sigma_y^2}\right) \exp\left(-\frac{w_{set}(z-H)}{2K} - \frac{w_{set}^2 \sigma_z^2}{8K^2}\right) \\ \times \left[\exp\left(-\frac{(z-H)^2}{2\sigma_z^2}\right) + \exp\left(-\frac{(z+H)^2}{2\sigma_z^2}\right) \\ - \frac{w_o \sigma_z \sqrt{2\pi}}{K} \exp\left(\frac{w_o(z+H)^2}{K} + \frac{w_o^2 \sigma_z^2}{2K}\right) \exp\left(\frac{w_o \sigma_z}{\sqrt{2K}} + \frac{z+H}{\sqrt{2\sigma_z}}\right)\right]$$
(4)

Where, $w_0 = w_{dep} - (0.5)w_{set}$ and $erfc_{(x)} = 1 - erf_{(x)}$ is a complementary error function.

Being the source height (*H*), the particulate emission rate (*Q*), coefficient of diffusivity (*K*), wind speed (*u*), sedimentation speed (w_{set}), deposition speed (w_{dep}), the parameters (σ_y) and (σ_z) are the width and height of the radioactive plume respectively.

PSODM program solves the atmospheric dispersion problem directly, using Equation 4 for calculates the concentration value of particulates emitted by four sources at ground level in mg/m^3 , given set of nine receptors located at ground level; Sums the particulate concentrations from each source at ground level as input data using Equation 5; Find the concentration at each receptor considering $A * dt * w_{dep}$ to obtain a total mass deposition in mg over the time interval dt by Equation 6.

$$glc = glc + ermak (xmesh-source.x (i), ymesh-source.y (i), 0,0, source.z (i), source.Q (i),$$

$$Uwind, Wdep, Wset)$$

$$den = den + (A * dt * Wden) * armak (recent x source x(i), recent y source y(i), recent z)$$
(5)

dep = dep + (A * dt * Wdep) * ermak(recept.x-source.x(i), recept.y-source.y(i), recept.z,source.z(i), source.Q(i), Uwind, Wdep, Wset)(6)

3. RESULTS AND DISCUSSION

In order to achieve the objective of this research, we used as a parameter for the release rates of sources S1, S2, S3 and S4, values 35, 80, 5 and 5 [8], respectively, whose unit is kg/s. The following results are due to the development of the present study, with values obtained through the PSODM program.

The PSODM model was developed using python. Different sensitivity tests of PSO parameters such as inertia weight w, number of particles (population), number of iterations and values of constants c_1 and c_2 were performed. The seed for each algorithm round was made randomly using python's random function.

Based on the population (p) parameter, the results obtained by PSODM will be presented and commented on below. In order to obtain the optimization of the results of the program, the values of the population quantity must be defined appropriately, since the choice of high values can cause slowness to reach the end of the LOOP. Moreover, for small values, PSODM may not converge towards good results. As observed in Table 2, whose population values vary from 10 to 50 and the number of iterations is equal to 100, being these small values, the results obtained were poor, once they diverge from the real values.

Table	2:	PSODM	results	[9].
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	Results Obtained – Mean Values				
р	Fitness	Source - S1	Source - S2	Source - S3	Source - S4
10	1,07599841274362E-08	35,07397447	80,0145399	4,75005694	3,06954355
15	8,27364170061403E-09	34,95943243	79,9180258	5,34175698	5,86475412
20	1,78183719729179E-09	34,97305862	79,9953527	5,03027527	5,18761202
30	7,04592848239190E-10	35,00386044	79,9996098	5,05327776	4,92775742
50	7,22890136167343E-10	34,99194268	80,0013072	4,96596723	5,07227585

Note: values of sources S_1 , S_2 , S_3 e S_4 em kg/s.

Table 3 presents the best results found with the PSODM, for values of w equal to 0,2, applied to Equation 2, with the population varying between 60 and 200, c_1 equal to 1,6, c_2 equal to 2,4, and iterations equal to 1000. Different tests were performed with different seeds for each parameter used in PSODM. It is observed that the PSODM presents better fitness results using a population value equal to or greater than 60, and number of iterations in 1000.

In Table 3, differently from Table 2, it is observed that regardless of the different values used in the populations, the values obtained by PSODM for sources S1, S2, S3 and S4 are equal. What shows that the result found by PSODM is a dominant global optimal, which even varying its parameters, it continues to converge to the same solution.

	Results Obtained – Mean Values				
р	Fitness	Source - S1	Source - S2	Source - S3	Source - S4
60	6,7382086744091E-20	34,999999993	79,999999999	4,999999992	4,99999933
80	6,7382086744091E-20	34,999999993	79,999999999	4,999999992	4,99999933
100	6,7382086744091E-20	34,999999993	79,999999999	4,999999992	4,99999933
150	6,7382086744091E-20	34,999999993	79,999999999	4,999999992	4,99999933
200	6,7382086744091E-20	34,999999993	79,999999999	4,999999992	4,99999933

Table 3: PSODM results [9].

Note: values of sources S_1 , S_2 , S_3 e S_4 em kg/s.

4. CONCLUSION

This paper presents an optimization model called PSODM, based on the particle swarm optimization (PSO), and Gaussian plume model in order to determine the emission rates of particulates into the atmosphere by multiple contaminant sources, after an accidental release using the concentration values collected by receivers distributed around these sources.

The values of the rates emitted by multiple sources, calculated by the PSODM, by means of the Ermak formula, which is a derivation of the Gaussian plume equation, plus the velocity of deposition and sedimentation of particulates in the ground. As output data the program presents the emission rates by the multiple sources, and the mean square error (fitness) obtained between the actual value and the calculated value of the data of the receivers.

Tests were performed, with different values for PSODM parameters, such as inertia factor (w), population number (p), number of iterations and values of constants c_1 and c_2 , It was observed that population values above 60 presented better results for the problem. It was also observed that with the variation of the values of the other parameters of the PSO, the developed model always converged to the same solution, showing that the solution found is a dominant global optimal.

The good results found with the PSODM show that the developed model is a good tool to determine the release rate of sources, through measurements using devices that detect the presence of radionuclides in the atmosphere.

The application in a nuclear accident with release of radionuclides into the atmosphere will be the identification of the plume, so that a more precise evacuation occurs according to the affected region. This can be used as a complement to the existing evacuation plan, by monitoring in real time the release rate of the sources.

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REFERENCES

- [1] OLIVEIRA L. F. S. and BARROSO A. C. O. Um sumário do acidente de Three Mile Island: do instante zero às lições para o futuro. Relatório técnico, COPPE/UFRJ, 1980.
- [2] BELLASIO R. and BIANCONI R. RTMOD: an Internet based system to analyze the predictions of long-range atmospheric dispersion models. Computers & Geociences, n. 25, p. 819-833, 1999.
- [3] PULLEN J., CHANG J. and HANNA S. Air-Sea transport, dispersion, and fate modeling in the vicinity of the Fukushima Nuclear Power Plant. A special conference session summary. American Meteorological Society, january, 2013.
- [4] CARBON B. Good Practice Guide For Atmospheric Dispersion Modelling. National Institute of Water and Atmospheric Research, Aurora Pacific Limited and Earth Tech Incorporated, Ministry for the Environment, Wellington, New Zealand, 2004.
- [5] LEELOSSY Á., MOLNÁR F., IZSÁK F., HAVASI Á., LAGZI I. and MÉSZÁROS R. Dispersion modeling of air pollutants in the atmosphere: a review, Central European Journal of Geosciences, n. 6, p. 257-278, 2014.
- [6] LEELOSSY Á., LAGZI I., KOVÁCS A. and MÉSZÁROS R. A review of numerical models to predict the atmospheric dispersion of radionuclides, Journal of Environmental Radioactivity, v. 182, p. 20-33, 2018.
- [7] KENNEDY J. and EBERHART R. C. A new optimizer using particle swarm theory. Proceedings of the IEEE international conference on neural networks, v. IV, p. 1942-1948. IEEE service center, Piscataway, NJ. 1995.

- [8] STOCKIE, J. M. Mathematics of Atmospheric Dispersion Modelling. SIAM Review, n. 53, p. 349-372, 2011.
- [9] BRASIL, D. R. Uma Modelagem Baseada no PSO para Estimativas das Taxas de Emissão de Particulados em um Acidente Nuclear. Master's dissertation, COPPE/UFRJ, 2021.
- [10] MOREIRA D. and TIRABASSI T. Modelo matemático de dispersão de poluentes na atmosfera: um instrumento técnico para a gestão ambiental. Ambiente e Sociedade, v. VII, n. 2, julho-dezembro, 2004.
- [11] ERMAK, D. L. An analytical model for air pollutant transport and deposition from a point source. **Atmospheric Environment**, v. 11, n. 3, p. 231–237, 1977.
- [12] LUSHI, E. and STOCKIE, J. M. An inverse Gaussian plume approach for estimating contaminant emissions from multiple point sources. Atmospheric Environment, n. 44, p. 1097–1107, 2010.