Journal of Applied Sciences

ISSN 1812-5654

ANSInet
an open access publisher
http://ansinet.com

Journal of Applied Sciences 8 (19): 3380-3388, 2008
ISSN 1812-5654

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

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Abstract: The objective of this research was to develop a methodology for calculation based on the networks of neurons for the calculation of axial dispersion in the fixed beds of linings parallelepipedic. In a first stage the results of the axial dispersion obtained on the fixed beds of linings parallelepipedic by the neuronal method was compared with the results resulting from the literature. In a second stage the performances of this method was showed and the computation results was modelled, in the form of mathematical models similar to those proposed by study many researchers, so that one can validate present results with those obtained by researchers, under the same operating conditions.

Key words: Networks neurons, fixed bed, axial dispersion, linings parallelepipedic, modelling

INTRODUCTION

Many methods enable to calculate axial dispersion in the fixed beds, most of them are interested only in classical analysis. Certain studies suggest models fairly performant, but few neuronal methods were established for the axial dispersion estimation. However, such methods could be very useful when one wishes to envisage axial dispersion in complex fixed beds.

In practice, one does not use the networks of neurons to carry out approximations of known functions. More often than not, the problem which comes up is as follows: one has a set of measurements of variables of a process of nature unspecified (physical, chemical, economic) and result of this process; it is supposed that there is a deterministic relation between these variables and this result and one seeks a mathematical form of this relation, valid in the field where measurements were carried out.

In other words, one seeks a model of the studied process, starting from the examples that one has. Once this phase is finished, the network of neurons black box is integrated in already existing software and make it possible to deal with problems, where the classical systems of data processing appear weak (Dreyfus, 2005; Haykin, 1999).

EQUATIONS OF THE MODEL OF FLOW PISTON WITH DISPERSION

Table 1 shows the three significant models of flow of Distribution of the Residence Time (DRT) with dispersion in the fixed reactors of fixed beds.

The major problem of the solutions is the boundary conditions which were largely discussed by Bischoff and Levenspiel (1962), Choy and Perlmutter (1976), Deckwer and Mahlman (1976), Gill (1975) and Parulekar and Ramkrishna (1984).

The process of mixture in the reactors is due mainly to the differences of speeds of the fluid elements, to the actions of local mixture due to the mobile of agitation, to the secondary swirls along the loop of circulation, to the phenomena of turbulent diffusion and molecular diffusion. All these effects can be characterized overally by a longitudinal or axial scatter coefficient. This coefficient represents the degree of retro mixture in the fluid and depends on the properties of the fluid, on the mode of flow and on the shape of the reactor (Levenspiel, 1999). Whereas axial dispersion in the fixed beds results mainly from the superposition of two mechanisms: molecular diffusion due to the gradient of dominating concentration for the low speeds of flow and the turbulent diffusion (geometric or mechanical dispersion) generated by the fluctuations of the speed of the fluid within the porous medium. Therefore it dominates strong speeds.

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Table 1: Significant models of flow of drt with dispersion in the reactors of fixed BED

Authors	Label of the model	Corresponding equation	
Van *et al.* (1969)	(DP)	$\frac{\partial c_T}{\partial t} - \frac{u_L}{H_T}\frac{\partial c_T}{\partial z} = Dax\frac{\partial^2 c_T}{\partial z^2}$	(1)
	(EDP)	Dynamic liquid zone : $\frac{\partial c_D}{\partial t} - \frac{u_L}{H_D}\frac{\partial c_D}{\partial z} + N\frac{u_L}{z.H_D}(c_D - c_S) = Dax\frac{\partial^2 c_D}{\partial z^2}$	(2a)
		Dynamic liquid zone : $\frac{\partial c_S}{\partial t} - N\frac{u_L}{z.H_S}(c_D - c_S) = 0$	(2b)
Iliuta *et al.* (1996)	EDP-DP	Dynamic liquid zone with : $\frac{\partial c_D}{\partial t} - \frac{u_L}{H_D}\frac{\partial c_D}{\partial z} + N\frac{u_L}{z.H_D}(c_D - c_S) + D_{eff}\frac{a_p.f_D.}{H_D}\frac{\partial c_I}{\partial r}\Big\vert_{r=R} = Dax\frac{\partial^2 c_D}{\partial z^2}$	(3a)
Iliuta *et al.* (1998)	EDP-DP	Stagnant liquid zone with : $\frac{\partial c_D}{\partial t} - N\frac{u_L}{z.H_D}(c_D - c_S) + D_{eff}\frac{a_p.f_D.}{H_D}\frac{\partial c_I}{\partial r}\Big\vert_{r=R} = 0$	(3b)
Iliuta *et al.* (1999)	EDP-DP	Intra particle liquid zone will : $\frac{\partial c_I}{\partial t} - \frac{D_{eff}}{r^2.H_D}\frac{\partial}{\partial r}\left(r^2\frac{\partial c_I}{\partial r}\right) = 0$	(3c)

Aris and Amundson (1957) and Sundaresan *et al.* (1980) proposed a theory based on the concept of cells of mixture to explain the phenomenon of axial dispersion (high Reynolds numbers). They show the criterion of interstitial Peclet thus:

$$Pe_i = \frac{u_0}{\varepsilon}\frac{d_p}{D_{ax}} \quad (4)$$

NEURONAL METHOD FOR DAX CALCULATION

Few works were published on the use of the neurons networks for the estimation of degree of mixing of a fluid crossing a porous medium laid out in fixed-bed. To our knowledge F Larachi it is the only one which developed two neuronal approaches to predict the axial scattering coefficient: the first approach (Piché *et al.*, 2002) concerns the diphasic reactors with fixes bed by using the number of Boldenstein:

$$(Bo = \frac{u_L}{a_p.Dax})$$

with an average absolute relative error (AARE) not exceeding 24%. The second approach (Belfares *et al.*, 2001) concerns the reactors for a column with pellets by adopting the Peclet number:

$$(Pe = \frac{u_{LS}.d_{eq}}{Dax}),$$

by using a bank of data and with a maximal AARE of 20%. The two approaches do not show the effect of the neuronal parameters on the AARE obtained by the network.

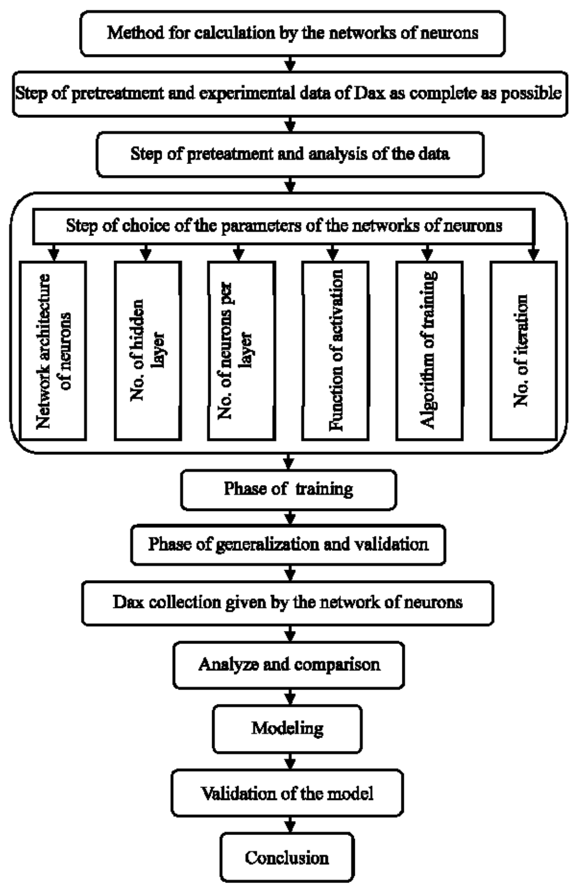

Fig. 1: Method for calculation of Dax by the networks of neurons

METHODOLOGY OF CALCULATION

The principle of calculation by the networks of neurons of axial dispersion in the fixed beds is shown in Fig. 1.

Table 2: Experimental correlations obtained by Comiti and Renaud (1989), on plates laid out fixed-BED

Nature of the porous medium (plate)	Equivalent diameter dp (cm)	Porosity ϵ	Kinematics viscosity ν ($cm^2\ sec^{-1}$)	Speed in empty U_0 ($cm\ sec^{-1}$)	Equations of correlation Dax ($cm^2\ sec^{-1}$)
First porous medium					$Dax = 3.57\, U_0^{0.86}$
Polystyrene	0.129	0.46	1.03×10^{-2}	$2.7\times10^{-3}<U_0<0.60$	$\frac{Dax}{\nu} = 20.2\, Re_i^{0.86}$
					$Pe_i = 0.049 Re_i^{0.14}$
Second porous medium					$Dax = 1.49\, U_0^{0.88}$
PVC	0.221	0,35	1.03×10^{-2}	$6.4\times10^{-3}<U_0<0.62$	$\frac{Dax}{\nu} = 3.85 Re_i^{0.88}$
					$Pe_i = 0.26 Re_i^{0.12}$
Third porous medium					$Dax = 2.06 U_0^{0.92}$
PVC	0.348	0.31	1.03×10^{-2}	$4.6\times10^{-3}<U_0<0.61$	$\frac{Dax}{\nu} = 2.67 Re_i^{0.92}$
					$Pe_i = 0.35 Re_i^{0.08}$

DATA BASE

The examples used for the training and the validation of the elaborate network of neurons are selected starting from the equations of experimental correlation suggested by Comiti and Renaud (1989), who worked on fixed beds packed of parallelepipedic particles at square base of weak thickness to side (PVC and polystyrene plates) laid out fixed-bed inside a cylindrical column. Table 2, recapitulates the experimental values of axial dispersion obtained by Comiti and Renaud (1989), as well as the operating conditions.

PRINCIPAL CHARACTERISTICS OF THE USED NETWORK OF NEURONS

The principal characteristics of the network used and the type of training can be summarized as follows:

Neurons network architecture: The fundamental property of the neurons networks is the universal approximation which can be stated in the following way: Any sufficiently regular limited function can be approximate uniformly, with an arbitrary precision, in a finished field of the space of its variables, by a neurons network comprising a layer of neurons hidden in a finished number, having all the same function of activation and a linear neuron of exit (Cybenko, 1989; Dreyfus, 2005; Funahashi, 1989). It is this property which justifies our choice of the network architecture of neurons to a hidden layer shown in Fig. 2.

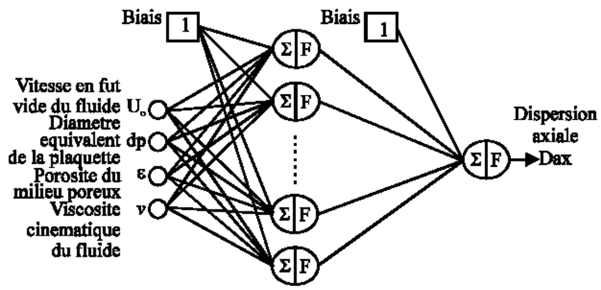

Fig. 2: Network of multi-layer neurons for the calculation of axial dispersion in the fixed beds of plates

Effect of the number of hidden layers: The effect of the number of hidden layers on the precision of the network is shown in Fig. 3. This last gives the average quadratic error according to the iteration number of several networks of different architectures. It is noted that really, the neurons network with only one hidden layer is the most efficient. As an example, after 100 iterations, the average quadratic error passes from 10^{-10} for the network of three hidden layers to 10^{-13} for the network to only one hidden layer with a multiplicative factor of 1000 Moreover, the only degree of freedom which remains for the determination of the network architecture is then the number of hidden neurons, which simplifies the optimization of the network architecture, as it will be seen later.

Effect of the activation function: The state of neuron depends on the various forms which can take the function of activation (Dreyfus, 2005). The influence of the activations functions currently the most used in the literature is shown in Fig. 4. However, it was noted that the exponential sigmoid function for the neurons of the hidden layer and a purely linear function at exit is the configuration best adapted and which gives the results of most efficient training and generalization. With an average quadratic error of training of 10^{-13} since the $60^{ième}$ iteration. The analytical treatment of the curves of Fig. 4, for small iteration numbers, show a great fluctuation of the average quadratic error, this whatever activation function are used. That is due to the arbitrary choice of the initial values of weight and skew by the algorithm of training. This variation is quickly attenuated and stabilized when it is about the function of exponential sigmoid activation. It is the reason for which this latter was retained.

Effect of the number of neurons: One of the fundamental unknowns to use the networks of neurons is the number

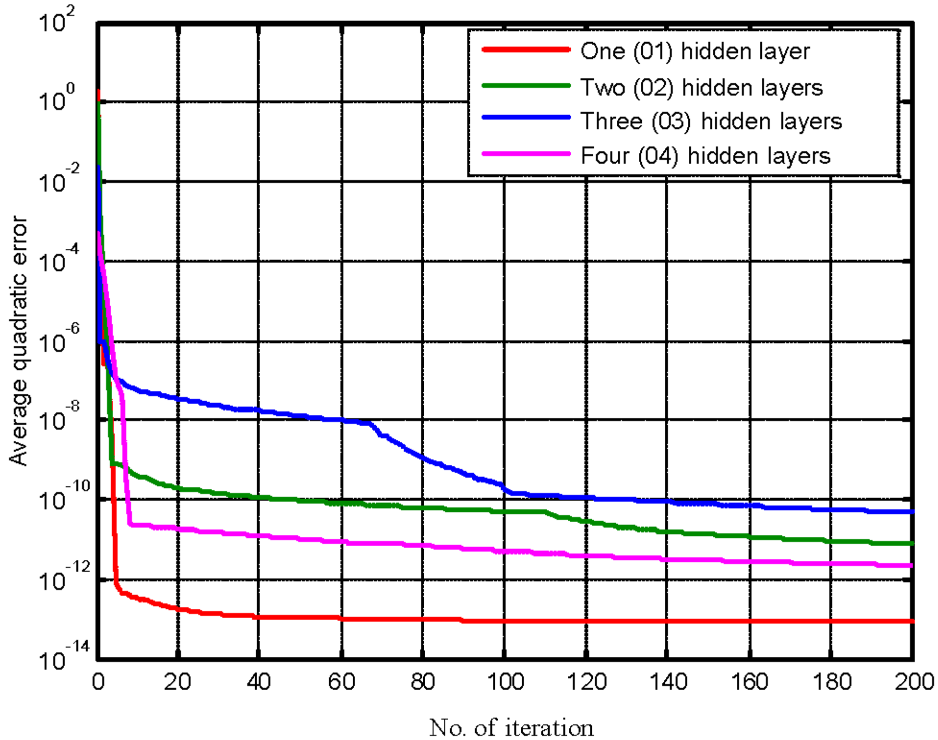

Fig. 3: Effect of the No. of hidden layers on the performance of training of the network of neurons

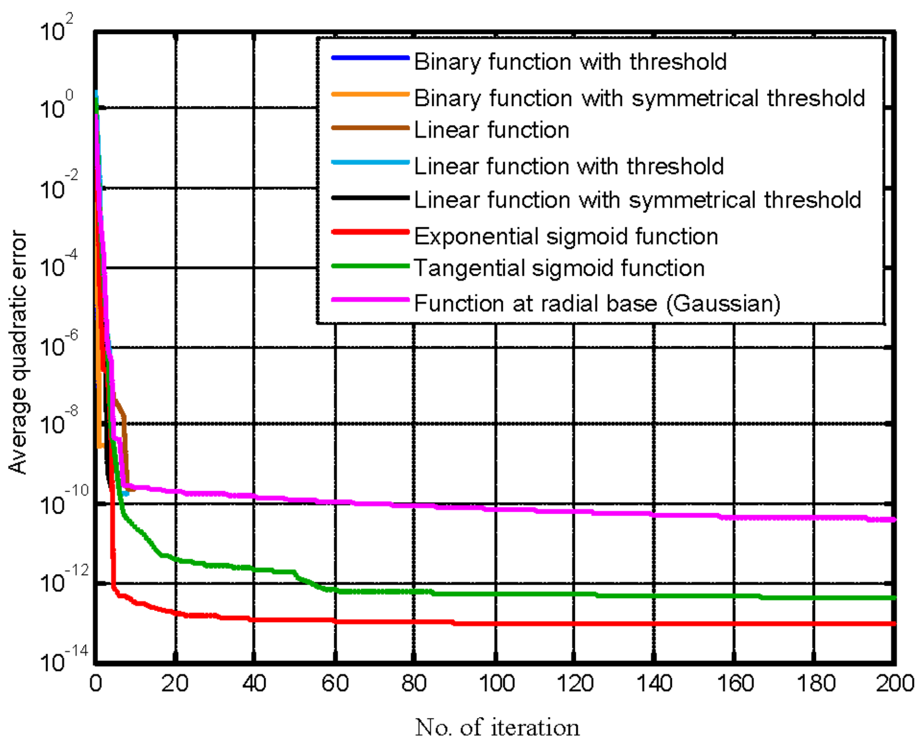

Fig. 4: Effect of the function of activation on the performance of training of the neurons network

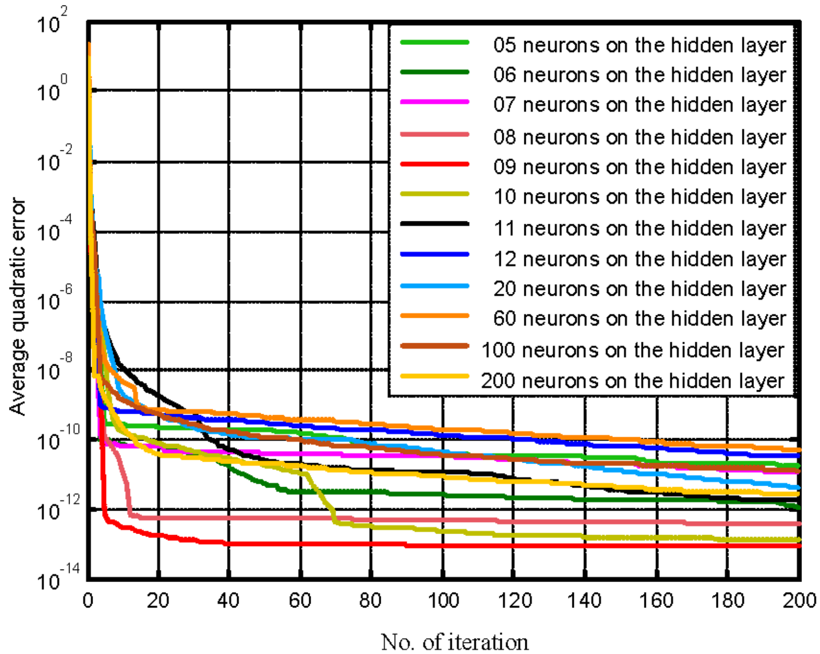

Fig. 5: Effect of the No. of neurons of the hidden layer on the performance of training of the neurons network

of neurons on the hidden layer. This one strongly depends on the complexity of the function to interpolate and the configuration of the inputs used during the training. If this number of neurons is too low, the network will not converge during the training, it will have too many data to learn and not enough neurons to store it. On the other hand, if the network has too many neurons, it will converge quickly, but apart from the points of training, the calculated answers will be poor (Boucheron, 1992; Dreyfus, 2005; Lamrini *et al*., 2005). It is difficult to find criteria allowing the addition or the withdrawal of neurons in the network. A very fine analysis by groping shows that the choice of nine neurons on the hidden layer is the best adapted number and most the performant to present problem, as the Fig. 5 confirms it. On the other hand, the output layer comprises only one neuron, since the network has only one size to calculate.

The difficulty which remainder is to fix the criterion of convergence or to stop of the training. In this step of procedure there are two methods: either one fixes the maximum number of iteration and one leaves with the program the care to find the global minimum or one fixes the minimal error for which the training stops. In this case, after preliminary tests, one noted that the maximum number of cycles of training where the network reaches the minimal error corresponds to a value of 200.

Effect of the training algorithm: Once the network is defined, one passes to the phase of training during which the network will try to learn one or more rules (or relations) by successive corrections from its weights and skew. For that, one imposes to him couples of input-output (series of training) and one modifies the weights and skew so that the answer turned over by the network converges towards the desired outputs. For present problem one has chosen the algorithm of Levemberg Marquardt, most usually used (Blayo and Verleysen, 1996), more rapid and allowing to treat in each iteration the whole of the couples input-output (Fig. 6).

Effect of the initial values of the weights and skews: The training is made several times, because the quality of the interpolation strongly depends on the initial values of the weights and skews of the network, catched chancy by the training algorithm. Figure 7 shows the effect of the choice of the initial values, by carrying out the training of the network several times, one notices that the performances differ from a test to another.

Generalization phase: In this phase, one applies to present network of neurons a new sample of examples where the AARE does not exceed 1%.

TEST ON THE REQUIRED PERFORMANCES

Figure 8 gathers the results of axial dispersion obtained by the neuronal method, it shows the existence of three classes of axial dispersion relating to the three

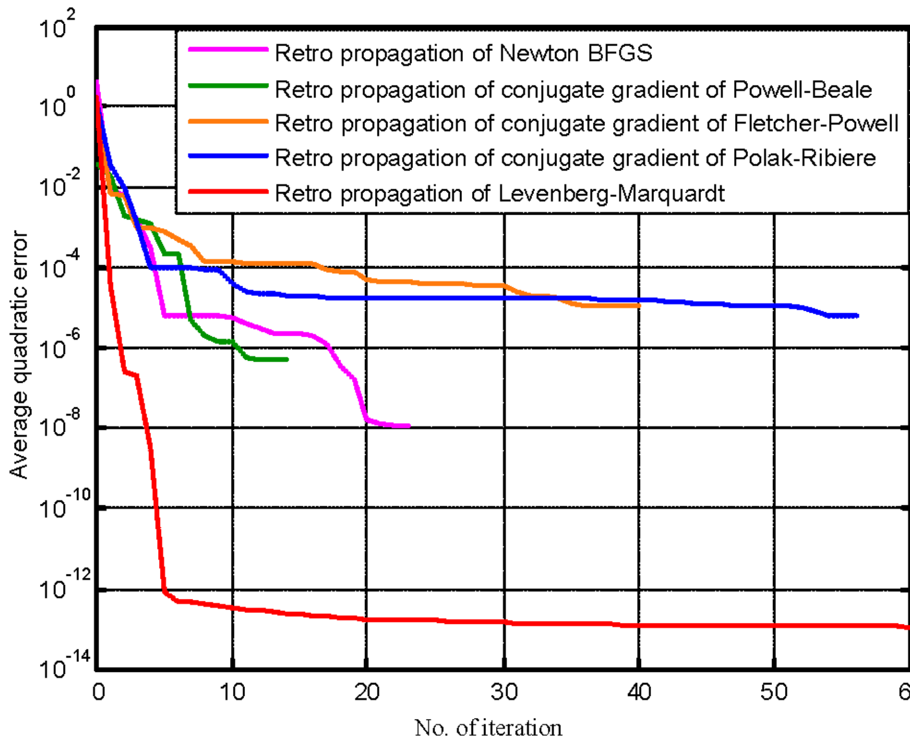

Fig. 6: Effect of the training algorithm on the training performance of the neurons network

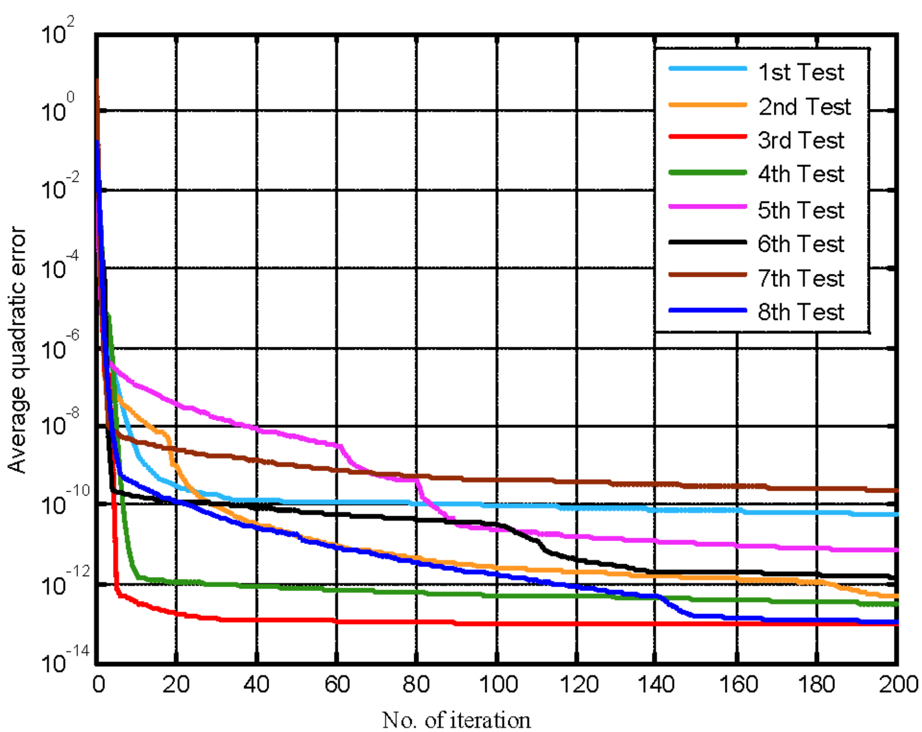

Fig. 7: Effect of the choice of the initial values of the weights and skews of the network on the training performance of the neurons network

Table 3: Comparison between the models of Comiti and Renaud (1989) and the models suggested by using the neuronal method

	Model of Comiti (1989)		Suggested model		Average relative variation (ERM) in (%)
First porous medium	$Dax = 3.57U_0^{0.86}$	(5)	$Dax = 3.593U_0^{0.867}$	(8)	
	Uo in cm sec^{-1} and Dax in $cm^2\ sec^{-1}$		Uo in cm/s and Dax in cm^2/s		0.34
	$\frac{Dax}{\upsilon} = 20.2Re_i^{0.86}$	(6)	$\frac{Dax}{\upsilon} = 19.907Re_i^{0.867}$	(9)	0.33
	$Pe_i = 0.049\ Re_i^{0.14}$	(7)	$Pe_i = 0.05Re_i^{0.133}$	(10)	0.58
	Nothing		$\varepsilon.Pe_i = 0.02 + 0.006\ \ Re^{0.415}$	(11)	------
	Nothing		$Pe_i = \frac{0.055\ Re_i^{0.15}}{1 + 0.09\ Re_i^{0.15}}$	(12)	2.03
Second porous medium	$Dax = 1.49U_0^{0.88}$	(13)	$Dax = 1.493U_0^{0.882}$	(16)	
	Uo in cm sec^{-1} and Dax in $cm^2\ sec^{-1}$		Uo in cm sec^{-1} and Dax in $cm^2\ sec^{-1}$		0.07
	$\frac{Dax}{\upsilon} = 3.85Re_i^{0.88}$	(14)	$\frac{Dax}{\upsilon} = 3.835Re_i^{0.883}$	(17)	0.55
	$Pe_i = 0.26\ Re_i^{0.12}$	(15)	$Pe_i = 0.261Re_i^{0.117}$	(18)	0.55
	Nothing		$\varepsilon.Pe_i = 0.02 + 0.084\ \ Re^{\ 0.139}$	(19)	------
	Nothing		$Pe_i = \frac{0.303\ Re_i^{0.15}}{1 + 0.179\ Re_i^{0.15}}$	(20)	0.52
Third porous medium	$Dax = 2.06\ U_0^{0.92}$	(21)	$Dax = 2.063U_0^{0.921}$	(24)	
	Uo in cm sec^{-1} and Dax in $cm^2\ sec^{-1}$		Uo in cm sec^{-1} and Dax in $cm^2\ sec^{-1}$		0.05
	$\frac{Dax}{\upsilon} = 2.67Re_i^{0.92}$	(22)	$\frac{Dax}{\upsilon} = 2.669Re_i^{0.92}$	(25)	0.04
	$Pe_i = 0.35\ Re_i^{0.08}$	(23)	$Pe_i = 0.375Re_i^{0.08}$	(26)	7.14
	Nothing		$\varepsilon.Pe_i = 0.02 + 0.108\ \ Re^{0.092}$	(27)	------
	Nothing		$Pe_i = \frac{0.555\ Re_i^{0.15}}{1 + 0.528\ Re_i^{0.15}}$	(28)	6.97

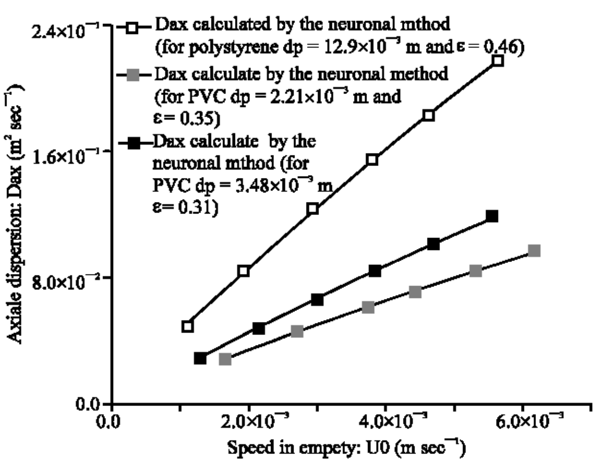

Fig. 8: Values of axial dispersion obtained by the neuronal method, according to speed empty for the three porous media

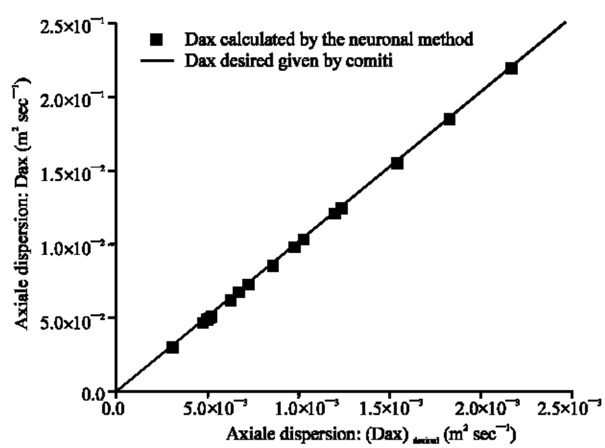

Fig. 9: Performances of the neurons network used for the calculation of the axial dispersion of the three porous media

porous media, of plates packed in the form of fixed beds, used by Comiti and Renaud (1989) (Table 3).

Figure 9 shows that the computed values by the neuronal method conform to those obtained by Comiti and Renaud (1989) with a relative error which does not exceed 1%.

MODELING

There are, in practice, two principal models of studies of the real flows: the mathematical model which appeals, according to cases, forms fairly simplified of vectorial relations, it provides an algebraic relation between the variables and the semi empirical semi model (dimensional analysis and the theory of the models), which provides information on the links which can exist between the various variables of the problem. In order to reinforce this study more, we tried to model the results obtained by the method of neurons network, by using simple models with the same type than those proposed by Comiti and Renauad (1989), so that the comparison is significant. In this stage and in order to put in evidence the speed effect in the empty and the nature of the porous medium on axial dispersion, it is convenient to gather the results of the three porous media in the Table 3.

CONCLUSION

Axial dispersion strongly depends on speed in empty, of the physicochemical characteristics of fluid and the structural organization of material constituting the porous medium. The neuronal method adopted for calculation of axial dispersion resulting from the flow of an aqueous solution through a porous medium of plate laid out fixed-bed and using the equations of correlation given by Comiti and Renaud (1989), is proved to be effective considering the good agreement between the desired values and the computed values. Its advantage is to simplify the numerical analysis and consequently the reduction of the computing time. It is always easy to propose a modeling according to a power full law, but the difficulty results from the physical significance of the parameters taken into account; this is not very restrictive for the industrial applications insofar as each particular problem appeals to a precise field of flow mode and nature of porous medium. Then a representation by the dimensional analysis provides informations on the links which can exist between different variables connecting axial dispersion to the physicochemical properties from the fluid and material constituting the fixed bed of the porous medium.

However, it is interesting to know if the neuronal method would be able to simulate axial dispersion for other garnishing. One thus will plan to check the validity of the method by analyzing the experiments carried out by other authors on the spherical and cylindrical garnishings.

NOMENCLATURE

AARE : Average absolute relative error
DP : Dispersion piston
DRT : Distribution of the residence time
EDP : Exchange dispersion piston
G_{has} : Specific surface of the grain (m^{-1})
p_{has} : Specific surface of the bed (m^{-1})
C_T : Total concentration of liquid (mole m^{-3})
Dax : Axial scattering coefficient (m^2 sec^{-1})
D_{EFF} : Coefficient of effective molecular diffusion, (m^2 sec^{-1})
D_H : Hydraulic diameter of Kobayashi (m) ($d_h = \frac{3D_c(1-\varepsilon)d}{1+2d}$)
D_m : Molecular diffusion coefficient of the considered species (m^2 sec^{-1})
d_p : Diameter of the particles (m)
D_{rad} : Radial scattering coefficient
$f_{\acute{a}}$: Fraction of the particle of the phase in the liquid zone
H_T : Total height of the bed (m)
N : Transfer unit numbers
R : Radial co-ordinates of the particle (m)
t : Time (sec)
u_{ls} : The superficial speed of the liquid through the porous medium (m sec^{-1})
u_L : Speed was empty liquid (m)
z : Axial co-ordinate (m)
ε : Porosity of the bed
ρ_α : Density of the phase α (kg m^{-3})
μ_α : Dynamic viscosity of the phase α (kg $m^{-1}sec^{-1}$)

Indices

D : Dynamic liquid zone
G : Gas
I : Intra particle liquid zone
L : Liquid
S : Stagnant liquid zone
T : Total liquid, combined zones
H : Hydraulic

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