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Particle dispersion modeling in ventilated room using artificial neural network

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Abstract Due to insufficiency of a platform based on experimental results for numerical simulation validation using computational fluid dynamic method (CFD) for different geometries and conditions, in this paper we propose a modeling approach based on the artificial neural network (ANN) to describe spatial distribution of the particles concentration in an indoor environment. This study was performed for a stationary flow regime. The database used to build the ANN model was deducted from bibliography literature and composed by 261 points of experimental measurement. Multilayer perceptron-type neural network (MLP-ANN) model was developed to map the relation between the input variables and the outputs. Several training algorithms were tested to give a choice of the Fletcher conjugate gradient algorithm (TrainCgf). The predictive ability of the results determined by simulation of the ANN model was compared with the results simulated by the CFD approach. The developed neural network was beneficial and easy to predict the particle dispersion curves compared to CFD model. The average absolute error given by the ANN model does not reach 5% against 18% by the Lagrangian model and 28% by the Euler drift-flux model of the CFD approach.

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1 Introduction

Indoor air quality is a significant concern, because people on average occupy most of their time in the built environment, where they are regularly exposed to pollutants in the interior atmosphere. Commonly, the contaminants diffuse into the ambient air around nuclear facilities in the radioactive fine particles form or gases radioactive form. Aerosols are considered as a primary factor for the indoor air pollution. To better assess the risks of internal contamination in ventilated areas, wherein the detailed information on aerosols transfer and particles concentration distribution is of great importance in the context of improving the radiological system (zoning control and classification). We think about improving the effectiveness of air filtration systems (HEPA filters for particulate and carbon filters for radioactive gas) in the ventilation systems of nuclear facilities, to undertake a study of the aerosol transfer in a ventilated room. We will continue along this path of study to choose optimal conditions (flow regime) that give minimum particles concentration in an ambient environment. For example, this technique is used to design the clean rooms for radioisotope production.

Generally, there are two approaches to simulate the particle transfer: experimental simulation and numerical simulation. As experimental simulation costs a lot, numerical simulation is often adopted to analyze the particle dispersion phenomenon [1–3], and is playing an increasingly important role nowadays in predicting particle behavior and air flow dynamics.

Most studies using computational fluid dynamic (CFD) followed particle's trajectory in the continuous phase (air) according to the Lagrangian or Eulerian approaches. The Eulerian particle tracking method considers the particle as a continuous phase and treats it as two fluid phases (air-particle). The momentum equations of the second phase (particles) are developed in a similar form of the gas phase (first phase: air). In the Lagrangian particle tracking approach, the fluid phase is considered as a continuous phase by solving the Reynolds-averaged Navier–Stokes equations (or RANS equations), whereas the particle phase is considered as a discontinue phase and the resultant motion equation relating the various forces exercising on an individual air-particle is resolved so as to get the single-particle trajectories [4]. Several groups in numerical fluid dynamics studied the condition effect over airflow (ventilation) and particle behavior [5–7], while others developed drift-flux model derived from Eulerian approach to study particle dispersion phenomenon in a closed environment [1, 4, 8–10]. The mixture model is a sub-Eulerian model for particles phase treatment [4], and the Lagrangian model, for particle trajectory tracking [4, 11–14].

In order to attain the objective of building accurate models in predicting behavior of indoor aerosol, we are oriented to the artificial neural network (ANN) simulation since it is successfully applied in other scientific fields. This work was elaborated in this context to develop a metamodel. Metamodeling enables a large analysis of the input variables, improves the generated model understanding and allows new studies to optimize the solution of systems [15, 16]. ANN is used widely in multidisciplinary varieties such as calibration of water distribution systems [17], modeling of nuclear chemistry applications [18], thermodynamic transport properties of fluids [19] and contamination of groundwater [20]. Recently, ANN has been trained and tested to optimize the ventilation systems in indoor environments [21, 22]. Being to replace conventional regression models, ANN is expected to evolve further in developing metamodel as it offers an alternative path to complex systems modeling. Based on several inputs and outputs, it is able to bring any nonlinear function to a random degree with a single hidden layer [16, 23].

In this work, a metamodel based on ANN was developed to describe the relationship between input variables governing the aerosols dispersion in a ventilated closed space. The predictive ability of ANN model was compared with experimental results and those given by CFD which are inspired from Ref. [1, 4]. Several simulations were designed to test and validate the metamodel. The predictive ability of the ANN model was compared to that of CFD approach (Lagrangian and Eulerian models) [4]. Graphical visualization of the particles concentration distribution along vertical direction at fixed axial position was done by a program written in MATLAB software. In addition, a second program for plotting the contours of normalized iso-concentrations to the central plane of the room (x, y). The best model for particle dispersion prediction is identified in a room for stationary flow regime.

2 Methodology

The most methodological way to develop an ANN model was to follow the flowchart steps in Fig. 1. The last two steps (training and test) mentioned in the proposed organization are treated in Sect. 3 [16].

2.1 Problem description

The room environment, as a model for particle concentration analysis, is shown in Fig. 2. Nineteen variables were selected to define the airflow and particle concentration. The air inlet is placed at the top opening on a wall and the exit at the bottom opening on the opposite wall. L, H and W are the room length, height and width, respectively. Coordinates of the concentration measurement points at the three directions (x, y, z) are, respectively, designated by x_1, y_1 and z_1. Coordinates of distance between the entrance and the exit of area A are denoted by x_{Ai-Ao}, y_{Ai-Ao} and z_{Ai-Ao} in three directions (x, y, z), and U is the inlet air velocity. As for the other parameters, τ is particle stay time in the room. ρ_f is density of air, μ is dynamic viscosity of air, ρ_p is aerosol density, and d_p is diameter of the aerosol particle. All quantities are expressed in the international system of units. The relation between the input parameters is

$$f\left(\frac{C}{C0}, L, W, H, x_1, y_1, z_1, A_i, A_o, x_{Ai-Ao}, y_{Ai-Ao}, z_{Ai-Ao}, U, \rho_f, \mu_f, \rho_p, d_p, \tau\right) = 0 \quad (1)$$

where C/C_0 is the normalized concentration of the particles in the indoor.

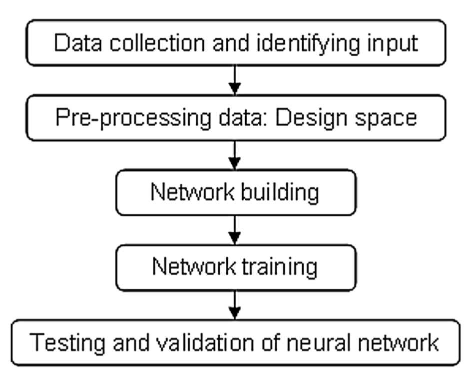

Fig. 1 Methodology flowchart

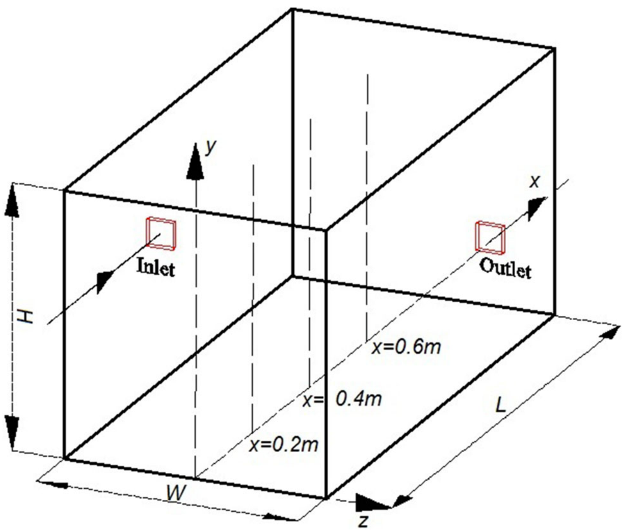

Fig. 2 Geometry of the model room

Table 1 Minimum and maximum values for the twelve groups

Parameters	Unit	Min	Max
d_p	m	5×10^{-7}	1×10^{-5}
U	m/s	0	1.5
x_1/L	–	0.17	0.83
y_1/H	–	0	0.9526
z_1/W	–	0.17	0.83
A_i	m^2	0.0016	0.06
A_o	m^2	0.0016	0.06
x_{Ai-Ao}	–	0.83	1
y_{Ai-Ao}	–	0	0.8
z_{Ai-Ao}	–	0	0.5
ρ_f	kg/m^3	1400	2100
$1/\tau$	s^{-1}	0	0.3

The use of dimensional analysis provides thirteen variables developed from Eq. (1) and reordered to obtain Eq. (2). The input variables were reduced to twelve: The two variables ρ_f and μ_f were simplified because the same environment fluid (air) with a constant temperature was considered, and three variables defining the study domain (L, H, W) were included in the measurement points coordinates to be dimensionless variables (x_1/L, y_1/H, z_1/W).

$$\frac{C}{C_0} = \beta\left(\frac{x_1}{L}, \frac{y_1}{H}, \frac{z_1}{W}, A_i, A_o, x_{Ai-Ao}, y_{Ai-Ao}, z_{Ai-Ao}, U, \rho_p, d_p, \tau\right) \tag{2}$$

2.2 Input parameters conception

The most important information regarding the relation between the output(s) and the space of input design has to be investigated effectively to reduce the experimentation time, numerical or physical simulations. To define the limits of numerical simulation domain, a minimal value and a maximal value were attributed at each parameter in Eq. (2) (Table 1). The database, defined by measured values deduced from Ref. [1–3], is constructed by 261 measured points of particles concentration, of which 80% affected for training, 10% for validation and 10% for test the ANN model.

2.3 Determination of the network model form

The neural network principle is similar to the nonlinear regression method. There are various types of neural networks, among which the multilayer perceptron (MLP) model is considered as the most popular network and usually used in scientific applications. It includes different layers at several levels: one input layer, one output layer and one or more hidden layers. Each layer consists of a number of neurons with an activation function between layers (Fig. 3).

The ANN, mathematically represented by Eq. 3, has three layers where n, m and p are, respectively, the numbers of neurons in the input, hidden and output layers [16].

$$\left(\frac{C}{C_0}\right)_k = f_{\text{output}}\left(\sum_{j=1}^{m} w_{jk} f_{\text{hidden}}\left(\sum_{i=1}^{n} w_{ij} x_i\right)\right) \tag{3}$$

where $y = (C/C_0)_k$ is the output; x_i is the input; w_{ij} is the weights input layer/hidden layer; w_{jk} is the weights hidden layer/output layer; and f is the activation function, which can be linear $f(a) = a$, sigmoid $f(a) = (1/(1+e^{-a}))$ or hyperbolic tangent $f(a) = \frac{e^a - e^{-a}}{e^a + e^{-a}}$.

2.3.1 Normalization of the inputs and output values

The normalization of values is an important ANN preparation step. The ANN input values may differ by

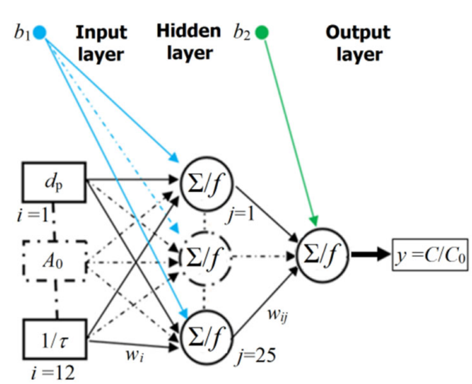

Fig. 3 ANN structure diagram

several orders of magnitude, which may not reflect the relative significance of the inputs predicting output particle concentration in this work. So, input and output variables data are normalized within the range limited between -1 and 1 using a mapminmax algorithm, given by Eq. (4), to normalize the maximum and minimum values of each row [24].

$$y = \frac{(y_{\max} - y_{\min})(x - x_{\min})}{(x_{\max} - x_{\min})} + y_{\min} \tag{4}$$

2.3.2 ANN performance

The differences between experimental and predicted values are filtered across the network and used to adapt the connections between the layers, so as to improve the performance. The root mean square error (RMSE) coefficient is the main criteria for evaluating the ANN performance, which is defined by [24]

$$\mathrm{RSME} = \left[\frac{1}{n}\sum_{i=1}^{n}\left(y_i - y_i^t\right)^2\right]^{1/2} \tag{5}$$

To improve the ANN quality based from the statistical point of view for the training, test and validation sets are evaluated using the squared correlation coefficient R, absolute error AE and average absolute error AAE,

$$R = 1 - \frac{\sum_{i=1}^{n}\left(y_i - y_i^t\right)^2}{\sum_{i=1}^{2}\left(y_i - y_0\right)^2} \tag{6}$$

with

$$y_0 = \frac{\sum_{i=1}^{n}\left(y_i - y_i^t\right)}{n} \tag{7}$$

$$\mathrm{AE}_i = \left[\frac{\left|y_i^t\right| - \left|y_i\right|}{\left|y_i^t\right|}\right] \times 100 \tag{8}$$

$$\mathrm{AAE} = \frac{1}{n}\sum_{i=1}^{n}\mathrm{AE}_i \tag{9}$$

where y_i, y_i^t and n are the ith trained, test or validation output value, the target value and the number of input vectors, respectively.

3 Results and discussion

To provide the best credible, reliable and valid results, the room geometry in Fig. 2 was selected as computational domain. Measured data of particle concentration realized by Chen et al. [1] using the Phase Doppler Anemometry (PDA) instrument were selected as reference values. The CFD simulation results, Lagrangian and drift-flux models, obtained by Bin Zhao et al. [4] were selected to confront the ANN model results. The room geometry was 0.8 m (L) $\times$ 0.4 m (W) $\times$ 0.4 m (H). The two openings (inlet and outlet) were sized at 0.04 m $\times$ 0.04 m, being symmetrical with the center plane at $Y = 0.2$ m. The aerosol density was 1400 kg/m^3. The inlet velocities were $U = 0.225$ and 0.45 m/s.

The parameters were evaluated to provide better configuration offering a compromise between the ANN performance and the best fit to describe the spatial distribution of the normalized particle concentration (x, y, z) in a workspace. To optimize the ANN model, the effect of several parameters were evaluated for network convergence, such as neuron number in the hidden layer, activation function between the layers (input layer, hidden layers and output layer), network training algorithm and the normalization function of input and output data.

Twenty-five neurons were chosen in the hidden layer after a series of simulations by varying the number of neurons and measuring the mean squared error (MSE). Additionally, there were large numbers of training algorithms producing an accurate network, fast and reliable. Six algorithms were tested to find an algorithm which performs better in our case, and the six networks established by their training algorithms were named as Net1, Net2, Net3, Net4, Net5 and Net6. The algorithms with their corresponding codes are presented in Table 2. Table 3 shows the selected ANN parameters.

The optimal configuration of the ANN has the following performances: $RMSE = 3.2518 \times 10^{-4}$, $R = 0.9994$, $Y_0 = 2.0128 \times 10^{-5}$, and $AE = 1.0661\%$. The best polynomial fit is $y = (C/C_0)_{\mathrm{pred}} = 1.0 \times (C/C_0)_{\mathrm{exper}} + 0.00089$.

Regression ANN analysis was performed to compare experimental and predicted data of particle concentration (Fig. 4). Figure 5 shows the comparison of simulated concentration by three numerical models: ANN model, drift-flux and Lagrangian CFD models versus the experimental data considered as reference values.

Modeling by ANN provides a better spatial distribution profile of particle concentration in indoor ambient and agree well with the experimental data almost in all calculate domain: interior domain and interpolated part. Using Eqs. (8) and (9), we compared the relative error and the average of the results simulated by CFD approach and the ANN model with the experimental values. The evaluated relative error was less than 5% for all concentrations obtained by ANN model as shown in Fig. 5, except the point with coordinates (0.2, 0, 30, 0.2) where a value of 13.48% was observed at $U = 0.225$ m/s.

The Lagrangian model gives acceptable values compared to the experimental data except the positions above the height of 0.3 m from room floor (jet flow) are relatively far from measured data.

Table 2 Training algorithms of the ANN

Network name	Training algorithms	MATLAB code	Acronym
Net1	Quasi-Newton/Levenberg–Marquardt	Trainlm	LM
Net2	Polak–Ribière Conjugate Gradient	TrainCgp	CGP
Net3	Fletcher–Powell Conjugate Gradient	TrainCgf	CFG
Net4	Quasi-Newton/One-Step Secant	TrainOss	OSS
Net5	BFGS Quasi-Newton	TrainBfg	BFG
Net6	Resilient Back-propagation	TrainRp	RP

Table 3 ANN parameters

Selected parameters	Properties
Layer hidden number	One hidden layer
Neurons number of hidden layer	25 neurons
Activation function	
Input/hidden layer	Log-sigmoid transfer function.
Hidden/output layer	Linear function
Normalized function	Premnmx (max and min) function
Training algorithm network	TrainCgf (Fletcher conjugate gradient) algorithm

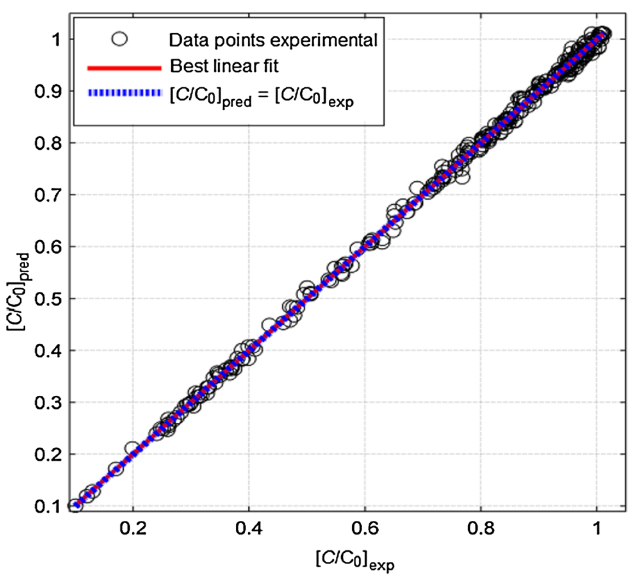

Fig. 4 Comparison of target and ANN predicted values for normalized concentration of particles from confined milieu

The average and the largest relative errors are 15.9 and 42.2%, respectively, at the point (0.2, 0.379, 0.2) for $U = 0.225$ m/s [4]. The drift-flux model gives fairly acceptable values in positions of above 0.3 m from room floor (jet flow) with 15% as average relative error. At room height of <0.3 m, the results are less than the experimental data and the largest relative error was 55.4% at coordinates (0.2, 0.14, 0.2) for $U = 0.225$ m/s [4].

Figure 6 shows the concentration errors using the simulations models of Lagrangian, drift-flux CFD and ANN, for three axial positions and inlet velocities of 0.225 and 0.45 m/s. The ANN model, with maximum average error of about 5%, performs the best, while the Lagrangian model comes in the second position with an average error about 16%.

In Fig. 5, the ANN-calculated values (black lines) coincide with the experimental points at $x = 0.2$, 0.4 and 0.6 m and at $U = 0.225$ and 0.45 m/s. The interpolation part, inside domain, is limited in the axial direction between x_1 and x_2, and the vertical direction between y_1 and y_2, as indicated in Figs. 7, 8, 9. To show better the particle concentration decrease in a closed environment, we graphically visualized the axial distribution of the jet flow at $y = 0.36$ m (Fig. 7). However, this model interpolates even spatial distribution of the particles concentration in other axial or vertical positions, indicating that the ANN model interpolates finely the particle dispersion phenomenon in a closed space.

The extrapolation values of particle concentration determined by the ANN in Fig. 7 indicate that they are tangible and perceptible if we see the graph allures of axial spatial distribution for inlet velocities of 0.225 and 0.45 m/s. From the data measured outside the interest domain limits, and from Fig. 7, the extrapolations values are acceptable. This means that the ANN model is a good extrapolator especially for positions near the computational boundary domain.

Figure 8 shows a graphical representation of the particles concentration distribution in a closed space in the central plane of the room. One sees an acceptable and reasonable shape of the concentration distribution with large particle concentration at air inlet area (as a pollution source in this case), decreasing gradually along the x-direction due to particle deposition on room walls. Based on these results for the iso-concentration contours at inlet

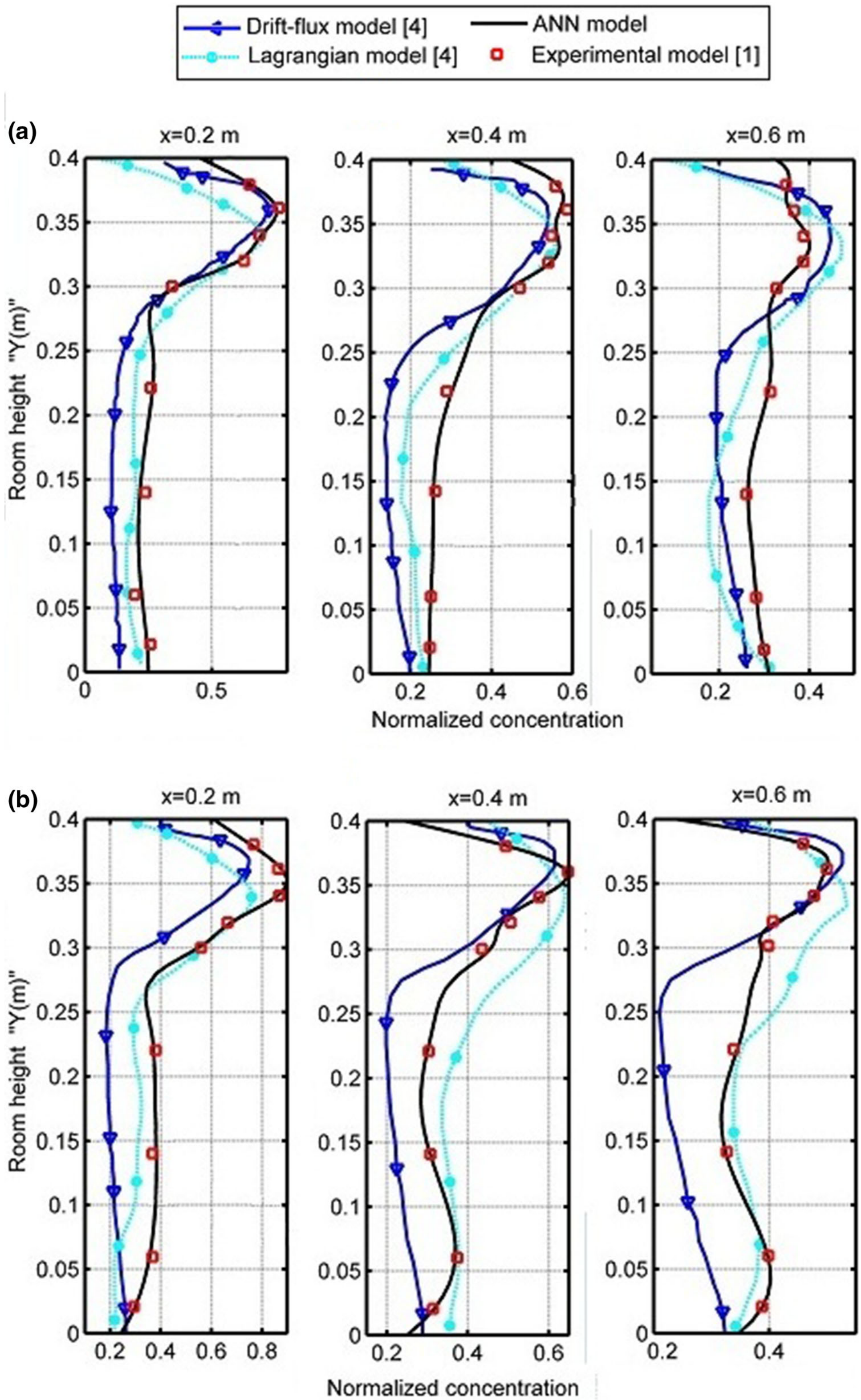

Fig. 5 Measured and predicted particle concentration at three different axial locations. **a** $U = 0.225$ m/s, **b** $U = 0.45$ m/s

velocities of 0.225 and 0.45 m/s (Fig. 8), we conclude that simulation results of particles concentration using the ANN were good on all over space of the domain and at different regimes of airflow.

In addition, Fig. 9 shows a detailed visualization of particles concentration distribution in the central plane of the room, in the axial and vertical directions, at inlet velocities of $U = 0.225$ and 0.45 m/s.

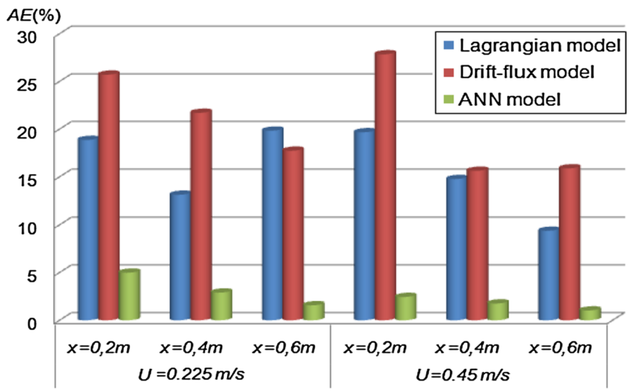

Fig. 6 Graphic visualization of the average error at three axial positions for two inlet velocity

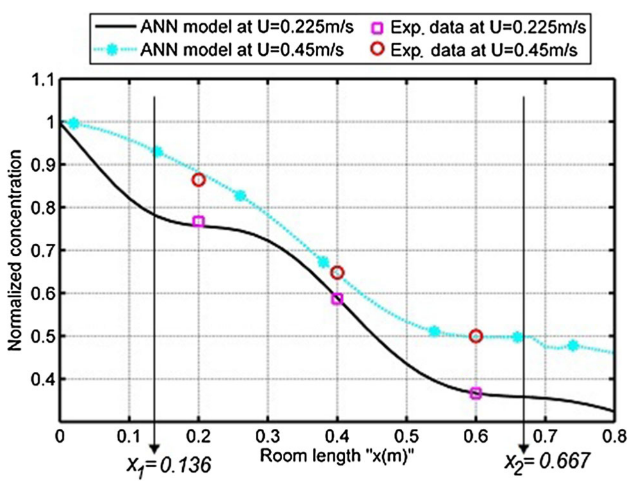

Fig. 7 Axial distribution of normalized concentration at room height of $y = 0.36$ m

4 Conclusion

The aim of this paper was focused on numerical modeling of particle dispersion in indoor environment and for stationary flow regime, using artificial neural network. The model was based on experimental data available in the literatures for smoothing the particle concentration distribution on all domain space and for different boundary conditions. Network performance was compared with CFD methods using the same assumptions and flow regime. The results led to the following conclusions:

1. The ANN model has better accuracy for performing smoothing particle concentration distribution in indoor environment, compared to CFD approach Lagrangian and drift-flux models. The ANN modeling gives an average relative error of <5%, compared to the experimental results.
2. The CFD methods give an average performance for the particle trajectory tracking in an indoor environment. For example, the Lagrangian model is acceptable for low particles concentrations, near walls, with an average relative error of around 18%; whereas the particle tracking by drift-flux model is good just at the core flow. So, unlike ANN modeling, the CFD approaches are limited by utilization to tracking model for smoothing of particles distribution in space.

As the ANN results are close to experimental data, it will be encouraging to develop this approach and consequently establish a platform for CFD simulation validation of different design parameters, so as to improve CFD

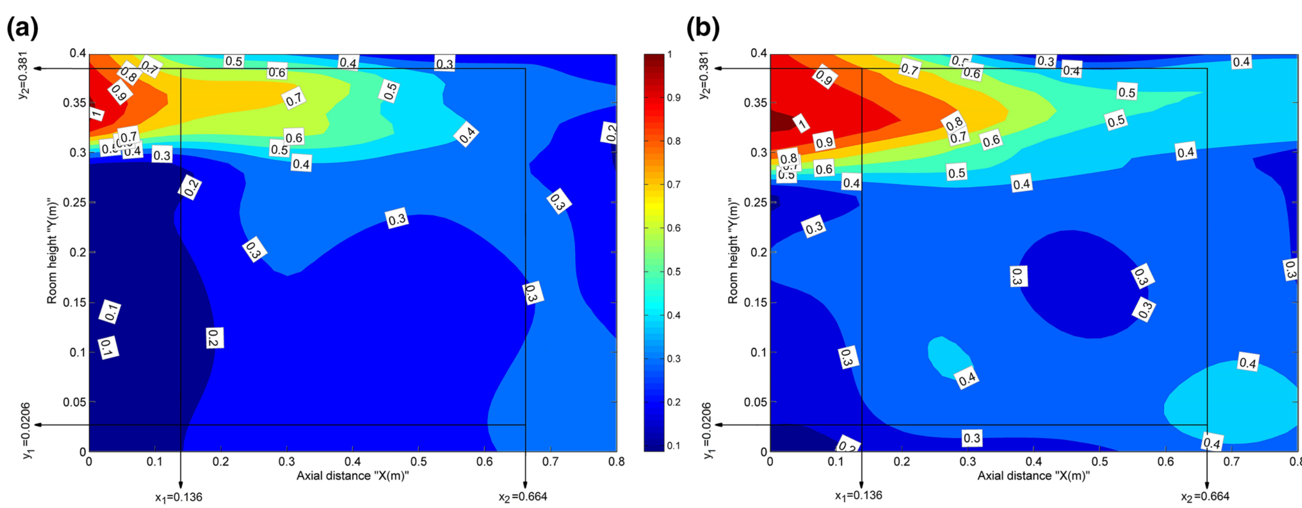

Fig. 8 Simulation results for the distribution of particle concentration at the surface center. **a** $U = 0.225$ m/s, **b** $U = 0.45$ m/s

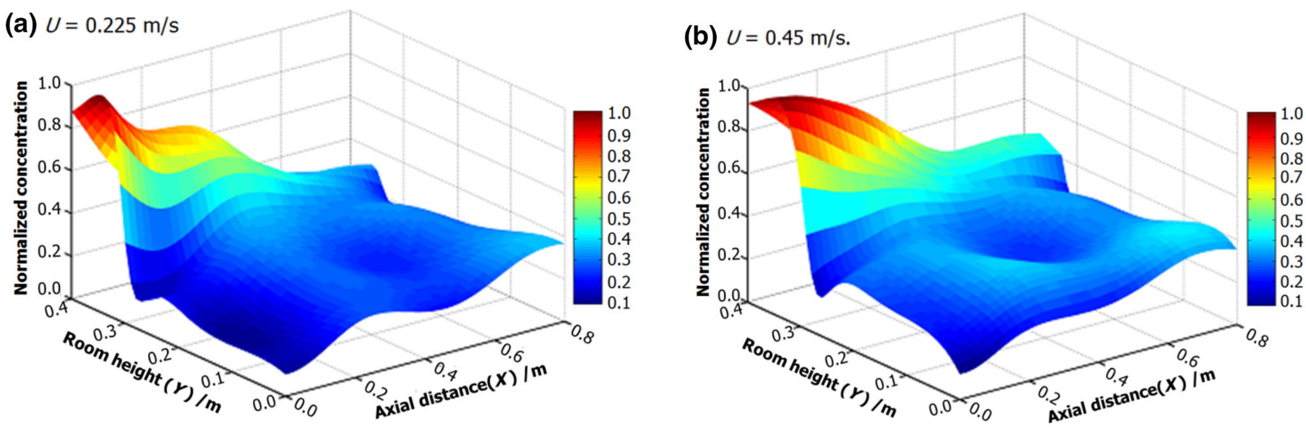

Fig. 9 3-D distribution of particle concentration in surface center at inlet velocity of **a** $U = 0.225$ m/s and **b** $U = 0.45$ m/s

methods and verify reliability of the simulation results. This will facilitate the cartography determination of particle concentration for purposes of safety issues and protection of workers within nuclear installation:

- Classification of controlled areas (red, orange or green),
- Calibration of monitoring equipment,
- Determination of filtration barrier in ventilation systems,
- Accumulation contaminants in the dead zones (bad ventilated areas).

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