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Application of the Neuronal Method for Calculating the Axial Dispersion in Fixed Beds of the Spherical Linings

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Abstract: The aim of this study was to examine the performances of this method for other type of spherical packing using the experimental data Comiti, Mauret, Chung and Mall. To prove the power of this method, the calculation results obtained were modeled in the form of mathematical patterns similar to those proposed by Comiti, Mauret, Chung and Mall, so we could compare our results with those obtained by these authors for the same operating conditions. At the end a new relationship between axial dispersion and Reynolds number was suggested.

Key words: Fixed bed, axial dispersion, spherical packing, neural networks, modeling

INTRODUCTION

The objective of this study is to determine the axial dispersion coefficient in fixed beds of spherical particles with the neuronal method and understand the methodology of this approach to better define the influence of all parameters that may affect the phenomenon of axial dispersion. The results will be reviewed later and compared with former work from the literature. To test the performance of the neural method, we studied the results of several researchers (Comiti and Renaud, 1989; Mauret and Renaud, 1997; Chung and Wen, 1968; Mall *et al*., 1976), who worked on the coefficient of axial dispersion in spheres fixed beds.

AXIAL DISPERSION IN THE SPHERES BEDS

When the velocity of the fluid in a porous medium is lower or nil the axial dispersion coefficient tends to a limit. Due to the tortuosity of the medium this value is less than the molecular diffusion coefficient for considered the chemical species (DeArcangelis *et al*., 1986; Bacri *et al*., 1987; Koplik *et al*., 1986). In case where flow velocities are lower or nil and beds of nonporous spheres, Koplik *et al*. (1986) showed that one could write:

$$D_{ax} \approx \frac{D_m}{\tau_e} = \frac{D_m}{\varepsilon \cdot F} = \frac{D_m}{\varepsilon} \cdot \frac{\sigma}{\sigma_0} \tag{1}$$

With the formation factor:

$$(F = \sigma_0 / \sigma) \tag{2}$$

which represents the ratio of the electrical conductivity of the fluid to electrical conductivity of saturated porous media. The electrical tortuosity is:

$$(\tau_e = \varepsilon \cdot F) \tag{3}$$

For higher Reynolds numbers, turbulent diffusion becomes dominant. We can explain this phenomenon from a model-type random walk. An element of fluid moves with an average speed ($u = u_0/\varepsilon$) and undergoes further random displacement l_d. The characteristic time is ($\tau d = l_d/u$) and the generated dispersion is l_d. For beads beds, l_d is about $0.5d_p$, (Koplik *et al*., 1986; Villermaux and Schweich, 1992; Villermaux, 1993; De Gennes, 1983; Carbonnel, 1979) then we get the equation describing the mechanical dispersion in a porous medium:

$$D_{ax} \approx \alpha \cdot d_p \cdot u \approx 0.5 \cdot d_p \cdot u \tag{4}$$

The effect of molecular diffusion is no longer quite negligible. Saffman (1959) and DeJosselin DeJong (1958) were the first to highlight this phenomenon from a modeling of medium using a pores network of equal length and diameter, but randomized: The fluid inside the cross section to the flow direction moves very slowly. Koch and Brady (1985) attributed this phenomenon to the existence of boundary layers on the surface of particles. Pomeau (1985) refered to areas of recycling the fluid. All this leads to a logarithmic correction of axial dispersion coefficient:

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$$D_{ax} = \alpha \cdot d_p \cdot u + \beta \cdot d_p \cdot u \cdot Ln\left(\frac{u \cdot d_p}{D_m}\right) \quad (5)$$

A second phenomenon involving molecular diffusion occurs when the particles of the medium are porous, absorb the tracer or where there are dead areas where the fluid velocity is zero (e.g., pores closed). This mechanism introduces a contribution to u^2 in the expression of the axial dispersion (Bacri *et al*., 1987; Rigord *et al*., 1990; Villermaux and Schweich, 1992; Han *et al*., 1985):

$$D_{ax} = \alpha \cdot d_p \cdot u + \beta \cdot d_p \cdot u \cdot Ln\left(\frac{u \cdot d_p}{D_m}\right) + \xi \frac{(u \cdot d_p)^2}{D_m} \quad (6)$$

In the case of non-porous spheres, the results are often correlated as follows:

$$D_{ax} = A \cdot u_0^B \quad (7)$$

The coefficient B is probably a logarithmic term and its value is generally in the 0.8 to 1.5 (Gist *et al*., 1990) and the value of α varies from 0.5 to 2 (Villermaux, 1993). However, there are media where the characteristic length of dispersion is much higher than 0.5 dp. This leads to an abnormal dispersion (Villermaux, 1993).

EFFECT OF HETEROGENEITY OF POROUS MEDIA ON THE AXIAL DISPERSION

Several phenomena can cause abnormally high values of axial dispersion in porous media, they are mainly related to local variations in permeability due to wall effects and size distribution of the diameter of pores or particles. Carbonnel (1979) modeled the effect of the size distribution of pore diameter, he shows that the axial dispersion increases when the size distribution of pore diameter increases. Han *et al*. (1985) measured the coefficient of axial dispersion in beds consisting of spheres and for three size distributions of particles: spheres of equal size ($d_{p,\,max}/d_{p,\,min} = 1$), a distribution with a ratio ($d_{p,\,max}/d_{p,\,min} = 2.2$) and a distribution with a ratio ($d_{p,\,max}/d_{p,\,min} = 7.3$). They show that the beds of uniform spheres which correspond to the distribution with a ratio of 1 are the same results. The areas of distribution of the ratio on 2.2 cause they dispersed at least twice more higher. DeArcangelis *et al*. (1986) have developed a method for describing the dispersion of a tracer into the phenomena of molecular diffusion. They apply this approach to a network of tubes arranged randomly and of same length in order to study the effect of dispersion section size of the pores. Villermaux and Schweich (1992) and Villermaux (1993) using a method based on fractal representation of the porous medium. This approach takes into account the preferential fluid pathways. The authors define a wildcard pattern representative of fluid flow, composed of parallel branches, each containing one or more identical cells. Each cell is replaced by the wildcard pattern and the procedure repeated to infinity, leads to a self similar system. The RTD (residence time distribution) obtained then depend on the number of cells per branch. If all the branches contain the same number of cells, then the flow is piston type. On the contrary, if the wildcard pattern offers paths of different lengths, RTDs are spreading and could potentially present several peaks or shoulders. Many of these works relate to the study of consolidated media for which the effect of heterogeneities is very sensitive. The study of these media, often based on the theory of percolation, generally leads to a characteristic length of dispersion l_d more than the diameter of the particles.

METHODOLOGY FOR CALCULATING

Upon the basic properties of neural networks and acting in the same way our previous work for the parallelepipedal packing (Hassani *et al*., 2008a) and fibrous packing (Hassani *et al*., 2008b), the development process of the neural network to calculate the axial dispersion in spherical beds can be illustrated by the flowchart in Fig. 1.

Database: We used the database for training the neural network that is generated from the study of Comiti and Renaud (1989), Mauret and Renaud (1997), Chung and Wen (1968) and Mall *et al*. (1976), who worked on the axial dispersion coefficient in fixed beds of spheres. The several researchers have used the Fourier analysis method to calculate the axial dispersion coefficient by the analysis of experimental curves of the Residence Time Distribution (RTD) for the fluid in the porous medium. Table 1 sums up the experimental results obtained by Comiti and Renaud (1989), Mauret and Renaud (1997), Chung and Wen (1968) and Mall *et al*. (1976) and the operating conditions (the nature for fixed beds of spheres, particles diameter, fluid velocity and Reynolds number).

ARCHITECTURE OF THE NEURAL NETWORK

The idea of artificial neural networks was inspired in the way biological neurons process information. This concept is used to implement software simulations for the massively parallel processes that involve processing elements interconnected in network architecture. The

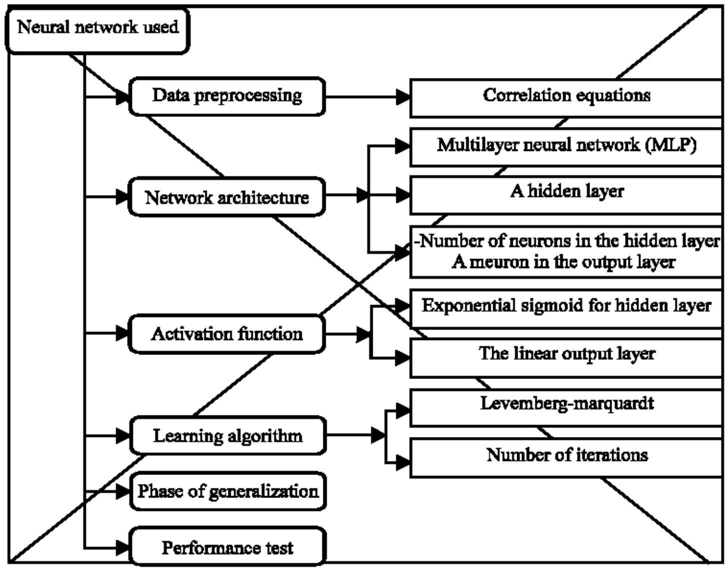

Fig. 1: Flowchart of procedure for the development of the neural networks to calculate Dax in fixed beds of spheres

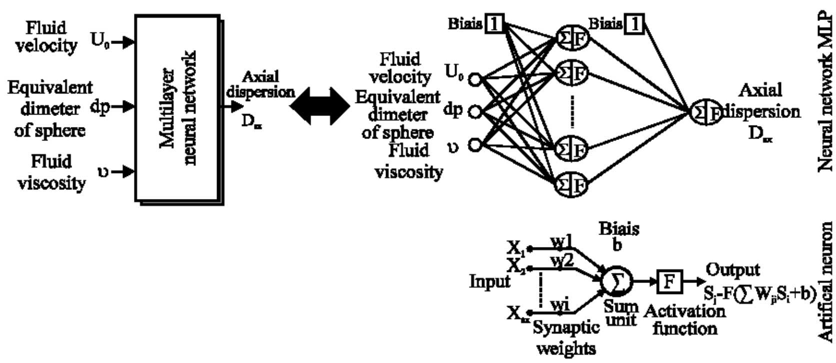

Fig. 2: Representation of generalized neuron formal and multilayer neural network to calculate the axial dispersion in fixed beds of spheres

Table 1: Summary of work of (Comiti and Renaud, 1989; Mauret and Renaud, 1997; Chung and Wen, 1968; Mall *et al.*, 1976) on the axial dispersion in fixed beds of spheres

Authors and reference	Particles	d_p (cm)	Re	U_0 (m sec^{-1})	Equation D_{ax} correlation (m^2 sec^{-1}) and U_0 in (m sec^{-1}) except for (Eq. 8) in (cm^2 sec^{-1}) and (cm sec^{-1})
Comiti and Renaud (1989)	Glass bead	0.499	0.145	2.10^{-4}	$\text{Dax} = 1{,}46\ U_0^{0{,}97}$ (8)
	Plastic pellet		à	à	
			29.07	6,2.10^{-3}	
Mauret and Renaud (1997)	Glass bead	0,221	---	5,9.10^{-4}	$\text{Dax} = 0{,}14\ U_0^{1{,}48}$ (9)
		0,397		à	$\text{Dax} = 0{,}026\ U_0^{1{,}15}$ (10)
		0,612		3,9.10^{-3}	$\text{Dax} = 0{,}00685\ U_0^{0{,}89}$ (11)
Chung and Wen (1968)	Glass bead	0,25	25	2.10^{-4}	$\varepsilon.\text{Pe}_i = 0{,}2 + 0{,}011\text{Re}^{0{,}48}$ (12)
	Aluminum ball	à	à	à	
	Steel ball	0,635	320	6.10^{-3}	
Mall *et al.* (1976)	Glass bead	0,733	39	2.10^{-4}	$\frac{\text{Dax}}{\nu} = 2{,}07\left(\frac{dpU_0}{\nu\,(1-\varepsilon)}\right)^{0{,}898}$ (13)
		à	à	à	
		1,71	201	6,2.10^{-3}	

artificial neuron receives inputs that are analogous to the electrochemical impulses that the dendrites of biological neurons receive from other neurons. Therefore, ANN can be viewed as a network of neurons which are processing elements and weighted connections.

The artificial neurons are arranged in layers (Fig. 2) wherein the input layer receives inputs (si) from the real world and each succeeding layer receives weighted outputs (wij.si) from the preceding layer as its input resulting therefore a feed forward ANN, in which each

Table 2: Characteristics of neural networks developed for calculating the Dax fixed beds of spheres

Neural network on the data	Comiti and Renaud (1989)	Mauret and Renaud (1997)	Chung and Wen (1968)	Mall *et al.* (1976)	All work
Data preprocessing (eq.)	(8)	(9 à 11)	(12)	(13)	(8 to 13)
Learning algorithm	Levemberg/ Marquardt	Levemberg/ Marquardt	Levemberg/ Marquardt	Levemberg/ Marquardt	Levemberg/ Marquardt
Number of hidden layer	01	01	01	01	01
Number of neurons					
Hidden layer	06	09	09	06	08
Output layer	01	01	01	01	01
Activation function of hidden layer					
Hidden layer	Exponential sigmoid	Exponential sigmoid	Exponential sigmoid	Exponential sigmoid	Exponential sigmoid
Output layer	Linear	Linear	Linear	Linear	Linear
Number of iterations	250	300	500	100	300
Learning standard (%)	$3,47.10^{-16}$	$3.,84.10^{-15}$	$9,48.10^{-11}$	$5,21.10^{-15}$	$1.10.10^{-10}$

input is fed forward to its succeeding layer where, it is treated. The outputs of the last layer constitute the outputs to the real world. In such a feed forward ANN a neuron in a hidden or an output layer has two tasks:

- It sums the weighted inputs from several connections plus a bias value and then applies a transfer function to the sum
- It propagates the resulting value through outgoing connections to the neurons of the succeeding layer where it undergoes the same process

The output is computed by means of a transfer function, also called activation function. It is desirable that the activation function has a sort of step behavior. Furthermore, because continuity and derivability at all points are required features of the optimization algorithms (Si-Moussa *et al.*, 2008).

The number of neurons in the input and output layers is determined by the number of independent and dependent variables respectively. The user defines the number of hidden layers and the number of neurons in each hidden layer. Model development is achieved by a process of training in which a set of experimental data of the independent variables are presented to the input layer of the network. The outputs from the output layer comprise a prediction of the dependant variables of the model. The network learns the relationships between the independent and dependent variables by iterative comparison of the predicted outputs and experimental outputs and subsequent adjustment of the weight matrix and bias vector of each layer by a back propagation training algorithm. Hence, the network develops a neural networks model capable of predicting with acceptable accuracy the output variables lying within the model space defined by the training set. Consequently, the objective of ANN modelling is to minimize the prediction errors of validation data presented to the network after completion of the training step.

Although, there is continuing debate on model selection strategies, it is clear that the successful application of ANN in modelling engineering problems is highly affected by four major factors:

- Network type
- Network structure (number of hidden layers, number of neurons per hidden layer)
- Activation functions
- Training algorithms

It is well established that the variation of the number of neurons of the hidden layer(s) has a significant effect on the predictive ability of the network. The most common way of optimizing the performance of ANN is by varying the numbers of neurons in the hidden layer(s) and selecting the architecture with the highest predictive ability (Si-Moussa *et al.*, 2008).

For the spherical packing we implement several neural networks to study separately the work of each author and at the end we have developed a single neural network that enables us to gather all the above studied works. We apply the inputs of neural networks the 3 major parameters characterizing the porous medium and the fluid (diameter, velocity and viscosity). Has the output of neural networks is obtained an only greatness (axial dispersion). Figure 2 shows the architecture adopted for all the neural networks.

Table 2 shows the characteristics of neural networks developed for the work studied by Comiti and Renaud (1989), Mauret and Renaud (1997), Chung and Wen (1968) and Mall *et al.* (1976) which provides the learning algorithm, number of hidden layer, number neuron in hidden layer, activation function, etc.

RESULTS AND DISCUSSION

Figure 3 shows the comparison between the results given with the neural method and the study of Comiti and Renaud (1989), Mauret and Renaud (1997), Chung and Wen (1968) and Mall *et al.* (1976). One finds in Fig. 3 that the scattering of axial dispersion in fixed beds of spheres determines from the neural network versus the velocity inside the empty coincides perfectly with the values estimated by the correlation equations given by Comiti and Renaud (1989), Mauret and Renaud (1997), Chung and Wen (1968) and Mall *et al.* (1976) despited the large difference of the results in their study, which shows the

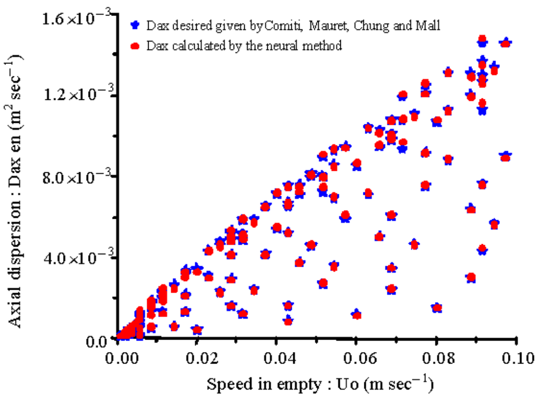

Fig. 3: Axial dispersion calculated by the neural network

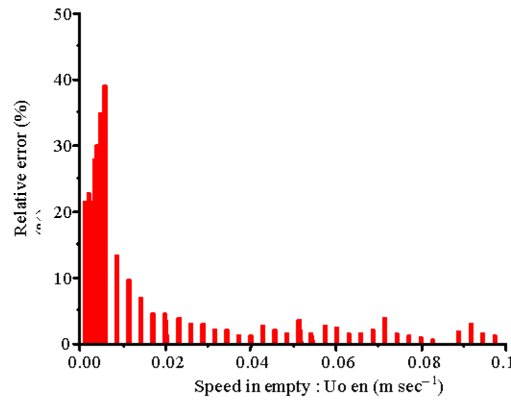

Fig. 4: Histogram of the percentage of error between the values of axial dispersion calculated by the neural network and the values given by the equations of correlation of the (Comiti and Renaud, 1989; Mauret and Renaud, 1997; Chung and Wen, 1968; Mall *et al*., 1976)

power of the neural model. A single neural network can cover the entire range of axial dispersion resulting from the studied works.

The analytical process of the cloud points of the axial dispersion calculated versus the velocity (Fig. 3), on one hand we showed that the phenomenon is even more important than the velocity of the fluid is high, on the other hand a strong dependence of the axial dispersion coefficient to particle diameter and fluid viscosity. Indeed, phenomenological view yields an increase of kinematic viscosity of the fluid causes slightly increase in axial dispersion, this is probably due to the fact that in the upstream part of the spherical particles where the flow is facilitated and the boundary layer is less thinner than it would in the downstream part, so there is separation of the boundary layer and as a result of the pressure gradient, it occurs a flow in the opposite direction to normal flow which radically changes the distribution of traffic speeds and pressures and therefore the formation of wake vortices and everything depends on the criterion of Reynolds. Similarly, an increase in the particle diameter causes a net increase of axial dispersion coefficient, due to the dimensions of wakes and vortices that are formed in the downstream of the spherical particle after the separation of the boundary layer that depends on the flow state and the particle size, rather than the size is larger along the wake and the intensity of wakes are larger therefore, the axial dispersion coefficient is important.

Figure 4 shows the comparison of the values of the coefficient of axial dispersion desired given by the equations of correlation of the Comiti and Renaud (1989), Mauret and Renaud (1997), Chung and Wen (1968) and Mall *et al*. (1976) and the values of axial dispersion calculated by the neural network.

There is an interval of two ranges of errors:

$$RE = 100\left(1 - \frac{(Dax)_{NN}}{(Dax)_{desired}}\right) \quad (14)$$

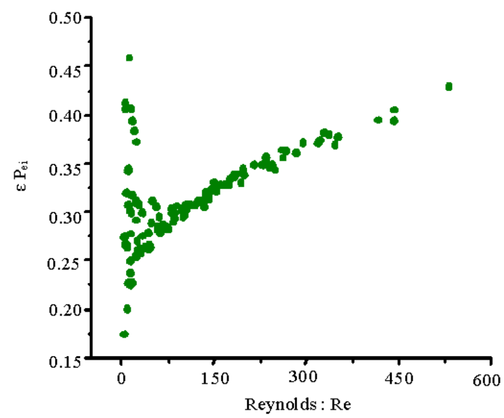

Fig. 5: Values $\varepsilon.P_{ei}$ obtained by the neural method, versus Reynolds number for fixed beds of studied spheres

a range with a relative error greater than 10% (10% <RE<40%) corresponds to a low speed range where the large dispersion of results of previous work (used as a database of learning), causes damage accuracy of neural network and a beach with an error less than 10% on a range of relatively high speed. These two behaviors are distinctly different with a dimensionless representation:

$$\varepsilon.Pe_i = f(Re) \quad (15)$$

as shown and confirmed in Fig. 5, where there is a decrease with Re and growth, hence the existence of a minimum of 0.25 which corresponds to RE = 25.

CORRELATION OF CALCULATION RESULTS

From the obtained results with the neural method, authors suggested two forms of dimensionless correlations that are shown in Table 3:

- The first form is similar to the correlation equation of Chung (Eq. 12):

$$\varepsilon.Pe_i = a + bRe^{0,48} \qquad (16)$$

- The second is a new correlation form:

$$\varepsilon.Pe_i = \alpha + \frac{\beta}{\sqrt[3]{Re}} + \gamma\sqrt{Re} \qquad (17)$$

Empirical constants (a, b) and (α, β and γ) are calculated sequentially from the results obtained by different developed neural networks.

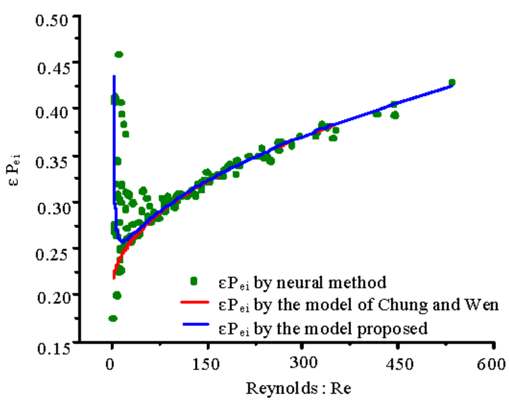

Fig. 6: Validation of the proposed model (Eq. 24) and its comparison with that of Chung and Wen (1968) (Eq. 12)

For the new form of correlation (Eq.17), the exponent 0.48 of the Chung relationship (Eq.12) is adjusted such as we get a fractional exponent (1/2) further we show an additional corrective term that is a random error is added to the classic phenomenon of axial dispersion which takes into account all the results. This correction term $\left(1/\sqrt[3]{Re}\right)$ is more important than the velocity of the fluid is low. This behavior can probably be attributed to the parameters of porous structure (tortuosity, specific surface area, porosity and permeability) which form the fixed bed.

Figure 6 shows the validation of the proposed model for all the work (Eq. 24) and its comparison with the correlation of Chung (Eq. 12).

Figure 7 shows the validation of the new form for the proposed correlation (Eq. 31) and its comparison with

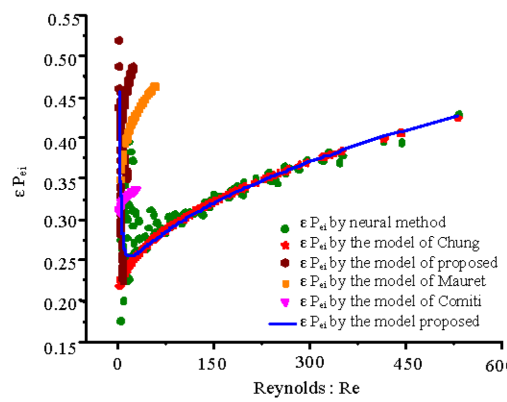

Fig. 7: Validation of the proposed model (Eq. 31) and its comparison with models of Chung and Wen (1968) (Eq. 12) Mauret and Renaud (1997) (Eq. 9 to 11), Mall *et al.* (1976) (Eq. 13) and Comiti and Renaud (1989) (Eq. 8)

Table 3: Correlation equation suggested from the neural method

Study	Proposed correlation equations from the neuronal method		News from correlations proposed method neuronal form: $\varepsilon.Pe_i = 0{,}732 - 0{,}193\ Re^{0,48}$	
Comiti and Renaud (1989)	$\varepsilon.Pe_i = 0{,}307 + 0{,}006\ Re^{0,48}$	(18)	$\varepsilon.Pe_i = 0{,}314 - \frac{0{,}05}{\sqrt[3]{Re}} + 0{,}0043\sqrt{Re}$	(25)
Mauret and Renaud (1997)	$\varepsilon.Pe_i = a + \frac{b}{\sqrt[3]{Re}} + c\sqrt{Re}$	(19)	$\varepsilon.Pe_i = 0{,}4 + \frac{0{,}425}{\sqrt[3]{Re}} - 0{,}0664\sqrt{Re}$	(26)
	$\varepsilon.Pe_i = 0{,}528 - 0.05Re^{0,48}$	(21)	$\varepsilon.Pe_i = 0{,}46 + \frac{0{,}211}{\sqrt[3]{Re}} - 0{,}0295\sqrt{Re}$	(27)
	$\varepsilon.Pe_i = 0{,}339 + 0{,}033\ Re^{0,48}$	(20)	$\varepsilon.Pe_i = 0{,}39 - \frac{0{,}298}{\sqrt[3]{Re}} + 0{,}0202\sqrt{Re}$	(28)
Chung and Wen (1968)	$\varepsilon.Pe_i = 0{,}203 + 0{,}0107Re^{0,48}$	(22)	$\varepsilon.Pe_i = 0{,}208 - \frac{0{,}05}{\sqrt[3]{Re}} + 0{,}0093\sqrt{Re}$	(29)
Mall *et al.* (1976)	$\varepsilon.Pe_i = 0{,}33 + 0{,}019Re^{0,48}$	(23)	$\varepsilon.Pe_i = 0{,}34 - \frac{0{,}05}{\sqrt[3]{Re}} + 0{,}0164\sqrt{Re}$	(30)
All work	$\varepsilon.Pe_i = 0{,}2 + \frac{1}{\sqrt[3]{Re}} + 0{,}011\ Re^{0,48}$	(24)	$\varepsilon.Pe_i = 0{,}197 + \frac{1.12}{\sqrt[3]{Re}} + 0{,}01\sqrt{Re}$	(31)

the models of Chung and Wen (1968) (Eq. 12) Mauret and Renaud (1997) (Eq. 9 to 11), Mall *et al.* (1996) (Eq. 13) and Comiti and Renaud (1989) (Eq. 8).

CONCLUSION

This study validates the neural network method adopted for calculating the coefficient of axial dispersion in fixed beds of spherical particles. The mean values of criterion interstitial Peclet calculated by the neural method correspond to the order of magnitude expected. If it refers to works consulted by Comiti and Renaud (1989), Mauret and Renaud (1997), Chung and Wen (1968) and Mall *et al.* (1976) can estimated that the neural method for calculating gives very satisfactory results and representative of the phenomenon of axial dispersion.

NOMENCLATURE

ANN	= Artificial Neural Networks
b	= Bias
Dax	= Axial dispersion coefficient (m^2 sec^{-1})
$(Dax)_{desired}$	= Axial dispersion coefficient desired (m^2 sec^{-1})
$(Dax)_{NN}$	= Axial dispersion coefficient calculated by the neural method (m^2 sec^{-1})
D_m	= Molecular diffusion coefficient (m^2 sec^{-1})
dp	= Equivalent diameter of sphere (m)
DRT	= Distribution of the residence time
F	= Form factor
l_d	= Characteristic length of dispersion (m)
Pe_i	= Peclet number of interstitial
Re	= Reynolds number
RE	= Relative error
s_i	= Output neuron
t	= Time (sec)
u	= Average speed of movement of the fluid (m sec^{-1})
u_0	= Superficial velocity (m sec^{-1})
U_0	= Speed in empty (m sec^{-1})
w_i	= Synaptic weights of neuron
x_i	= Input of the neuron
α, β	= Settings
ε	= Porosity of the bed
σ	= Electrical conductivity of porous medium
σ_0	= Electrical conductivity of the fluid
τ	= Hydraulic tortuosity
τ_d	= Temps caractéristique de dispersion (s)
τ_e	= Tortuosité électrique
υ	= Fluid viscosity

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