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Study of radioactive particle tracking using MCNPX code and artificial neural network

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ABSTRACT

Agitators or mixers are highly used in the chemical, food, pharmaceutical and cosmetic industries. During the fabrication process, the equipment may fail and compromise the appropriate stirring or mixing procedure. Besides that, it is also important to determine the right point of homogeneity of the mixture. Thus, it is very important to have a diagnosis tool for these industrial units to assure the quality of the product and to keep the market competitiveness. The radioactive particle tracking (RPT) technique is widely used in the nuclear field. In this paper, a method based on the principles of RPT is presented. Counts obtained by an array of detectors properly positioned around the unit will be correlated to predict the instantaneous positions occupied by the radioactive particle by means of an appropriate mathematical search location algorithm. Detection geometry developed employs eight NaI(Tl) scintillator detectors and a Cs-137 (662 keV) source with isotropic emission of gamma-rays. The modeling of the detection system is performed using the Monte Carlo Method, by means of the MCNPX code. In this work, a methodology is presented to predict the position of a radioactive particle to evaluate the performance of agitators in industrial units by means of an Artificial Neural Network.

Keywords: radioactive particle tracking, artificial neural network, MCNPX code, gamma densitometry.

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1. INTRODUCTION

Agitators or mixers are highly used in the industry when processes such as dispersion and homogenization are desired. Several industrial segments need this equipment, for example, to process products in the chemical, food, pharmaceutical and cosmetic industries. This equipment is used to: mix liquids, promote reactions of chemical substances, keep homogeneous liquid bulk during storage, or increase heat transfer. This industrial equipment is designed for each application with specific configurations, depending on the characteristics, such as density, phase and viscosity of the agitated product. The principle of agitation occurs in several ways, for example: in the mechanical agitator, the movement of the heterogeneous mass to the impeller achieves the agitation. During the production process, the equipment may fail and compromise the appropriate stirring or mixing procedure. Besides that, it is also important to determine the right point of homogeneity of the mixture. Thus, it is very important to have a diagnosis tool for these industrial units to assure the quality of the product and to keep the market competitiveness. In the nuclear field, the radioactive particle tracking (RPT) technique is a non-invasive method widely used.

RPT consists of monitoring a radioactive particle inside a volume of interest, for example inside the agitator or the mixer. It is important to note that the tracer must have the same characteristics of the fluid where it is inserted. To track the particle, it is necessary to have a detection system composed by an array of radiation detectors. RPT technique has been used in different fields. For example: to obtain flow field information about solid-phase motion in fluidized beds [1], to reconstruct online flow visualization in multiphase reactors [2], to reconstruct the position of a radioactive particle moving in a fluid as a sequence of small cubic cells occupied by successive particle positions [3] and more applications.

The instantaneous particle position is calculated through a reconstruction algorithm that converts the detector counts as a function of coordinates of the particle. Many reconstruction algorithms have been developed, such as a weighted regression scheme [4], a modified weighted regression scheme [5], the cross correlation technique [6], the Monte Carlo approach [1, 7-9] and feedforward Artificial Neural Network [2].

Artificial Neural Networks (ANN's) [10] has been used for some decades in different fields of study. With an ANN it is possible to study and reconstruct online flow visualization in multiphase reactors [2], study the chaotic behavior of a three-phase fluidized bed [11], predict volume fractions in multiphase flows [12,13] and identify flow regime [13].

This work consists of eight NaI(Tl) scintillator detectors displaced in two plans (the detectors are positioned in a 90º angle, and each plan has four detectors), a Cs-137 (662 keV) point source with isotropic gamma-ray emission and a PVC (Polyvinyl Chloride) tube filled with dry air. The Monte Carlo method is used to model the detection system and the simulations are provided by means of the Monte Carlo N-Particle eXtended (MCNPX) computer code [14]. In this work, the reconstruction algorithm used is given by a 5-layer feedforward ANN with a backpropagation algorithm to calculate the instantaneous position of the radioactive particle.

2. THEORETICAL FOUNDATIONS

2.1. Principles of the Radioactive Particle Tracking (RPT) Technique

Gamma rays are highly penetrating electromagnetic radiation that can travel long distances until detected by a radiation detection system. The number of photons recorded depends on the distance between the emitted gamma ray and the detector. This is the basic principle explored in the radioactive particle tracking technique, which uses an array of radiation detectors, generally scintillator detectors, to locate a single radioactive particle. It is important to highlight that the radioactive particle must have identical physical characteristics to the fluid investigated inside the volume of interest. The determination of the coordinates (x, y, z) of the radioactive particle is given by algorithms based on phenomenological or empirical approaches, which consider the relation between the number of photons recorded by each of the detectors and the location of the particle. The counts registered in each detector during a time interval is expressed by Equation 1 [15]:

$$C_i = \frac{T\nu A\phi\varepsilon_i(\mathbf{p},t)}{1+T\tau\nu A\phi\varepsilon_i(\mathbf{p},t)}, i = 1, \ldots, n \quad (1)$$

Where T is the dwell time, τ is the dead-time of the detectors, A is the source activity, ν is the number of photons emitted by disintegration, ϕ is the photopeak-to-total ratio and $\varepsilon_i(\mathbf{p}, t)$ is the efficiency of ith detector with respect to a position p in a time t. Besides the distance to the particle, the number of photons recorded depends on the attenuation properties of the materials disposed between the particle and the detector, and on the properties of the detector [16]. For a greater accuracy in particle location, a high number of detected photons is required and this occurs because the number of photons detected is subject to statistical fluctuations during the detection process.

The detection system employed depends on some aspects that affect the interaction of the gamma-rays with the detectors materials [16]. The most important aspects are the characteristics of the radioactive particle such as gamma-ray energy and activity; the types of gamma-rays interaction with matter (in this work: photoelectric effect and Compton scattering); the solid angle at which the irradiated surface of the detector is subjected, as seen by the particle; the detection efficiency; the photopeak fraction; and the dead-time of the acquisition system.

2.2. MCNPX Code

The computational code Monte Carlo N-Particle eXtended is a code based on the Monte Carlo Method that considers the effects of the interaction of radiation with matter with thirty different particles and four light ions [14]. For photons, for example, the Rayleigh and Compton scatterings and Bremsstrahlung are take into account. MCNPX code allows the construction of tridimensional and complex geometries, serving as a tool of extreme relevance for modeling nuclear installations, radiation detectors, shielding studies and other applications. Because it is a well-founded and valid code, its results and calculation methodology are widely accepted.

An advantage of this code is the existence of an input file that contains all the information about the source distribution, energy, time, position, surfaces or cells of where the radiation is emitted. In this way, the user does not need to have knowledge about programming languages like FORTRAN, C++, etc. Therefore, the MCNPX code is a consolidated and well accepted code in the scientific area, because it allows carrying out simulations of situations less ideals and closer to the real considering the phenomena of radiation transport and interaction of radiation with matter. MCNPX code will be used in the first step of this work, aiming to stablish a more appropriated geometry to apply the RPT technique. This code is also used to determine the materials that will be used as a source and the fluid inside the volume of interest.

2.3. Artificial Neural Network (ANN)

An artificial neural network (ANN) is a mathematical model capable to reproduce the human neuron function. In this way, its most important characteristic is to learn through examples [10]. If an appropriate set of data is given to the ANN, it is able to recognize patterns, generalizing knowledge during the learning process, that is, ANN is able to assign a response to situations that are not included in the training set. There are two phases of the ANN: i) Training phase that is also called learning process. This is where the ANN is supposed to learn and recognize patterns by using a learning algorithm. It is often an offline phase; ii) In the working phase, the trained ANN is used to respond to new situations. It is the online phase and the ANN does not need the training set anymore. In this work, a 3-layer feedforward ANN with a backpropagation algorithm will be used as a location algorithm to predict the radioactive particle instantaneous position. The ANN was trained with 108 different cases, following approximately the set distribution: 60% training, 30% test, 10% validation.

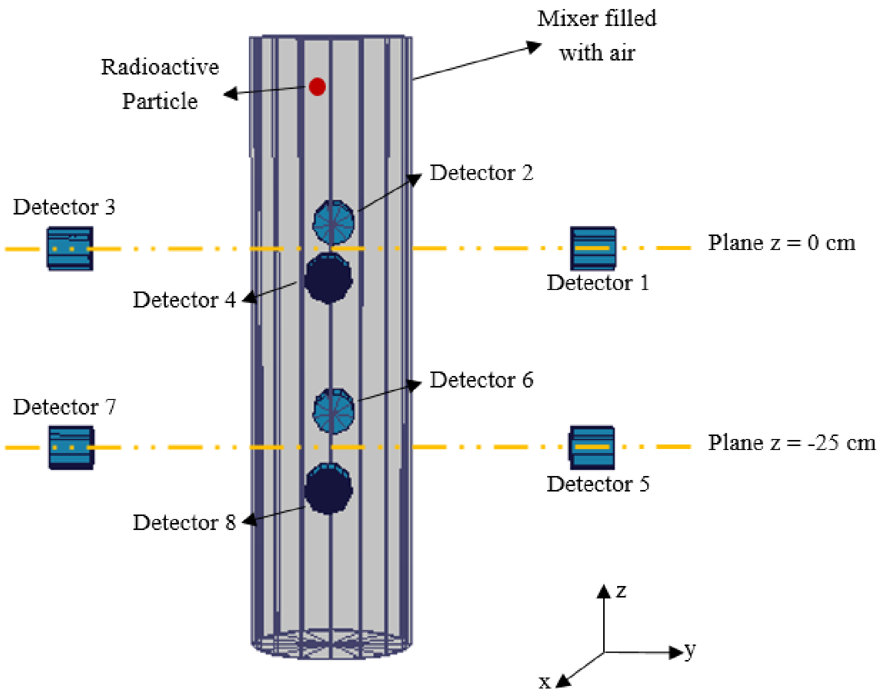
3. MATERIALS AND METHODS

In this section will be described the simulated geometry using the MCNPX code and the method used to predict the radioactive particle position inside de volume of interest. The calculation of the instantaneous particle position was made with a location algorithm by an artificial neural network.

3.1. Simulated Geometry

Simulated geometry in this work was performed with the MCNPX code, and it consists of a PVC (Polyvinyl Chloride) tube with 10 cm of radius and 100 cm of length containing air in its interior, eight scintillator detectors of NaI(Tl). The radioactive particle is a Cs-137 (662 keV) point source with isotropic emission. The eight detectors were distributed in two planes along the tube: the first plane is positioned at z = 0 cm and the second plane at z = -25 cm, as shown in Figure 1.

Figure 1: *Simulated geometry using MCNPX code.*



Each plane has four NaI(Tl) detectors, which are spaced at a 90° angle from each other. The distance between the detectors and the tube is 20 cm. Simulated detectors has a 2"x2" NaI(Tl) crystal, it is surrounded by a reflective layer composed by 0.1 cm thick magnesium oxide (MgO) and it has a 0.1 cm thick aluminum (Al) layer. The crystal is surrounded and sealed by an aluminum layer 0.1 cm thick. It is necessary to emphasize that the photomultiplier was not simulated in this work.

In the MCNPX code input file, through the tally card F8, the response of the simulation is the pulse height distribution of the source. In this work, only the region corresponding to the photoelectric absorption was used for the ANN training. To ensure that the relative error remains below 5% in the photopeak region, it was used 1E07 as number of histories (NPS) in the simulations. Considering the frontal and side distance between the source and the detector, the absolute efficiency was evaluated. It is important to highlight that all the detectors have the same efficiency curve.

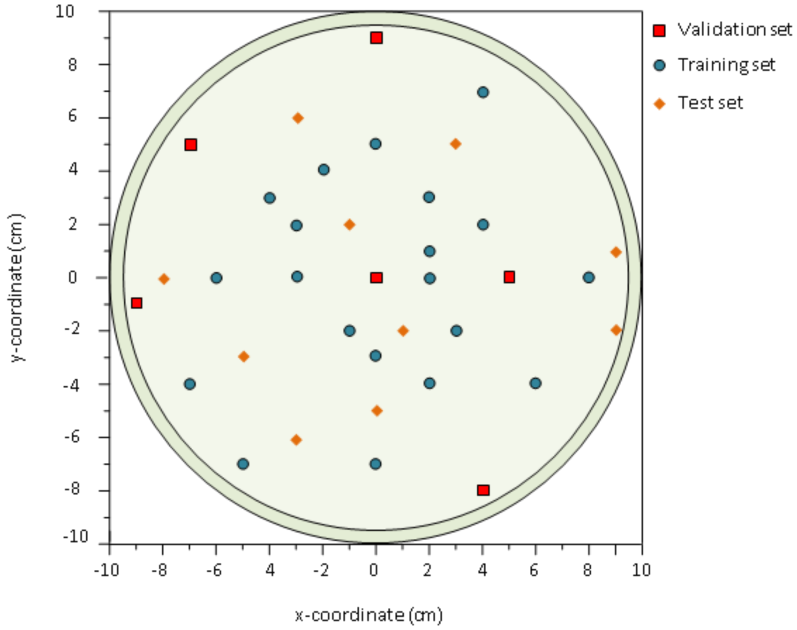
3.2. Artificial Neural Network (ANN) Training

The principle of the RPT technique is to correlate each detector counting to the instantaneous particle position inside the volume of interest. In this study, the instantaneous position of the particle is calculated by a location algorithm given by an ANN.

To train a neural network is necessary a training set of data that was chosen in a certain proportion about: 60% Training, 30% Test, 10% Validation. Radioactive particle was positioned in 108 different positions (x,y,z), including positions between the detectors planes, and all these positions were created randomly. The x coordinate range from -9 to 9 cm while the y coordinate range from -8 cm to 9 cm in each plane. These positions were replicated in the planes, and the z-coordinate was varied in three different positions: z = 0 cm, z = -12.5 cm and z = -25 cm.

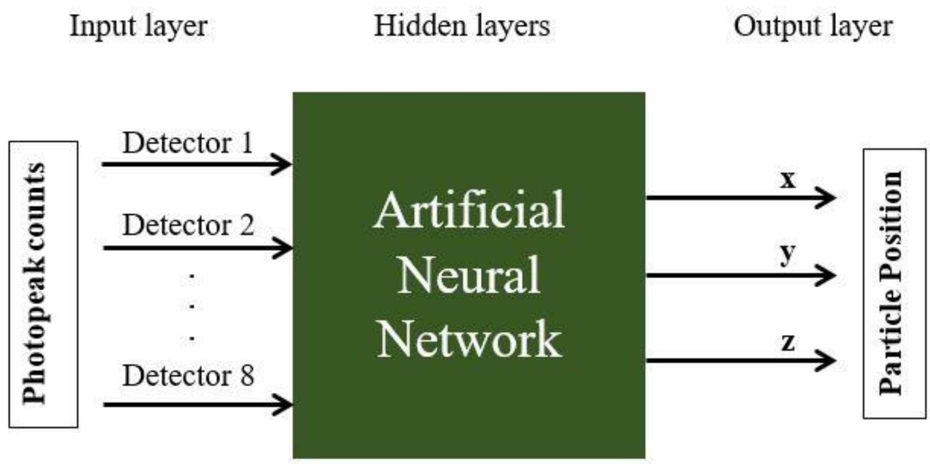
Figure 2 shows the positions x and y for one plane only. Data set with 108 simulations to train the ANN was divided into sets of Training (60 simulations), Test (30 simulations) and Validation (18 simulations). Test set is used to evaluate the ANN generalization and to avoid the overtraining. A 3-layer feed-forward multilayer perceptron with the backpropagation algorithm has been used. Data sets were distributed empirically and randomly.

Figure 2: *Positions X and Y for training, test and validation sets for plane.*



ANN training patterns are composed by inputs and outputs. Inputs are the registered counts of the eight detectors and the outputs are the positions (x,y,z) of the radioactive particle. As said in section 3.1, only counts of the region corresponding to the photoelectric absorption were used in the ANN training. The pulse high distribution was divided into 800 channels with 10 keV each. The count related to the total absorption was in the 670 channel. For a better understanding, the ANN structure is arranged in Figure 3.

Figure 3: *Schematic representation of the ANN.*

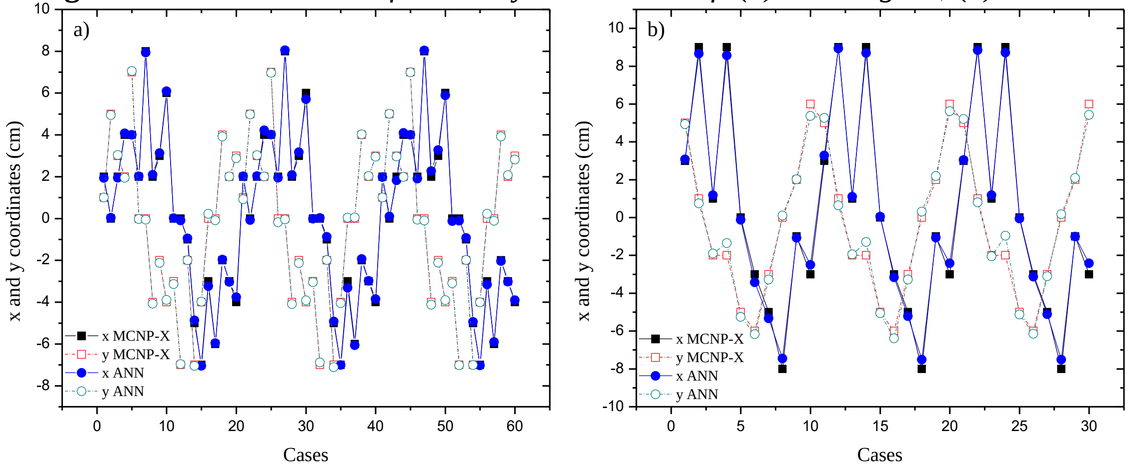


4. RESULTS AND DISCUSSIONS

The results presented in this section represent the processed data from the trained ANN to predict the instantaneous radioactive particle position. Simulations were performed with the MCNPX code, using the tally card F8 for pulse height distribution estimative, but only the corresponding region of the photoelectric absorption was used to generate the results. To ensure that the relative error associated with the counts of each detector was less than 5% for all the cases, the calculation accounted to 1E7 NPS.

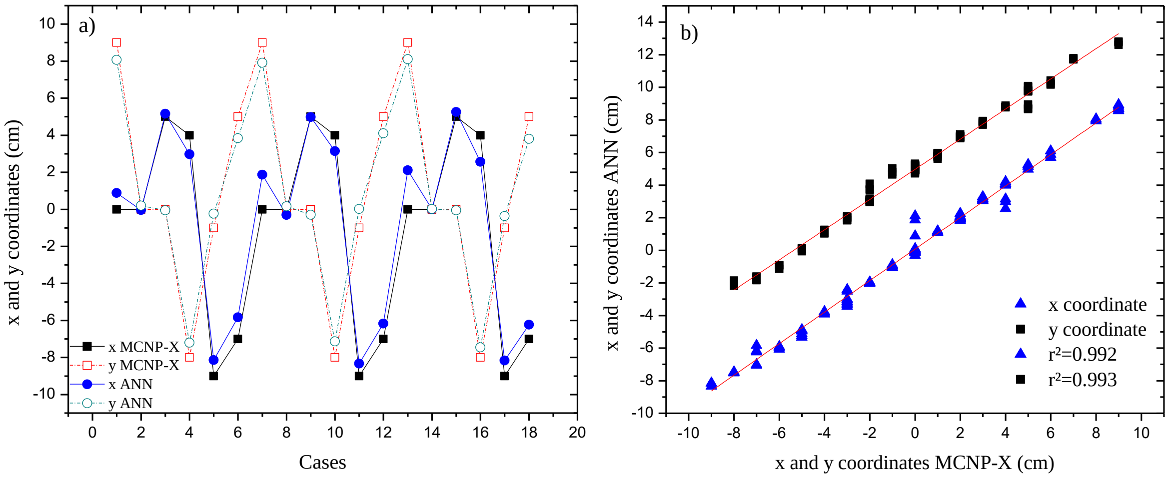
The coordinates x and y obtained by ANN in comparison to the MCNPX data are shown in Figure 4. Results are related to the Training and Test sets. The results from the training and test sets shows that the ANN follows the pattern from the simulations with MCNPX code.

Figure 4: *Results obtained for x and y coordinates of: (a) Training set; (b) Test set.*



The Validation set is an important step because here the ANN shows its potential to recognize new patterns that were not used in Training and Test sets. The comparison between trained ANN with MCNPX code for Validation set is one of the final tests to evaluate the off-line phase is represented the Figure 5(a). It is possible to observe the tendency of ANN to follow the coordinate's values given by MCNPX code. For a better evaluation of the results of the ANN, a minimum squares method was applied to a linear fit to correlate coordinates x and y from MCNPX code with ANN. The linear fit of the coordinates x and y for all data is shown in Figure 5(b), and it is important to mention that the linear coefficient of the y coordinate was modified to a better visualization.

Figure 5: *Results obtained for x and y coordinates for: (a) Validation set: (b) linear fit for all data.*



Correlation coefficient (r^2) from the linear fit for x-coordinate is 0.992 and it shows that the ANN is converging well. Meanwhile, for y-coordinate, r^2=0.993, which is also a good indicative of the ANN convergence. These results points to a good acceptance of the proposed methodology. Correlation coefficient (r^2) for Training set is 0.998 for x and y coordinates. In the Test set, r^2=0.997 for x and y coordinates. Results indicates a good compatibility between data generated by MCNPX and the ANN. As the z-coordinate has been varied in a few positions (z=0 cm, z=-12.5 cm, z=-25 cm), the results for the Training, Test and Validation sets will be presented in Table 1, as well as processed data generated by the ANN. Most important parameters to evaluate the ANN convergence are relative errors and the correlation coefficient.

Table 1: Processed data from the trained ANN.

Processed data	**Coordinates**		
Relative Error	**x**	**y**	**z**
< 5%	50.00	50.932	61.11
5% – 10%	19.44	14.81	3.70
10% – 20%	11.11	5.56	1.85
20% – 30 %	1.85	2.78	0
> 30%	0.93	6.48	0
Correlation coefficient	0.996	0.996	0.999

Analyzing the processed data, r^2=0.99 for all cases shows a good convergence of the ANN for the three coordinates. Over 60% of the results for x and y coordinates were below 10% of relative error. Meanwhile, for the z coordinate, over 60% were below 5% of relative error. The results show a good convergence of the ANN and it indicates that the ANN could be capable to predict the z-coordinate as well. Few cases above 30% of relative error, for all cases, is also a good parameter to evaluate the good convergence of the ANN.

5. CONCLUSIONS

In this work is presented a non-invasive methodology, based on the principles of the radioactive particle tracking (RPT) technique, to predict the position of the radioactive particle to evaluate agitators in industrial units. The modeling was performed by MCNPX code, and the reconstruction algorithm is given by a 3-layer feedforward artificial neural network (ANN) with a Backpropagation algorithm. The results presented by the trained ANN indicates its great potential to predict the instantaneous position P(x,y,z) of the radioactive particle inside a volume of interest. Over 69% of the cases were below 10% of relative error for x-coordinate and over 64% of the cases were below 10% of relative error for y-coordinate. For z-coordinate, over 60% of the cases were below 5% of relative error. The correlation coefficient (r^2) were 0.99 for all cases. These results indicate that the methodology here presented could be a good diagnosis tool for industrial units.

6. ACKNOWLEDGMENTS

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