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A NEURAL NETWORK FOR PREDICTING WITH THE DIFFUSION EQUATION: A CASE STUDY OF LONG ROOMS

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ABSTRACT

The diffusion equation model with a constant diffusion coefficient underestimates the sound pressure level and reverberation time when elongated rooms are considered in room acoustics. In fact, for these types of rooms, it has been established that the diffusion coefficient is spatially variable and depends on the acoustics properties of the surfaces. This study presents a novel method for estimating the spatially dependent diffusion coefficient of the diffusion equation model for the case study of long rooms using an artificial neural network. The network is trained to relate the dimensions of the room, the absorption coefficients of the surfaces and the 3D source and receiver positions to the corresponding diffusion coefficient using supervised learning. The databases are generated using the sound particle tracing approach (SPPS) and Fick's law. Results show that the neural network model, with the appropriate considerations and architecture, can quickly recover the space-varying diffusion coefficients over the room based only on the model's inputs (geometries, properties of the room, and source positions). When the predicted diffusion coefficients of the neural network are used in the diffusion equation, the sound pressure level and reverberation time of the room can be accurately predicted.

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1. INTRODUCTION

In the past few decades, simulating how sound behaves in spaces has been essential to enhancing interior comfort. As a result, numerous simulation techniques are created to improve the accuracy of prediction methods. Some examples are ray and beam tracing [1], the diffusion equation approach [2,3], the image source method [1], the radiosity method [1], and various wave-based methods [4]. In particular, the diffusion equation has been used recently due to its efficiency in computational time [5].

However, the limiting parameter of the diffusion equation is the diffusion coefficient (in units m^2/s). This is often considered a constant value, depending on the room's volume and the surface areas of the boundaries. However, for non-proportionate rooms, this assumption is incorrect. Effectively, Fick's law assumes a proportionality relationship between the reverberant sound intensity vector \mathbf{I} and the gradient of the reverberant energy density $w(\mathbf{r})$ (in $\text{kg}/(\text{m s}^2)$) through the diffusion coefficient:

$$\mathbf{I}(\mathbf{r}) = -D(\mathbf{r})\nabla w(\mathbf{r}) \quad (1)$$

where $\mathbf{r} = (x, y, z)$ is the position vector. Researchers have shown that it should be spatially varying depending on the dimensions of the room and also dependent on source position and the mean absorption coefficient α of the room [5–8]. The diffusion coefficient can be determined using Equation (1), which requires knowledge of





the intensity of the sound and the energy density. These parameters can be calculated using a reference method such as the sound particle tracing model (SPPS) [9]. The present study explores using an artificial neural network to estimate the diffusion coefficient directly. In the domain of room acoustics, previous work has shown that it is possible to use neural networks [10], where the estimation of the mean absorption coefficients was derived from a room impulse response using virtually supervised learning [10].

In a second step, the diffusion equation model using these estimated neural network diffusion coefficient values is used to calculate the sound pressure level (SPL) and the reverberation time (T_{30}), two main parameters in room acoustics, and compared to a reference acoustics approach of the sound particle tracing model (SPPS).

In Section 2, an introduction to the diffusion equation model is given. Section 3 describes the methodology used for the study, including the neural network architecture. The results of the neural network are discussed in Section 4 and compared to the diffusion coefficient values obtained by SPPS. In Section 5, the predicted diffusion coefficients from the neural network are introduced in the diffusion equation model, and the results of SPL and T_{30} are compared with those calculated with the reference method. The paper concludes in Section 6 with an overview of the results and limitations of the method.

2. DIFFUSION EQUATION AND DIFFUSION COEFFICIENT IN ACOUSTICS

The diffusion equation is a partial differential equation used to predict the time-dependent energy density for the diffuse part of the sound field, enabling the calculation of the room's acoustic parameters. It is an energy-based method that allows the calculation of the sound energy density over space and time. Under the assumption of Fick's law of diffusion described in Equation (1), the behaviour of the sound in a room can be described by the time-dependent diffusion equation model, for acoustic energy density $w(\mathbf{r}, t)$ in $[\text{kg}/(\text{m}^2 \text{s}^2)]$ [11]:

$$\frac{\partial w(\mathbf{r}, t)}{\partial t} = \nabla \cdot (D(\mathbf{r}) \nabla w(\mathbf{r}, t)) + q(\mathbf{r}, t), \text{ in } V \quad (2)$$

where $D(\mathbf{r})$ is a proportionality factor between the sound intensity and the gradient of the sound energy density with units $[\text{m}^2/\text{s}]$ and q is the energy per volume of a sound source. The diffusion equation is associated with some boundary conditions that describe how the sound behaves

at the surface boundary of the room as follows [12, 13]:

$$D(\mathbf{r}) \frac{\partial w(\mathbf{r}, t)}{\partial n} + cAw(\mathbf{r}, t) = 0 \text{ in } \partial V \quad (3)$$

where n is the normal to the surface and A is the absorption factor. The absorption factor depends on the absorption coefficient of the specific surface and has been modified over the years to allow the use of higher absorption coefficients in the model by Picaut [14] and Jing and Xiang [13, 15]. The absorption factor, defined by Picaut as the Sabine Absorption Term ($A = \alpha/4$), is used for the simulations of this article [14]. The diffusion coefficient represents a limiting factor for the diffusion equation, which is often considered as a constant value for proportionally shaped rooms depending on the volume and total surface area of the room, as highlighted in Equation (4) [11]:

$$D_{\text{th}} = \frac{\lambda c}{3}, \quad (4)$$

where D_{th} stands for theoretical diffusion coefficient, and λ is the mean free path of the room defined as $4V/S$, where V represents the room's volume and S represents its entire boundary surface area. The condition for using this definition of D_{th} is that it holds for diffuse fields and proportionate rooms [11].

The diffusion coefficient has been studied extensively, and it has been discovered that for non-proportionate rooms, the assumption of using a constant diffusion coefficient does not hold, as it incorrectly predicts the SPL and the T_{30} of the room, along with most of the other parameters. By using Fick's law, multiple researchers have highlighted that the diffusion coefficient for non-proportionate rooms depends on different variables [5–8], like the distance between source and receiver, mean absorption and scattering coefficient [6–8] but also the source position [5]. In [6], the researchers consider the normed approximated diffusion coefficient [6]:

$$D_{\text{Fick}}(\mathbf{r}) = \frac{\sqrt{I_x^2 + I_y^2 + I_z^2}}{\sqrt{\left(\frac{\partial w}{\partial x}\right)^2 + \left(\frac{\partial w}{\partial y}\right)^2 + \left(\frac{\partial w}{\partial z}\right)^2}} \quad (5)$$

where I_x, I_y, I_z are the components of the intensity vector $I(\mathbf{r})$ and the $\left(\frac{\partial w}{\partial x}\right), \left(\frac{\partial w}{\partial y}\right), \left(\frac{\partial w}{\partial z}\right)$ are the component of the gradient of the energy density vector $w(\mathbf{r})$. The gradient of the energy density is calculated using the second order of accuracy central difference. Using the approach



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described above, Figure 1 shows the diffusion coefficient along the central axis of the elongated room of dimensions $[L_x, L_y, L_z] = [40, 4, 4]$ with mean absorption coefficient of 0.1, with the source position at (2.0 m, 2.0 m, 2.0 m) and the receiver position at $(x, 2.0 \text{ m}, 2.0 \text{ m})$, where x indicates that the receiver coordinate x changes over the length of the room.

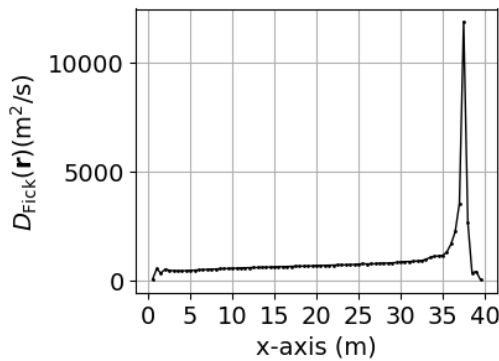


Figure 1: Numerical estimate $D_{\text{Fick}}(\mathbf{r})$ on the central line over the x -axis.

As can be seen in Figure 1, this diffusion coefficient presents a maximum value close to the end of the elongated room. This peak is probably due to the backward propagation reflections from the extremities, and it represents a challenge when proposing a neural network architecture.

Visentin shows that if the $D_{\text{Fick}}(\mathbf{r})$ is only calculated on the main axis and if it is assumed that the value is equal in the cross section, then the diffusion model correctly predicts the SPL and T_{30} over the main axis. Multiple researchers have assumed that the diffusion coefficient in elongated rooms is constant over the cross-section [5, 6, 16]. This is also the assumption used in this paper.

3. METHODOLOGY

As seen in Section 2, studies have indicated that the diffusion coefficient is spatially dependent. However, predicting these values prior to solving the diffusion equation for an elongated room remains a challenge. In fact, there are two possibilities to find the diffusion coefficient: (1) conducting real measurements in elongated rooms, however, there is no standard procedure or methodology to conduct these measurements and (2) estimating the diffusion coefficient by simulations but it is necessary to use

another acoustic model approach to calculate it. In order to overcome this limitation, a third option will be to analytically estimate a function for $D_{\text{Fick}}(\mathbf{r})$ depending on the room variables. However, it is quite challenging due to the form of the diffusion coefficient as seen in Figure 1 (more specifically due to the peak).

Therefore, in this study, a neural network architecture is designed and fine-tuned to estimate the diffusion coefficient in a supervised fashion, given only the room's dimensions, the mean absorption coefficient, and the source and receiver positions as input. The sound particle tracing model (SPPS) serves as a reference method both to calculate the diffusion coefficient $D_{\text{Fick}}(\mathbf{r})$ and to calculate the acoustic parameters of the room (SPL and T_{30}).

3.1 Simulated database

To create the database necessary for the neural network, the SPPS is used in this study to calculate both the intensity and the gradient of the energy density. These quantities are obtained by considering the energy density and intensity of the particles passing through a small sphere centered at the receiver point [9]. The gradient of the energy density is then computed using the second-order accurate central difference scheme.

For each room, a 3D grid size of receiver position spaced by $\Delta = 0.5 \text{ m}$ is used to discretize the volume. The sound power of the source is considered equal to 0.01 W. The direct sound energy between the source and the receiver is removed.

The simulations are conducted by emitting 200,000,000 particles. This number of particles decreases with time. At each reflection with the surface, the considered particle could be absorbed or reflected depending on the absorption coefficient. For example, a surface with a mean absorption coefficient of 0.3 gives a 30% probability of being absorbed and 70% probability to be reflected [9]. There is no atmospheric attenuation in any of the simulations. The scattering coefficient for each simulation is 1, therefore, only diffusely reflective boundaries are considered. The receivers are points on a grid every 0.5 m between each other.

A data set of 400 room configurations is simulated with the SPPS to calculate the diffusion coefficient at each point in the 3D room grid. The data set is formed by the target data ($D_{\text{Fick}}(\mathbf{r})$) and the following input: the length, width, and height of the room (L_x, L_y, L_z , respectively), the coordinates of the source position (S_x, S_y, S_z), the coordinates of the receiver positions (R_x, R_y, R_z) and the



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mean absorption coefficient (α).

The input data are chosen considering the previous literature [5–7]. The configurations chosen are elongated rooms within these limits:

- Length between 10 m to 40 m with steps of 0.1 m;
- Width between 2 m to 5 m with steps of 0.1 m;
- Height between 2.5 m to 4 m with steps of 0.1 m;
- Mean Absorption from 0.05 to 0.3 with steps of 0.05.

The position of the source is chosen at random but with a minimum distance from the boundary of 0.5 m. The coordinates are multiples of 0.1 m.

To make sure that the rooms are elongated, the compactness value of a room, the ratio of its whole cubed surface area to its squared volume, divided by the same ratio of an equal-volume sphere [17] is chosen to be more than 3.5.

The database is divided into training, validation, and test datasets. The training set (55% of the full database) is used by the neural network to learn from, and the validation set (35% of the database) is used to tune the model by preventing overfitting. The training and validation dataset comes from the same rooms but different grid receiver points. On the other end, the test set (10% of the full database) is used to evaluate the capacity of the neural network to predict the diffusion coefficient inside new unseen rooms.

3.2 Pre-processing of data

Since there are peaks (singularities) in the diffusion coefficient values in the database, as seen in Figure 1, the scale of the observations is quite large. In addition, the distribution of the observation is non-Gaussian, as can be seen in Figure 2. Both these features are known to be problematic for neural network training. To resolve these two points, the data $D_{\text{Fick}}(\mathbf{r})$ are divided by the room-specific D_{th} (denoted as D_{norm}) and then by taking the logarithm of base 10 of the value, as shown in Figure 3.

Figure 2 shows that the majority of $D_{\text{Fick}}(\mathbf{r})$ values lie in the low range, predominantly between 0 and 1000. Values greater than 1000 are rare, accounting for only 0.56 % of the total data. These higher values are not displayed in the figure due to their low frequency.

Figure 3 shows that the $\log_{10}(D_{\text{norm}})$ can be more closely approximated by a Gaussian curve (which means that the original data are more or less lognormally distributed). This normalization significantly improved neural network estimation performance in practice.

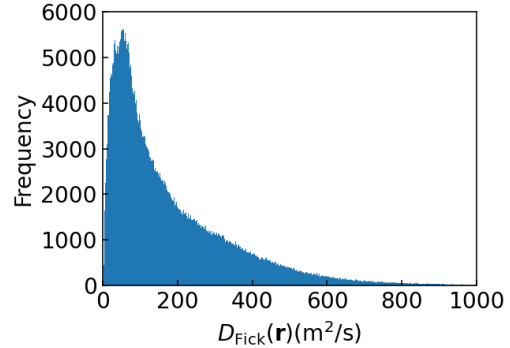


Figure 2: Histogram of $D_{\text{Fick}}(\mathbf{r})$ for 400 rooms

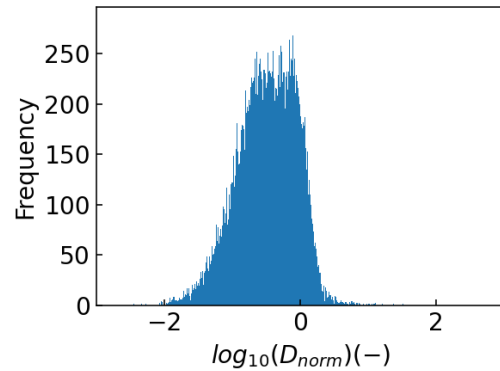


Figure 3: Histogram of $\log_{10}(D_{\text{norm}})$ for 400 rooms

3.3 Network architecture

The neural network architecture used in this study is the multilayer perceptron (MLP). The MLP architecture is illustrated in Figure 4 below.

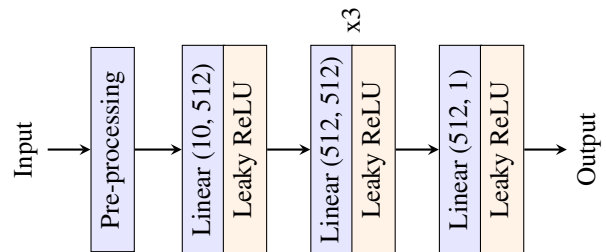


Figure 4: MLP network architecture

The starting point of the neural network architecture is the input vector, which has ten features: the room di-



mensions (L_x, L_y, L_z) , source coordinates (S_x, S_y, S_z) , receiver coordinates (R_x, R_y, R_z) and the mean absorption coefficient α . The MLP architecture is fully connected and comprises one input layer and three hidden layers of linear functions of dimensions 512 followed by an output layer with no activation function, as this is a regression problem. The input layer goes from dimension 10 indicating the input $(L_x, L_y, L_z, S_x, S_y, S_z, R_x, R_y, R_z, \alpha)$ to dimension 512, while the output layer goes from dimension 512 to 1, since the diffusion coefficient value for that specific grid point in that specific room is a scalar. The output layer is a single linear neuron predicting the logarithm (base 10) of D_{norm} . The loss function is the mean-squared error loss function. The network is optimized in the training set using batches of size 1000 and the ADAM optimizer [18] with a learning rate of 0.0005. The activation function for the architecture is the Leaky ReLU, which is appropriate for the type of output, since the log-normed target values can have negative values. Early stopping is used based on validation loss to prevent overfitting, and the model with the best validation performance is retained.

4. RESULTS OF THE NEURAL NETWORK

In this section, an analysis is conducted to estimate the reliability and relevance of the neural network model. Figure 5 shows the evolution of the loss function of the training and validation data sets.

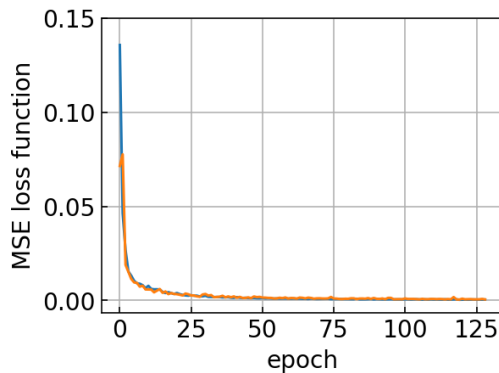


Figure 5: Loss evolution on training and validation datasets; — Training loss, — Validation loss.

Zooming in Figure 5, it can be seen that the training loss tends to be lower than the validation loss and never intersects. This is a good indication of no overfitting. When

the validation loss no longer decreased for more than 10 epochs, the training loop is stopped, and the weights of the model minimizing the validation loss are kept.

Figure 6 compares the diffusion coefficient given by Fick's law (Equation (5)) and calculated with the SPSS to the estimated diffusion coefficient given by the neural network and denoted by $\tilde{D}_{\text{Fick}}(\mathbf{r})$. It is shown that a good agreement is observed between the $D_{\text{Fick}}(\mathbf{r})$ and the $\tilde{D}_{\text{Fick}}(\mathbf{r})$ values except for some high values of the diffusion coefficient. In these cases, the network tends to under-fit the values of $D_{\text{Fick}}(\mathbf{r})$. It also shows that the pre-processing method seems to work most of the time but probably not for the highest peak values of the database. For the test dataset, the mean, median and standard deviation of the absolute error $|\tilde{D}_{\text{Fick}}(\mathbf{r}) - D_{\text{Fick}}(\mathbf{r})|$ are calculated. These are, respectively, 21.9, 8.4 and 81.6 and account for the fact that the majority of $D_{\text{Fick}}(\mathbf{r})$ are low in values. Looking at Figure 2, the results of absolute and relative errors are promising since a mean absolute error of 20 is quite small compared to the values of $D_{\text{Fick}}(\mathbf{r})$.

In Table 1 second column, the mean, median and standard deviation of the relative errors (RE) have also been calculated:

$$RE(\%) = \frac{|D - D_{\text{Fick}}(\mathbf{r})|}{|D_{\text{Fick}}(\mathbf{r})|} \cdot 100 \quad (6)$$

where $D = \tilde{D}_{\text{Fick}}(\mathbf{r})$.

These values are much lower than the same relative errors using the D_{th} , which yields 400 % for the mean, 200 % for the median, and 900 % for the standard deviation, as shown in Table 1, third column. Therefore, in all cases, using the estimated diffusion coefficient predicted by the neural network is always better than using D_{th} .

Table 1: Relative error calculated with the theoretical value of D_{th} and with the value $\tilde{D}_{\text{Fick}}(\mathbf{r})$ obtained with the neural network.

with	$\tilde{D}_{\text{Fick}}(\mathbf{r})$ [%]	D_{th} [%]
RE mean	15.8	460.0
RE median	8.0	193.1
RE standard deviation	23.6	870.0



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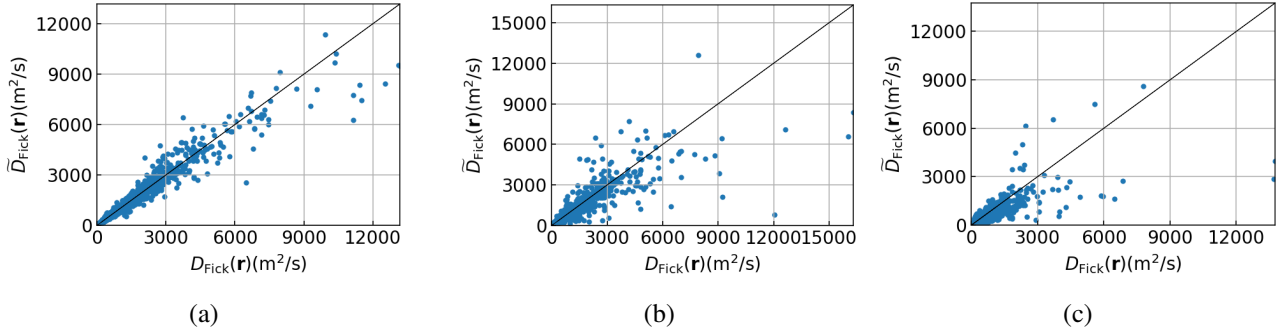


Figure 6: Comparison between target values and output value of $D_{\text{Fick}}(\mathbf{r})$ for training (a), validation (b), and test set (c).

Based on these results, it is now possible to predict the diffusion coefficient accurately within the range covered by the generated data. Rooms outside this range, as noted in Section 3.1, were not considered.

5. VALIDATION OF THE DIFFUSION MODEL

This section shows the validation process of the results obtained by the neural network in Section 4. The idea is to verify whether the estimated diffusion coefficient, which differs on average by approximately 16% from the diffusion coefficient given by the SPPS, can give accurate results when introduced into the diffusion equation model (Equations (2) and (3)). In order to conduct this analysis, the SPL and T_{30} of the room given by this modified diffusion model and the reference method SPPS are compared. The diffusion equation model used for the calculations is based on the second-order finite difference numerical method of DuFort and Frankel [19] but with a spatial variational diffusion coefficient. The mesh chosen in the diffusion equation is identical to the mesh grid chosen for estimating the diffusion coefficient (Section 3). As highlighted by Visentin [6] the diffusion coefficient value at the center of the cross section is considered equal over the cross section. This is also being done in this study for the $D_{\text{Fick}}(\mathbf{r})$ and $\tilde{D}_{\text{Fick}}(\mathbf{r})$. Multiple rooms are checked, but only the results of a corridor of dimensions $[L_x, L_y, L_z] = [39, 3, 3]$ are shown in this paper. The results for this room are obtained using the source position at (1.5 m, 1.5 m, 1.5 m) and the receiver position at $(x, 1.5 \text{ m}, 1.5 \text{ m})$, where x indicates that the receiver coordinate x changes over the length of the room with a mean absorption coefficient of 0.1 and 0.3. This room is not part of the training, validation or test dataset of the neural network.

The predicted diffusion coefficient $\tilde{D}_{\text{Fick}}(\mathbf{r})$ area is calculated using the weights of the neural network and the input variables: room dimensions (L_x, L_y, L_z), source coordinates (S_x, S_y, S_z), receiver coordinates (R_x, R_y, R_z) and the mean absorption coefficient α .

Figure 7 shows the SPL and T_{30} curves over the length of the room (x-axis) calculated with the SPPS and those calculated with the diffusion model with the theoretical diffusion coefficient (D_{th}), the diffusion coefficients $D_{\text{Fick}}(\mathbf{r})$ and $\tilde{D}_{\text{Fick}}(\mathbf{r})$.

It is shown that the use of $D_{\text{Fick}}(\mathbf{r})$ and the use of $\tilde{D}_{\text{Fick}}(\mathbf{r})$ produces almost no difference in the results of SPL and T_{30} , although the values are slightly different mainly at the end of the corridor, where the peak value is present. The trained neural network can correctly estimate the diffusion coefficients for most of the receiver points in the room, leaving the highest values of $D_{\text{Fick}}(\mathbf{r})$ underestimated. Although this happens, if comparing the SPL and T_{30} calculated with $D_{\text{Fick}}(\mathbf{r})$ and calculated with $\tilde{D}_{\text{Fick}}(\mathbf{r})$ the difference is slight. Therefore, the neural network can estimate the diffusion coefficient to accurately predict the SPL and T_{30} of elongated rooms within the range considered in this study compared to the SPL and T_{30} calculated with $D_{\text{Fick}}(\mathbf{r})$. Once the neural network is trained, this method does not need another room acoustic method to estimate the energy density gradient as Visentin et al. [6], and it is, therefore, much faster.

However, it can be seen that the SPL and T_{30} calculated by the diffusion equation and the SPPS do not match, even when using the $D_{\text{Fick}}(\mathbf{r})$, especially when the distance between source and receiver increases and at higher absorption coefficients (Figure 7 (d)). In addition, there is a small mismatch also close to the source; however,



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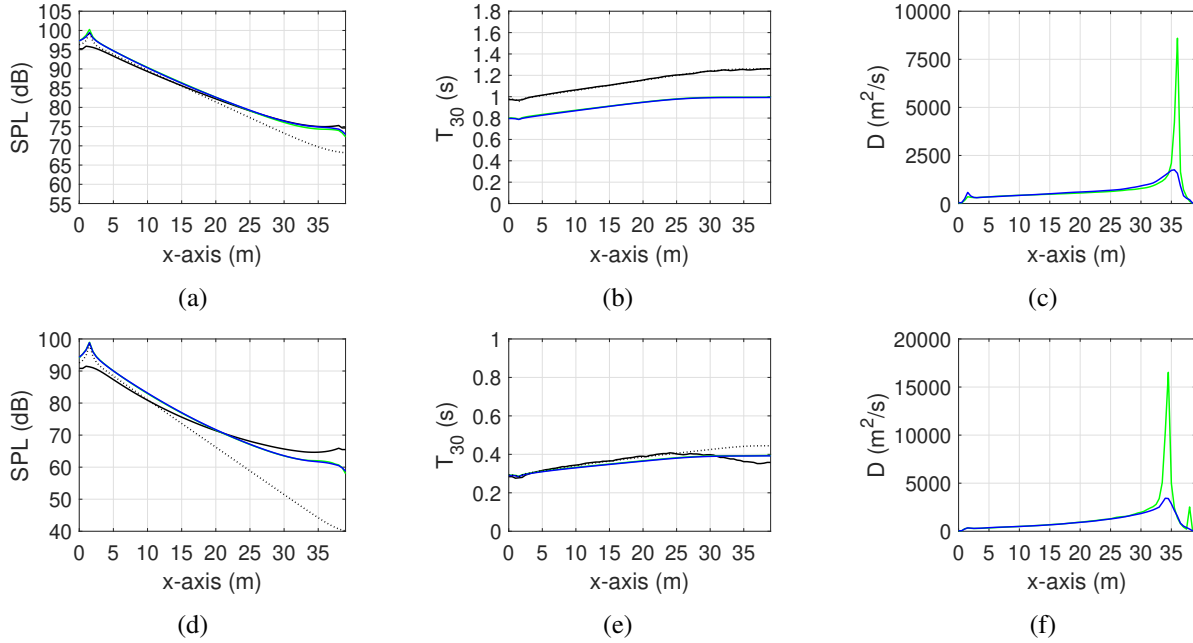


Figure 7: Comparison SPL, T_{30} and Diffusion coefficient D for a $39 \times 3 \times 3 \text{ m}^3$ with source position at (1.5 m, 1.5 m, 1.5 m) and the receiver position at $(x, 1.5 \text{ m}, 1.5 \text{ m})$ with an absorption coefficient of 0.1 (a, b and c) and an absorption coefficient of 0.3 (d, e and f); SPL and T_{30} calculated with —SPPS, — $D_{\text{Fick}}(x)$, — $\tilde{D}_{\text{Fick}}(x)$, D_{th} .

this is because the diffusion equation wrongly predicts the sound field close to the sound source and a correction will need to be applied as researchers have already highlighted [6, 12]. It is therefore demonstrated that using D_{th} and $D_{\text{Fick}}(\mathbf{r})$ as in Equation (5) in the diffusion model has some limitations. Further research is required to address this issue.

6. CONCLUSIONS

For non-proportionate rooms, in particular elongated rooms, the diffusion equation model using the theoretical diffusion coefficient estimates the variable properties in a room incorrectly. Therefore, this paper proposes a novel method to estimate the diffusion coefficient based on the room's dimensions, source position, and absorption coefficient via an artificial neural network. The database of diffusion coefficient $D_{\text{Fick}}(\mathbf{r})$ data, assuming the correctness of Fick's law, is created by running the sound particle tracing model (SPPS). The artificial neural network is created and defined to minimize the loss during the training

loop for the training, validation, and test data sets. The target to optimize is chosen to be the logarithm value in base 10 of the normalized values versus the theoretical diffusion coefficient of $D_{\text{Fick}}(\mathbf{r})$ as defined in Equation (5) in Section 2.

Results have shown that the neural network can estimate the correct value of the diffusion coefficient $D_{\text{Fick}}(\mathbf{r})$ with a 15% mean relative error. This error is also much smaller than that using the theoretical diffusion coefficient.

A validation study is conducted to see if the $\tilde{D}_{\text{Fick}}(\mathbf{r})$ predicts correctly the SPL and T_{30} of different rooms compared to those of the SPPS. Results show that using the predicted $\tilde{D}_{\text{Fick}}(\mathbf{r})$ and the $D_{\text{Fick}}(\mathbf{r})$ does not change the SPL and T_{30} of the room.

It is also shown that there is a limit in using the $D_{\text{Fick}}(\mathbf{r})$ and therefore two possibilities would need to be investigated further: (1) considering a direction dependent diffusion coefficient, (2) to add an advection term in the Fick's law as it appears to approach the limits of its assumptions [11].



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