

Improvement Axial Dispersion Calculation in Fibrous Garnished Fixed Beds Using the Neural Method

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Abstract: To determine accurately the physical modeling of flow through porous media and / or in chemical reactors, especially in the field of low Reynolds numbers, it is essential to compute the coefficient of axial dispersion. In prior studies, we employed the neural method to compute axial dispersion within fixed beds with parallelepiped and spherical packings. In the present study we apply the same method of calculation on heterogeneous fixed beds with large anisotropy using data from Poirier and Trinh on fibrous beds. Such an investigation could be however very useful while one has the desire to predict the mixing process to characterize the axial dispersion in fixed beds of anisotropic particles and when experimental measurements are not accessible and / or difficult to implement as for reactors and / or industrial complex porous media. To show also the robustness and applicability of this method, the calculation results obtained will be modeled using expressions similar to those proposed by Poirier and Trinh, so that we can compare our results with those obtained by these authors, under the same operating conditions. Furthermore, our study offers a comprehensive analysis encompassing all three examined fixed bed configurations, namely parallelepiped, spherical, and fibrous arrangements.

Keywords: Fixed bed, porous media, axial dispersion, fibrous beds, neural networks, modeling.

1. INTRODUCTION

Abnormally elevated levels of axial dispersion within porous materials result from a complex interplay of various factors. Local permeability variations, arising from the intricate networks of interconnected pores and channels, create imbalances in flow distribution and contribute to increased dispersion. Additionally, the heterogeneous nature of the surrounding environment, marked by wall effects and variations in pore or particle diameters, plays a significant role in this phenomenon. Interactions between solutes and the porous material's walls further complicate the dispersion process. Moreover, research highlights the substantial impact of bed length on axial dispersion coefficients (D_{ax}), with longer beds offering increased opportunities for solute dispersion. Understanding these multifaceted factors is essential for optimizing processes involving porous materials, such as chromatography columns or chemical reactors, to minimize axial dispersion and enhance overall process efficiency.

2. FIBROUS GARNISHING

In a fixed bed formed by stacking particles for padding, the shape of these particles dictates the fluid's flow lines as it bypasses them, along with the resulting wake downstream of the object, and consequently, influences the coefficient of axial dispersion.

After exploiting the performance of the neural method with media whose behavior is relatively well known (spherical and parallelepiped packing), and in order to better highlight the structuring of the medium on the axial dispersion, in this part we study a very particular environment by the neural network method. It is a fibrous mattress of high porosity, made up of anisotropic particles (fibers), characterized by a distribution in size of the diameter of the pores much greater than the beds of beads or platelets. When a fluid flows through a fibrous mat, it results in a faster circulation in the large pores than in the small ones, thus leading to a greater dispersion of the flow [1]. This phenomenon has already been observed in other works, which has led certain authors [2] to criticize the use of a

representation of the flow based on the axial dispersion. In their opinion, the preponderant phenomena in the fibrous mats are linked to the preferential passages and the axial dispersion in the classical sense of the term is then negligible. So an anomaly in the description and quantification of the phenomenon of axial dispersion.

Poirier [3], [4] and Trinh [5], [6] conducted tracing experiments on fixed beds of unbleached softwood kraft pulp, arranged in a fixed bed in a cylindrical column with an internal diameter of 8 cm and variable height H. They studied the influence of the principal parameters of operation of paste washers (circulation speed of the solution of washing "water", the thickness of the fibrous mattress and the consistency of the mattress). Basing themselves on an experimental design, the authors proposed a correlation binding the evolution of the Peclet number to the principal parameters quoted above.

$$Pe_H = -0,91 H^2 - 0,58 H C - 27,32 C U_0 + 17,90 H + 3,12 C + 219,67 U_0 - 43,08 \quad (1)$$

Equation (1) clearly shows that the three parameters studied (U_0 , H, C) are linked variables. With:

U_0 : the speed of the fluid in (cm/s) $0,01 \text{ cm/s} \leq U_0 \leq 0,08 \text{ cm/s}$

H : the thickness of the porous medium expressed in (cm) $2,5 \text{ cm} \leq H \leq 8,5 \text{ cm}$

$C = \frac{1}{1 + \frac{\varepsilon \rho V_s}{1 - \varepsilon}}$: the consistency of the fibrous mattress in percentage $3 \% \leq C \leq 17 \%$

$\rho = 1 \text{ g/cm}^3$: volumetric mass of the washing solution (water),

$V_s = 2,17 \text{ cm}^3 / \text{g}$: the specific volume of the fibers mouthfuls of water,

ε : the porosity of the fibrous mattress.

Equation (1) was retained as a training and generalization database for the development of our neural network for the calculation of axial dispersion in fibrous mattresses. We note here that the literature is very poor in expressions directly or indirectly linking the coefficient of axial dispersion with the parameters influencing the phenomenon of dispersion in fibrous mattresses and in our opinion the correlation (eq.1) remains the most elaborate and representative expression of the axial dispersion despite the restricted range of operating conditions.

3. ARTIFICIAL NEURAL NETWORK MODEL

The idea behind artificial neural networks is influenced by how biological neurons process information. As a result, artificial neural networks can be thought of as a group of processing units and weighted connections that mimic a network of neurons biological.

The organization of artificial neurons (Fig. 1a) in layers, involves the input layer receiving data's (s_i) from the external environment. Subsequent layers then take in weighted outputs ($w_{ij} s_i$) from the previous layer as its input. This architectural arrangement gives rise to a feedforward artificial neural network ANN (Fig. 1b). In this network type, each input is forwarded to the next layer for processing. The outputs generated by the final layer act as the network's outputs to the external world. Neurons within the concealed or output layers of a feedforward ANN serve two fundamental purposes: they compute the cumulative summation of weighted inputs from multiple connections and following this, they subject this computed sum to a transfer function. Furthermore, they transmit the resultant value through outbound connections to the neurons located in the subsequent layer, where an identical process ensues.

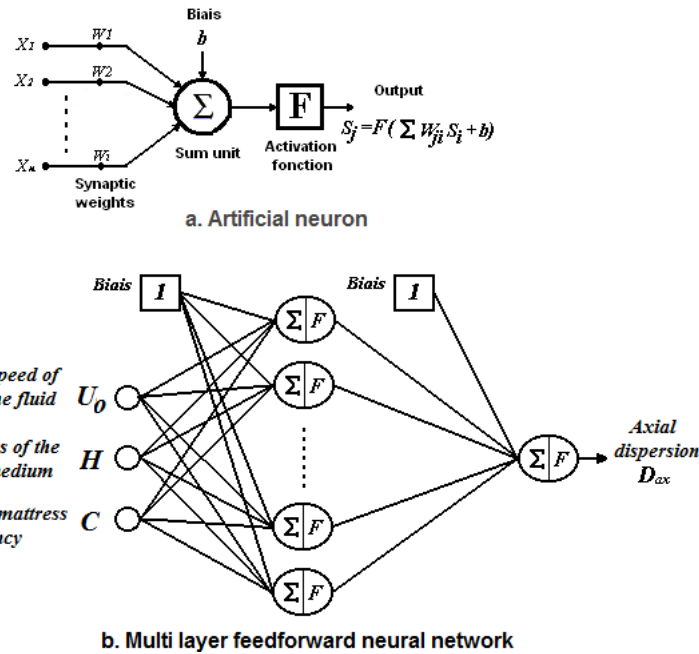


Figure 1: Representation of neuron formal and Multi-layer feed forward neural network for the calculation of axial dispersion in the fibrous fixed beds.

It's well established that varying the number of neurons in the hidden layer(s) significantly impacts the predictive ability of the network. The most common approach for optimizing ANN performance is to adjust the numbers of neurons in the hidden layer(s) and select the architecture that demonstrates the highest predictive ability. The design and optimization of our neural network used for the calculation of the axial dispersion in fibrous mats can be carried out in several steps:

- Data collection and processing: equation 1
- Neurons network architecture: multi-layer neurons network
- Number of hidden layers: one hidden layer
- Number of neurons: thirteen (13) neurons on the layer hidden and one (01) neuron on the output layer
- Function of activation : exponential sigmoid for hidden layer and linear for the output layer
- Algorithm of training : Levenberg - Marquardt
- Number of iteration : 200 iterations
- Training : EQM of training $5,2 \cdot 10^{-16} \%$
- Generalization and validation: relative error ERA $\leq 5 \%$.

4. MODELING

The mathematical modeling of all the calculated values of the axial dispersion from the neural method can be empirical, i.e. it can be based on the search for a purely descriptive mathematical function and therefore fit into an activity of comparisons between models and measurements. In this context, modeling requires the correct choice of relevant quantities and of the mathematical function. Indeed, since the parameters which directly influence the axial dispersion are linked variables, the calculation results can be represented in the following form:

$$Y = a_0 + \sum_{i=1}^3 a_i X_i + \sum_{i=1}^3 a_{ii} X_i^2 + \sum_{i=1}^2 \sum_{j=i+1}^3 a_{ij} X_i X_j + \sum_i^1 \sum_{j=i+1}^2 \sum_{k=i+2}^3 a_{ijk} X_i X_j X_k \quad (2)$$

With $(a_0, a_{ii}, a_{ij}$ et $a_{ijk})$ are constants of calculations without physical meaning and $X = (H, C, U_0)$ the main variable.

In accordance with the form of the proposed model (eq.2) close to that of Poirier [3], [4] and Trinh [5], [6] (eq.1), an expression has been proposed which takes into account the combination of all the main variables governing the phenomenon:

$$Pe_H = -41,7 + 1,5 \cdot 10^4 U_0 + 1,8 \cdot 10^3 H + 2,7 C + 5,8 \cdot 10^6 U_0^2 - 9,2 \cdot 10^3 H^2 + 22,45 C^2 + 2 \cdot 10^4 U_0 H - 4,8 \cdot 10^3 U_0 C - 146 HC + 4,4 \cdot 10^4 U_0 HC \quad (3)$$

This empirical formulation is then a particular facet that enables quantitative predictions and has some advantages namely to reduce the data volume, the easy comparison of data sets and prediction.

It is interesting to compare the results obtained in this paragraph with previous work concerning dispersion in fibrous mats. It should be noted here that a direct quantitative comparison is difficult because the values of the axial dispersion can vary greatly from one test to another and this for identical operating conditions as mentioned by several authors, in particular Mauret [1], Poirier [3], [4] and Trinh [5], [6]. As a result, the discrepancies noted in the literature are high; if we do not take into account the effect of the diffusion of the tracer in the stagnant zones, the dispersion becomes purely geometric and we can define a dispersion characteristic length:

$$I_d = \frac{Dax}{U_0} = \frac{H}{Pe_H} \quad (4)$$

The results obtained are summarized in the following table:

Table 1: Comparison of axial dispersion in fibrous mats in terms of dispersion characteristic length I_d (*: α is calculated assuming $d_f = 40 \mu\text{m}$)

| Authors | Experimental conditions | $\frac{H}{Pe_H} = I_d \text{ (m)}$ | $\alpha = \frac{I_d}{d_f}$ |
|----------------------------|---|--|----------------------------|
| Poirier [3] Trinh [5] | $2,5 \text{ cm} \leq H \leq 8,5 \text{ cm}$ $1 \cdot 10^{-4} \text{ m/s} \leq U_0 \leq 8 \cdot 10^{-4} \text{ m/s}$ $3 \% \leq C \leq 17 \%$ Unbleached paste kraft of conifer | $1,3 \cdot 10^{-3}$ to $8,3 \cdot 10^{-3}$ | 32,5 to 208 * |
| Grähs [7] | $10 \text{ cm} < H < 17 \text{ cm}$ $1,7 \cdot 10^{-4} \text{ m/s} < U_0 < 9,2 \cdot 10^{-4} \text{ m/s}$ $6 \% < C < 10 \%$ Unbleached paste kraft of conifer | $4,4 \cdot 10^{-4}$ to $1,0 \cdot 10^{-3}$ | 11 to 25 * |
| Järveläinen [8] | $5 \text{ cm} < H < 11 \text{ cm}$ $3,8 \cdot 10^{-4} \text{ m/s} < U_0 < 6,3 \cdot 10^{-4} \text{ m/s}$ $C = 6 \%$ Paste kraft of conifer | $9,8 \cdot 10^{-4}$ to $1,25 \cdot 10^{-2}$ | 24,5 to 313 * |
| Sherman [9] Pellet [10] | $3 \text{ cm} < H < 8 \text{ cm}$ $2 \cdot 10^{-4} \text{ m/s} < U_0 < 1,0 \cdot 10^{-2} \text{ m/s}$ $0,7 < \varepsilon < 0,9$ Viscose fibre / of Dacron | $3,0 \cdot 10^{-4}$ to $1,3 \cdot 10^{-3}$ for d_f varying de 16 à 122 μm | 4 to 80 |
| Mauret [1] | $3,4 \text{ cm} < H < 5,25 \text{ cm}$ $2,4 \cdot 10^{-4} \text{ m/s} < U_0 < 3,88 \cdot 10^{-3} \text{ m/s}$ $0,67 < \varepsilon < 0,82$ Viscose fibre 20dtex | $7,3 \cdot 10^{-4}$ to $7,1 \cdot 10^{-3}$ for $d_f = 50 \mu\text{m}$ | 14,6 to 142 |
| | $H = 3,4 \text{ cm}$ $2,4 \cdot 10^{-4} \text{ m/s} < U_0 < 1,1 \cdot 10^{-3} \text{ m/s}$ Unbleached paste kraft of conifer | Deflocculated : $5,4 \cdot 10^{-3}$ Flocculated : $5,25 \cdot 10^{-3}$ to $2,6 \cdot 10^{-3}$ | 135 * 13 to 65 * |
| Our results | $3,5 \text{ cm} \leq H \leq 8,5 \text{ cm}$ $1 \cdot 10^{-4} \text{ m/s} \leq U_0 \leq 8 \cdot 10^{-4} \text{ m/s}$ $3 \% \leq C \leq 17 \%$ Unbleached paste kraft of conifer | $1,4 \cdot 10^{-3}$ to $3 \cdot 10^{-3}$ | 34,98 to 75,45 |

From the table above, it can be seen that the dispersion characteristic length is much greater than the diameter of the fibers (a variation of 4 to 300 times the diameter of the fiber depending on the work). Consequently, these differences in axial dispersion in a fibrous mat can be attributed to: the association of fibers in the form of flocks, preferential passages, the large pore diameter size distribution, and diffusion of solutes.

5. RESULTS AND ANALYSIS

Figure 2 shows the layout of the axial dispersion coefficient calculated by the method of neuronal versus coefficient that is calculated from equation 1. It is noted that all values are adequately represented by the neural network developed.

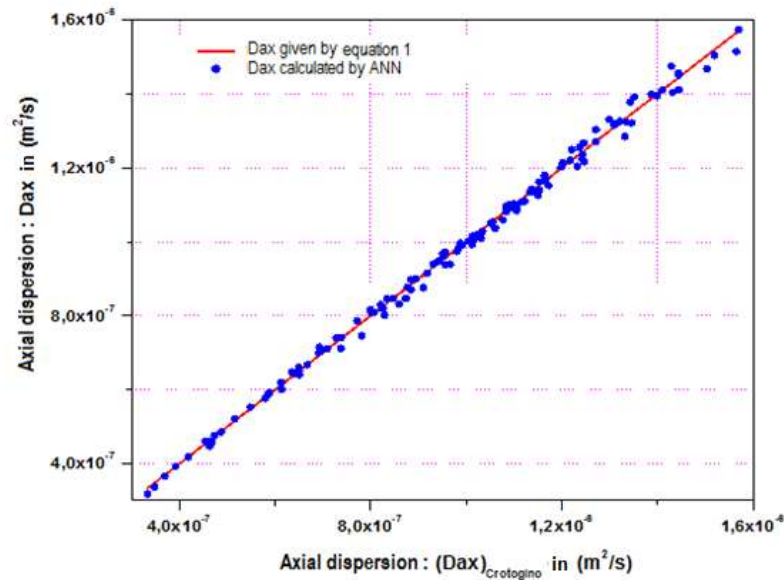


Figure 2: Performance of the neural network used for calculating the coefficient of axial dispersion in fixed beds of fibers.

Figure 3 illustrates the impact of the fibrous mat's thickness on the axial dispersion coefficient for a porosity of $\epsilon=0.693$ ($C = 16.95\%$). In general, for a given velocity within the studied range, an elevation in the height H of the fibrous mat leads to a corresponding increase in axial dispersion.

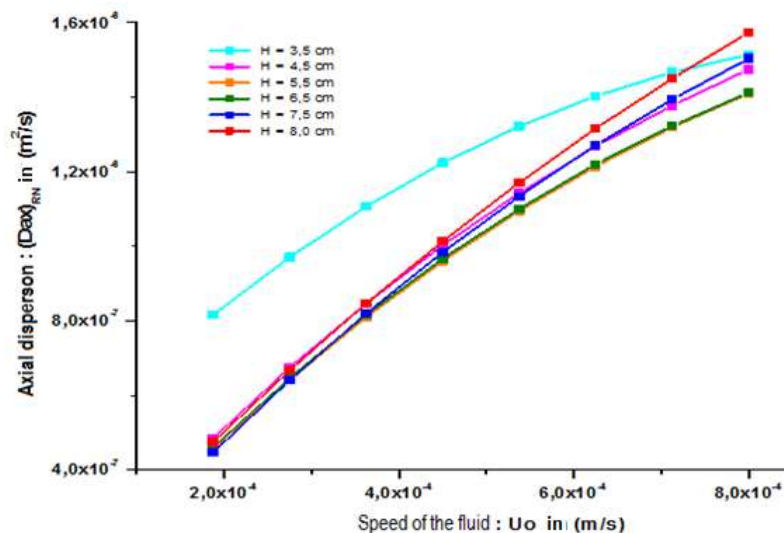


Figure 3: Effect of the thickness of the porous medium on the axial dispersion

Figure 4 depicts the influence of porosity on axial dispersion, while maintaining a constant mattress thickness ($H=6.5$ cm). It is noted that, the higher the porosity, the greater the volume of the void contained in the fibrous mat and consequently the axial dispersion is significant.

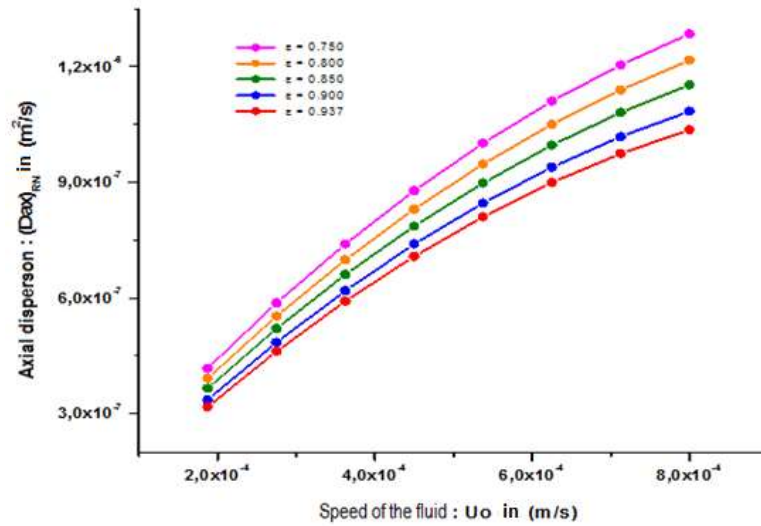


Figure 4: Effect of porosity on axial dispersion for $H = 6.5$ cm

Figure 5 represents the evolution of the Peclet number, calculated by the neural network, as a function of the empty barrel flow velocity, for different operating conditions examined.

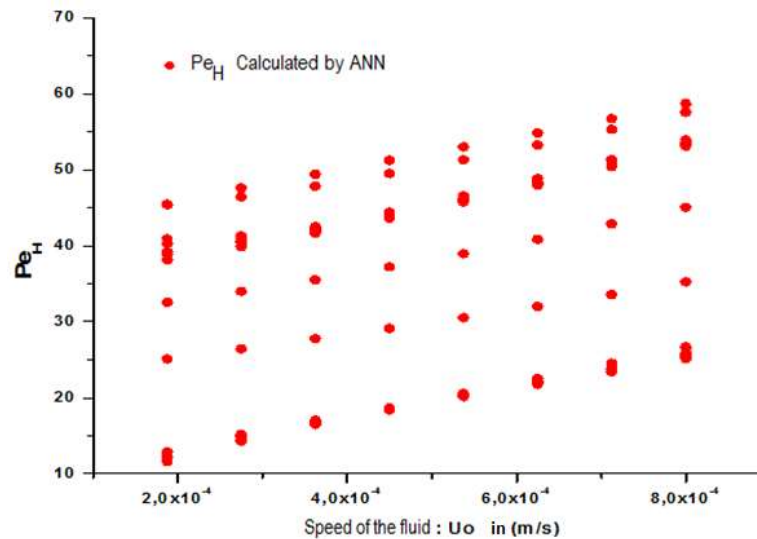


Figure 5: Values of Peclet number (Pe_H) obtained by the neural method for fibrous fixed beds.

From Figure 5, it is noted the greater height H of the fibrous mat the greater the axial dispersion. Moreover, the higher the porosity the higher the volume of the larger void content in the fibrous mat and hence the axial dispersion is important.

To illustrate depict the influence of the three interrelated parameters (height, consistency, and velocity) on axial dispersion, it is necessary to construct a three-dimensional representation of the proposed model (Eq.3). Three cases are possible:

First case: the axial dispersion is represented as a function of the speed of the fluid and the height of the bed at different consistencies (porosities).

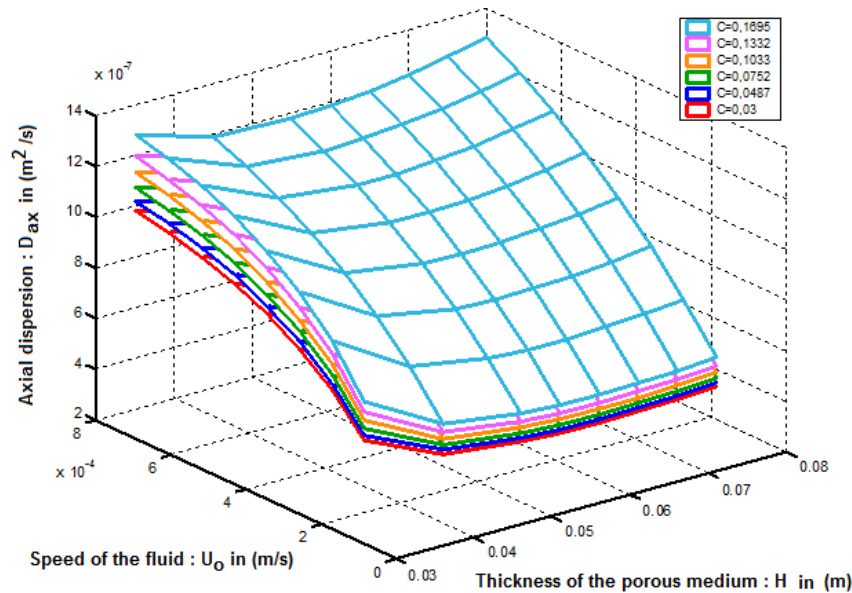


Figure 6: Three-dimensional representation of axial dispersion in a fibrous mattress for a consistency (porosity) of the variable bed.

Second case: the axial dispersion is represented as a function of the speed in the empty barrel and of the consistency of the mattress at different heights of the bed

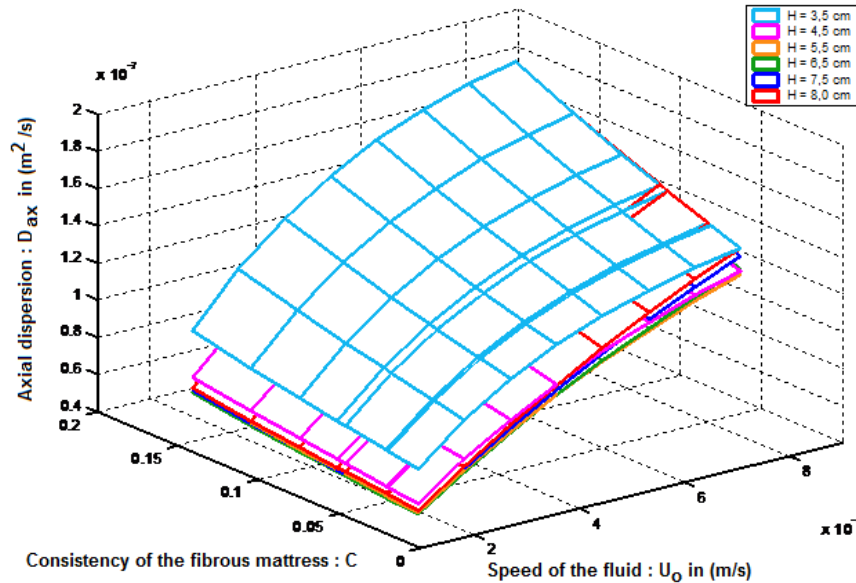


Figure 7: Three-dimensional representation of axial dispersion in a fibrous mattress for a height of the variable bed.

Third case: the axial dispersion is represented as a function of the height of the bed and the consistency of the mattress at different speeds.

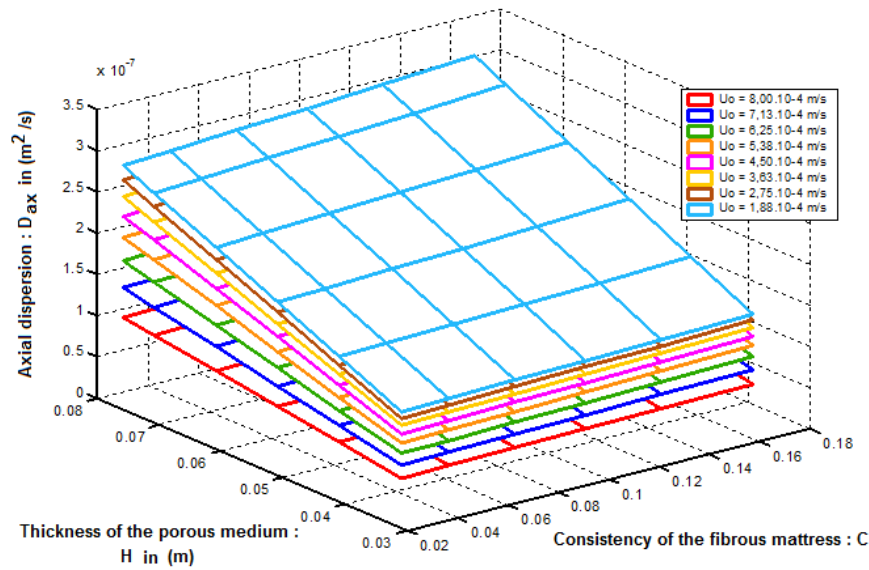


Figure 8: Three-dimensional representation of axial dispersion in a fibrous mattress for a variable speed.

6. COMPARISON OF AXIAL DISPERSION OF THE THREE PACKINGS STUDIED

In order to emphasize the impact of particle shape on the axial dispersion coefficient during the flow of a fluid through a fixed bed of identical particles, it is essential to compare the results obtained for the three studied packings: Platelets [11], spherical [12], and fiber. The results for the three studied packing and the main operating conditions are listed in Table 2.

Table 2: Proposed correlation equations from the neural method for the three packing

| Garnishing | Equations of correlation suggested from the neuronal method | Operating conditions |
|---------------|---|---|
| Platelets [9] | $Pe_i = \frac{0,055 Re_i^{0,15}}{1 + 0,09 Re_i^{0,15}}$ | 0,12 cm < dp < 0,35 cm 0,3 < ε < 0,5 2,7.10-3 cm /s < Uo < 0,62 cm /s |
| Spheres [10] | $\varepsilon.Pe_i = 0,197 + \frac{1,12}{\sqrt[3]{Re}} + 0,01 \sqrt{Re}$ | 0,2 cm < dp < 0,65 cm 2.10-4 m/s < Uo < 6.2.10-3 m/s |
| Fibres | $Pe_H = -41,7 + 1,5.10^4 U_0 + 1,8.10^3 H + 2,7 C + 5,8.10^6 U_0^2 - 9,2.10^3 H^2 + 22,45 C^2 + 2.10^4 U_0 H - 4,8.10^3 U_0 C - 146 H C + 4,4.10^4 U_0 H C$ | 3,5 cm ≤ H ≤ 8,5 cm 1.10-4 m/s ≤ Uo ≤ 8.10-4 m/s 3 % ≤ C ≤ 17 % |

Figure 9 allows the comparison of axial dispersion according to the speed between the three studied garnishings (spherical, Platelets and fibrous). This figure shows that: axial dispersion is all the more significant since the speed is raised and this whatever the type of garnishing is, axial dispersion in a fixed bed of plates is more significant than that of a fixed bed of spherical particles and in this last it is more significant than that of a fibrous mattress.

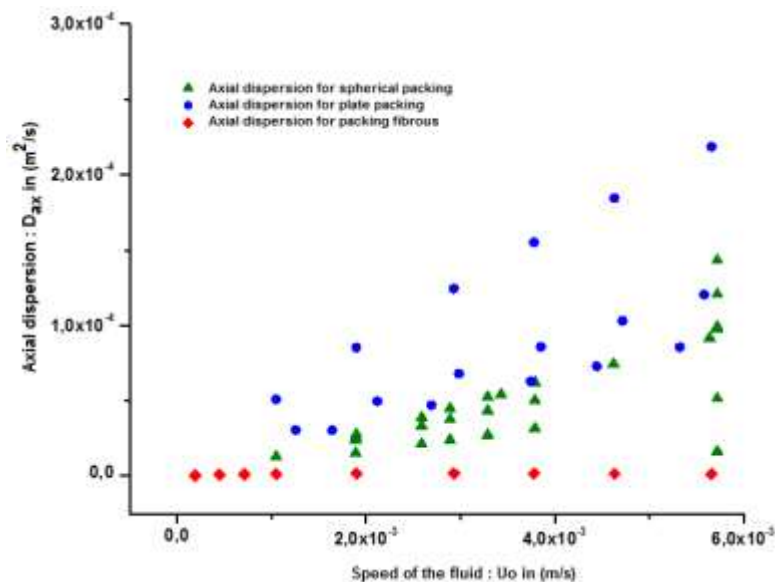


Figure 9: Comparison of axial dispersion coefficient in fixed beds of the three types of packings studied (zoom between $0 \leq U_0 \leq 6.10^{-3}$ m/s).

7. CONCLUSION

The dispersion within a fibrous mattress appears to be influenced by various parameters, particularly fluid velocity, fixed bed height, fibrous mattress density, as well as fiber and floc dimensions. Despite the multitude of factors affecting axial dispersion within fibrous mattresses, the neural approach remains effective, satisfactory, and representative for assessing the axial dispersion coefficient. The potency of this methodology is demonstrated by the robust agreement observed when comparing results obtained through neural networks with the conclusions of prior literature. Furthermore, the obtained results also illuminate the correlation between the axial dispersion phenomenon and the geometry of the particles comprising the porous medium. In fact, axial dispersion in a fixed bed of platelets proves to be more significant than that observed in a fixed bed of spherical particles, which in turn surpasses that of a fibrous mattress.

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