Application of Neural Networks to Mass-Transfer Predictions in a Fast Fluidized Bed of Fine Solids

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In this study back-propagation, feed-forward neural networks are applied to estimate mass-transfer parameters in fast fluidized beds of fine solids. These networks are trained to predict mass-transfer rates using measurements of the sublimation rate of coarse naphthalene balls in fast fluidized beds of fine glass beads at several solid-to-gas mass flow rates within the relevant superficial gas-velocity range. When tested to predict the effective diffusivities from a coarse particle to the bulk of the fast bed of fine solids, trained neural networks calculated the Sherwood number with high accuracy. It is demonstrated that back-propagation, feed-forward neural networks provide a more accurate correlation for the mass-transfer coefficient compared to those obtained by the currently used heuristic models.

Introduction

Basic knowledge of the combustion of suspended coal particles in the gas-suspension flow in vertical pipes is important in the design of energy-related systems such as fluidized-bed combustors. In general, the surface burning rate of the solid carbonaceous char particles determines the efficiency of coal combustion in such systems. In most industrially important applications the concentration of char particles in a riser is very low. Consequently the number of cases in which two char particles interact with each other can be neglected. This implies that the problem can be considered as the reactivity of a single char particle in a vertical gas-suspension flow. Recent tests by Basu and Halder (1989) on burning rates of coarse carbon particles (diameter between 5 and 9 mm) indicated that both chemical kinetics and mass transfer are important in determining the combustion rate in a fast bed. Hence, an accurate prediction of the char combustion rate in the fast fluidized bed of fine solids requires knowledge of the mass transfer rate to the surface of the burning particle. To provide a background knowledge of mass transfer, Halder and Basu (1988) have measured the rate of sublimation of 11-mm naphthalene balls in fast fluidized beds of 54-and 260-μm glass beads at several solid-to-gas mass flow rates within the superficial gas-velocity range of 3 to 4.5 m/s. The experimental results were compared to those obtained from their mechanistic model using a modified form of the expression for the Sherwood number for mass transfer to an isolated sphere in bubbling-bed conditions proposed by La Nauze and Jung (1982). For the fast bed the proposed Sherwood number (Basu and Halder, 1989) is as follows:

$$Sh = \frac{k_g D_p}{D_G} = 2\epsilon + 0.69\left[(U_g - U_p)\frac{D_p}{\epsilon \nu_g}\right]^{0.5} Sc^{0.33}, \qquad (1)$$

where k_g is the mass-transfer coefficient; D_p is the naphthalene ball diameter; D_g is the diffusivity of naphthalene in air; ϵ is the bulk voidage of the bed; U_g is the gas velocity; U_p is the particle velocity; ν_g is the kinematic viscosity of gas; and Sc is the Schmidt number.

Their theoretical predictions, however, showed that the Sherwood number based on gas–particle slip velocity de-

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creases with the size of the inert particles, which disagrees with their experimental observations. Their observations can be rationalized by considering the fine-particle velocity fluctuations in the boundary layer around the coarse particle. These fluctuations may induce a dispersive gaseous motion that can aid mass-transfer rates resulting from the motion of fluid particles across the boundary layer due to the turbulent core. This augmentation in gaseous transport in the large-particle boundary layer is thus closely linked to the fine-particle fluctuating velocity, which was recently confirmed by experiments (MacNeil and Basu, private communication, 1995). Apparently, the theoretical approach of Halder and Basu does not have the necessary foundation for describing the effect of particle velocity fluctuations on mass transport in fast fluidized beds.

Essential progress can be made if one constructs theories such as that of Dasgupta et al. (1994) that take into account the effect of particle fluctuations in the transport processes involved in a turbulent gas-suspension flow of small particles at a moderately high mass loading of solids. They explored some aspects of the interaction between the diffusive processes, which lead to a process of homogenization, and the instabilities of gas or particle phase, which lead into formation of large-scale solid structures (clusters). In the presence of clusters in gas–solid flows in vertical tubes, the relative velocities between single particles and clusters, which may be induced by body forces, lead to collisions. The result is an accelerating effect on the more slowly moving cluster as it is overtaken by the faster moving single particles. This also results in an increasing relative velocity between a single particle and the gas. Hence, a single small particle, which would be expected to follow the motion of gas closely, poorly correlates with the corresponding fluid points, and as a result, reacts sluggishly to the turbulent velocity fluctuations of the surrounding gas. In such systems, one expects the particle slip velocity to be much higher than the single-particle terminal velocity, as was previously observed by Horio and Kuroki (1994). Interest in nonequilibrium aggregation processes has recently been stimulated by the direct-simulation Monte Carlo calculations of Tanaka et al. (1995), which predicted the existence of large-scale solid structures with well-defined scaling. Clusters generated by their model have a fractal dimensionality (Mandelbrot, 1982) that is smaller than the dimensionality of the space in which the cluster is formed. However, it is not obvious how the cluster translational and rotational diffusion coefficients, which significantly affect the rate of mass transfer, depend on the cluster size.

The highly complicated flow behavior of the particles in a fast fluidized bed of fine solids accounts for the lack of a rigorous model for predicting the mass-transfer processes in these systems. As such, it is essential to develop new approaches and the associated tools for dealing with this complex system. In this article, a method is presented to study mass transfer in dense gas–solid flows that is different from the classic method by Halder and Basu (1988). The present nonclassic method is based on artificial neural networks, which are large interacting systems of simple units (Hertz et al., 1991). Neural networks are useful for the logically accurate formulation of complex systems. The purpose of the neural-network model in studying mass transfer in fast fluidized beds is to extract a more accurate correlation for the mass-transfer coefficient from the available measurement. To this end, a neural-network topology is designed for mass-transfer prediction from coarse naphthalene balls to a fast fluidized bed using the experimental results presented by Halder and Basu (1988). Foremost among the difficulties associated with the attrition of the naphthalene ball is that of dealing with the collisional events between the ball and fine-bed particles. Hence, it is scarcely surprising to find that the theory for particle attrition in a fluidized bed (Kono et al., 1987) is in a rather early stage. As an initial speculation, it is assumed that the mass transfer does not affect the attrition rate of naphthalene balls. The present design has been shown to give results that compare favorably to those obtained by Halder and Basu (1988), though using much fewer computational resources. However, the present results are not based on any fundamental physical theories. We use the present neural network to give the perspective views of the Sherwood number as a function of the bed density and superficial gas velocity for 54-μm particles.

Architecture and Parameters of the Networks

In this study, the feed-forward, back-error propagation network architecture, which is shown in Figure 1, is applied exclusively to the prediction of mass-transfer rates in a riser of a fast fluidized bed by learning the optimal mapping between the input vectors ξ_k^μ and the output ζ_i^μ. The inputs are functionals of the mean solids fraction at the upper entrainment region ξ_1, the superficial gas velocity ξ_2, the fine-particle diameter ξ_3, and the through flow of solids ξ_4, and the output is the mass-transfer coefficient ζ_1. Here different vectors are labeled by a superscript μ. The data set consists of 45 vectors from the experiment, which was based on the sublimation of coarse naphthalene balls in fast fluidized beds of 54 and 260 μm fine glass beads in a 102-mm-dia. and 5.5-m-tall circulating fluidized-bed apparatus (Halder and Basu, 1988).

The data set is divided into two groups: the training set, including sublimation rates of coarse naphthalene balls in fast fluidized beds of fine glass beads at several solid-to-gas mass flow rates within the relevant superficial gas-velocity range, and the testing set. The network design comprises two layers, one of nonlinear processing units, followed by an output layer of linear processing units, with adjustable connection strengths (weights) between them. This design allows the network to learn nonlinear and linear relationships between input–output pairs $\{\xi_k^\mu, \zeta_i^\mu\}$. The hidden units in between the input and output layers increase the network memory, and therefore allows the network to be trained to higher accuracy. In the present study, nine hidden units produced the best fit to the test data. Learning is performed by the network by means of a back-propagation algorithm, which involves minimizing the following error function (Hertz et al., 1991) that vanishes as the final calculated outputs of the network match the observed output for a training set of input–output pairs $\{\xi_k^\mu, \zeta_i^\mu\}$:

$$E = \sum_\mu \sum_i [\zeta_i^\mu - O_i^\mu]^2, \tag{2}$$

where ζ_i^μ are the mass-transfer rates reported by Halder and

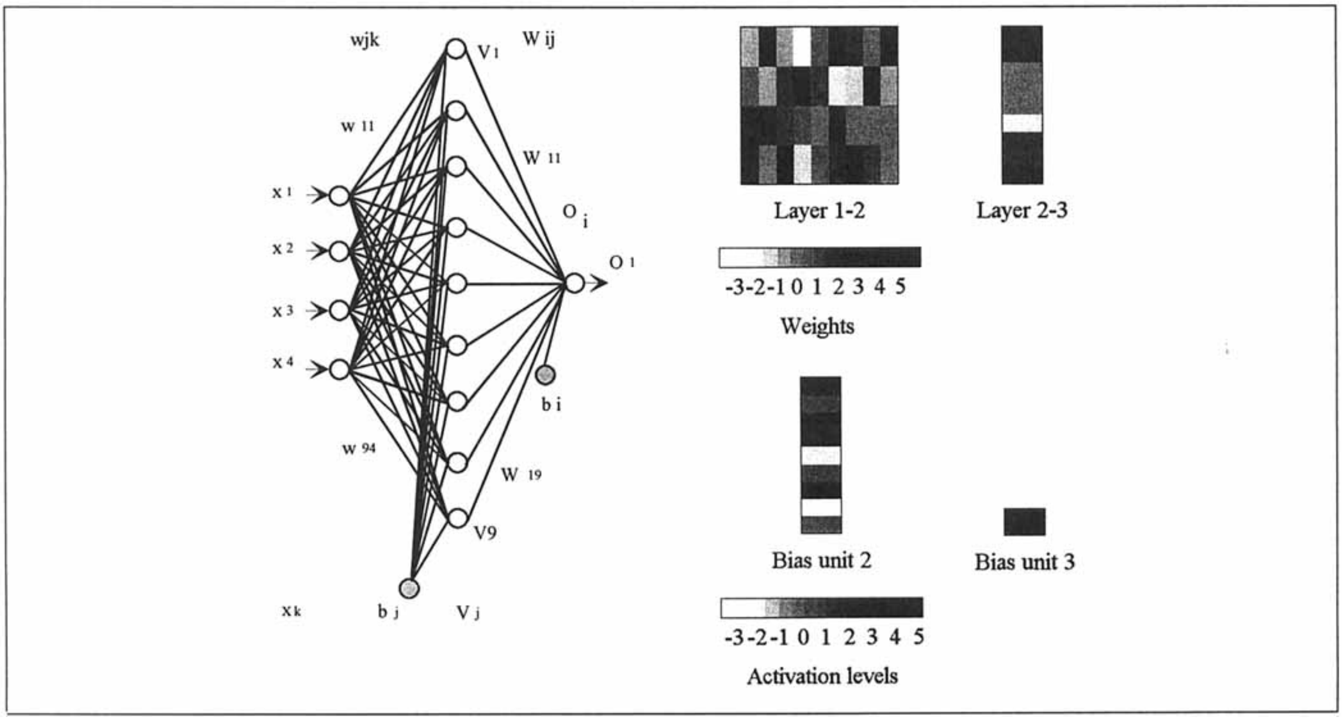


Figure 1. Three-layered, feed-forward, back-propagation neural network, and activation levels and weights calculated with the neural network trained on the training data set.

Basu (1988), and O_i^μ are the calculated outputs of the present network. Information processing begins by applying an input vector ξ_k^μ to the input layer, which outputs the values of the vector elements V_j^μ. These values are fed forward through the network, which produces the final outputs as follows:

$$O_i^\mu = \sum_j W_{ij} \tanh\left[\beta\left(\sum_k w_{jk}\xi_k^\mu + b_j\right)\right] + b_i, \tag{3}$$

where β is the steepness factor of the hyperbolic tangent function, which is set to unity in this study; w_{jk} is the weight on the connection from the kth input unit to the jth hidden unit; W_{ij} is the weight on the connection from the jth hidden unit to the ith output unit; b_j and b_i are the bias terms of the hidden and output layers, respectively. The Levenberg–Marquardt update rule (Levenberg, 1944; Marquardt, 1963) is used to learn the appropriate weights and biases associated with each interconnection. According to the network approach the adjustable parameters are the number of units in the hidden layer and the initial values of the connections.

An additional adjustable parameter may be defined by considering the hydrodynamic complexity of the gas binary solids mixture flow in vertical tubes. Using the concept of granular temperature, introduced in the kinetic theory of rapid granular flow (Jenkins and Savage, 1983), Ippolito et al. (1995) demonstrated a lack of equipartition of fluctuation kinetic energy for the binary granular mixture. This leads to the deposition of fine particles in the boundary layer of the coarse naphthalene ball, which may control the process of mass transfer from the coarse particle to the bulk. It is worth noting that the coarse particles in a fast-fluidized-bed riser do not always move up with the gas. Sometimes, they fall due to collisions with the down-flowing clusters. Hence, the assumption that the time-averaged solids fraction around a coarse naphthalene ball is identical to the mean solids fraction in the upper entrainment region may not be valid. It is not obvious how to rigorously treat this problem, but there is an approximation that is discussed as follows. Assuming that a turbulent gas–laminar particle suspension flow model such as that proposed by Louge et al. (1991) can describe important characteristics of a particulate flow around a coarse naphthalene particle, the expression for particle diffusivity can be obtained (Zamankhan et al., 1997)

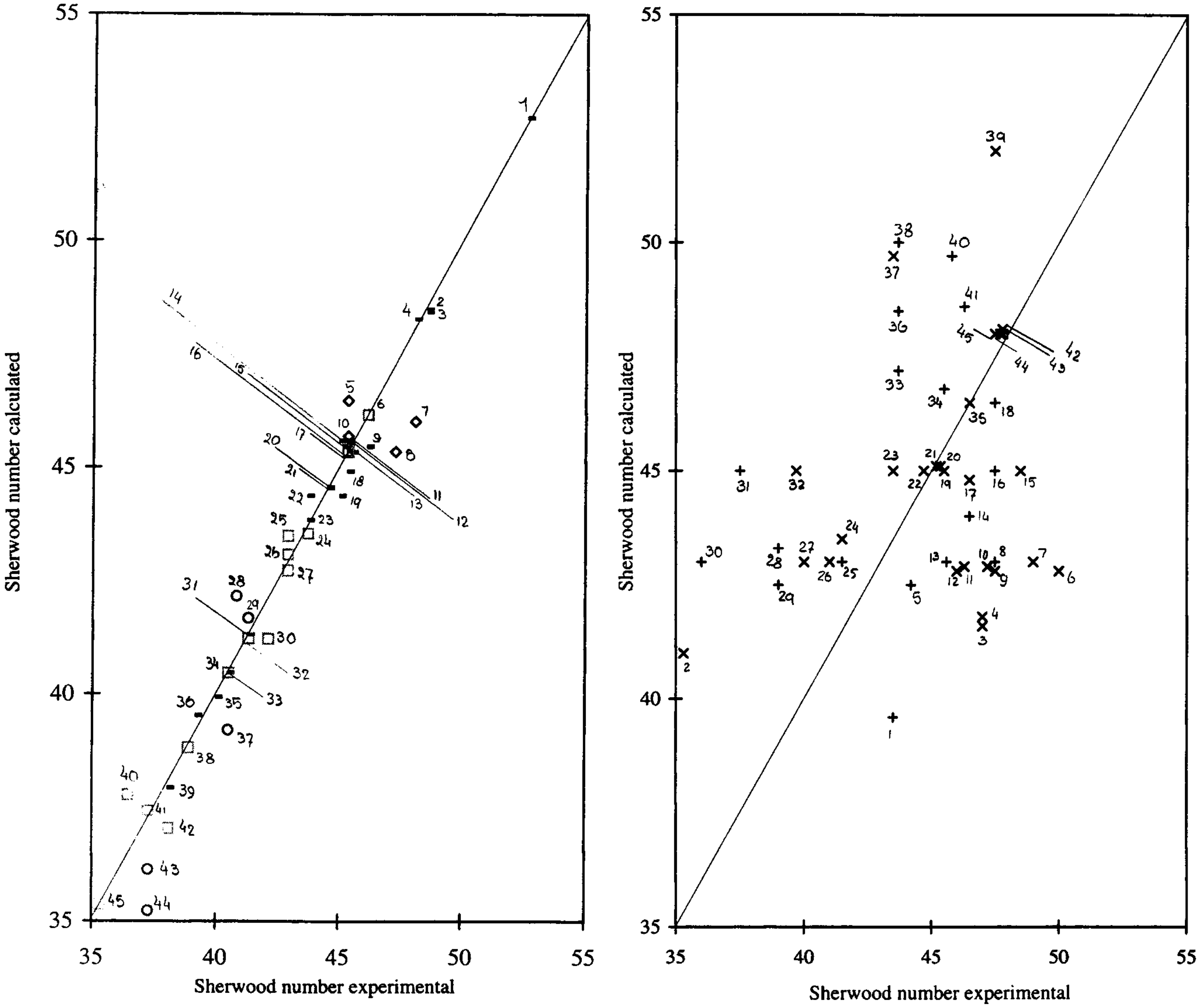
$$D = \frac{\sigma\pi^{1/2}}{8(1+e)\phi\chi_c}\left(\frac{T}{m}\right)^{1/2}, \tag{4}$$

where σ is the diameter of fine particles; ϕ is the solid fraction; e is the coefficient of restitution, which represents the dissipative nature of a granular system; χ_c is the contact value of the equilibrium radial distribution function evaluated at the solid fraction ϕ; T is the granular particle temperature; and m is the mass of fine particles. Substituting for particle diffusivity from Eq. 4 into the expression for fluid diffusivity proposed by Friedlander (1957), the following relationship for ξ_1 can be obtained:

$$\xi_1 = \frac{1}{K\overline{\phi_s}\chi_c(K\overline{\phi_s})}, \tag{5}$$

where $\overline{\phi_s}$ is the mean solids fraction at the upper entrainment region; and K is the additional adjustable parameter where $K\overline{\phi_s}$ represents the time-averaged solid fraction around the coarse naphthalene particle. Using Eq. 5 to evaluate ξ_1 requires knowledge of χ_c. At this time an exact equation for χ_c in terms of solid fraction and particle diameter is not available. Therefore, the so-called Carnahan–Starling (1969) approximation, which is in almost exact agreement with the exact molecular dynamics calculations for values of volume fraction up to about 0.5, is used in the present study.

The weights and biases are initially assigned random values in the range $[-5\times10^{-2}, 5\times10^{-2}]$. Changing the absolute value of the initial weights and biases in the interval $[10^{-3}, 1]$ leads only to negligible changes in the performance of the prediction. Training is continued until the error goal, which is properly selected to avoid overtraining, is met. After the network is trained, a testing set is used to evaluate its performance. Perhaps a meaningful measurement of accuracy is the Pearson correlation coefficient (Fisher, 1970). It is worth noting that the learning and testing capabilities of a neural network depend on the size of the training set, which represents the number of associations between the input and output vectors on which the network has been trained. A network trained on a small training set memorizes patterns that are quite distinctive, and therefore may not be reliably generalized on the never-seen-before cases of the testing sets. In the present study, the network is trained with input vectors of size 36, that are selected randomly from the data set. To investigate the effect of the coefficient K on the mass-transfer rates, different sets of weights are generated by training the network on different training sets prepared by varying the coefficient K.



(a) **(b)**

Figure 2. (a) Sherwood numbers: experimental vs. calculated when training and testing data sets are predicted with the neural network in Figure 1 trained on the training data set, which includes 36 points, for the coefficient $K=10$; (b) experimental vs. from heuristic model data of Halder and Basu (1988).

The testing data set includes 9 points. Symbols and conditions are as follows: bed particle size 260 μm (training set □ and testing set ○); bed particle size 54 μm (training set ◇ and testing set -); bed particle size 260 μm (Halder and Basu, 1988) +; and bed particle size 54 μm (Halder and Basu, 1988) ×.

Results and Discussion

The experimental results of the Sherwood number, based on the sublimation rate of coarse naphthalene balls in fast fluidized beds of fine glass beads, are compared to those obtained using the trained network, which is shown in Figure 1, for the coefficient $K=10$ in Figure 2a. The excellent agreement of the results suggests that the present design can provide an accurate correlation for the mass-transfer coefficient in fast fluidized beds for the range of experimental conditions of Halder and Basu (1988). Figure 2b, on the other hand, represents the experimental results and those obtained from the heuristic model of Halder and Basu (1988). An overestimation of mass transfer for 260-μm fine particles and an underestimation for 54-μm particles indicate that in the boundary layer of the coarse naphthalene particle the flow regime is not fluid-dominated, but instead, that momentum transport due to collisions between particles plays the most important role in the particle motion. In a vertical riser of the circulating fluidized bed, the relative velocities between fine particles and the coarse naphthalene particle, which are induced by body forces, will lead to collisions between fines and the coarse particle. This causes an increase in the relative velocity between fines and the gas. The change in velocity of a fine particle after a collision therefore increases the probability of collisions between the fine particles. Consequently, fine particles, which would be expected to closely follow the motion of gas correlate poorly with the corresponding fluid elements, and as a result the response of particles to the motion of the gas is more or less limited to the influence of the gas on the mean velocity of the particle. In this condition, where the random component of the particle velocity is generated mainly by solid-body collisions between the particles, the particle diffusivity can be calculated using Eq. 4. There is, however, little reason to apply this relation in the cases where the process of mass transfer of gas from the coarse particle to the bulk is controlled by the diffusional motion of clusters (Zamankhan, 1997).

When viewed on a local scale, say on the order of fine-particle dimension, the random motion of the fluid elements and those of particles are coupled via a constraint like the approximation proposed by Friedlander (1957) for massive particles. This sheds more light on the significance of the proposed expression, Eq. 5 for the input ξ_1. However, a rigorous treatment of gas–particle suspension flows over a large spherical obstacle is needed to provide knowledge essential for the understanding of the mechanism of mass transfer from a coarse particle to a fast bed of fine solids.

The effect of coefficient K on the mass-transfer rate predictions is examined by training the network on different training sets prepared by varying the coefficient K. This results in the generation of different sets of weights and biases for the network. The performance of the network with the coefficient $K=10$ is compared to that with the coefficient $K=3$ for 54-μm particles. The experimental results of the Sherwood number are compared to those obtained using the trained network with different coefficients K in Figures 2a and 3. The excellent agreement of results suggests that the variations of coefficient K might not exceed the predictive capacity of the neural network. However, the smaller success of the trained network with the coefficient $K=3$ in predicting mass-transfer coefficients in the relevant superficial gas-

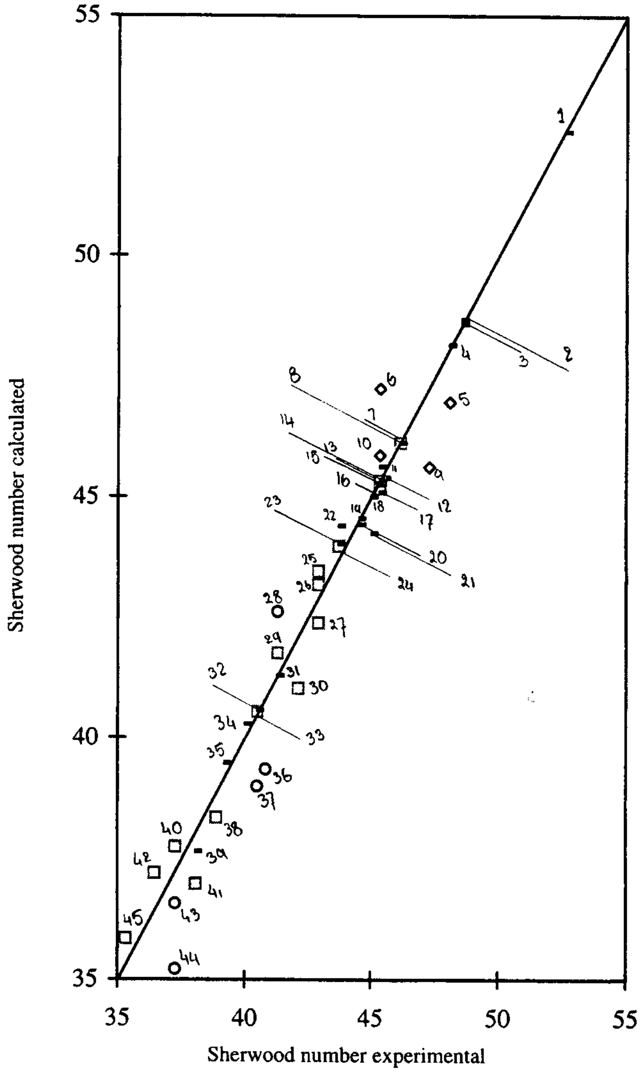


Figure 3. Sherwood numbers: experimental vs. calculated when training and testing data sets are predicted with the neural network in Figure 1 trained on the training data set, which includes 36 points, for the coefficient $K=3$.

The testing data set includes 9 points. Symbols and conditions are as follows: bed particle size 260 μm (training set □ and testing set ○); and bed particle size 54 μm (training set ◇ and testing set -).

velocity range compared to that of the network with the coefficient $K=10$ (the results are given in Figures 4 and 5), suggests that mass-transfer parameters in a fast bed of fines cannot be successfully extrapolated using the lower values of coefficient K. This suggessts the possibility that a network design using higher values of coefficient K might supply a more efficient correlation for the mass-transfer coefficient from the existing data set, although further testing of this possibility is required. It is worth noting that the proposed empirical method may yield large errors when it is used to extrapolate far outside the range of the experiments on which it is trained. The advantage of the heuristic model of Halder and Basu (1988) is that it can be extrapolated to different operating conditions. Results of additional experiments similar to those

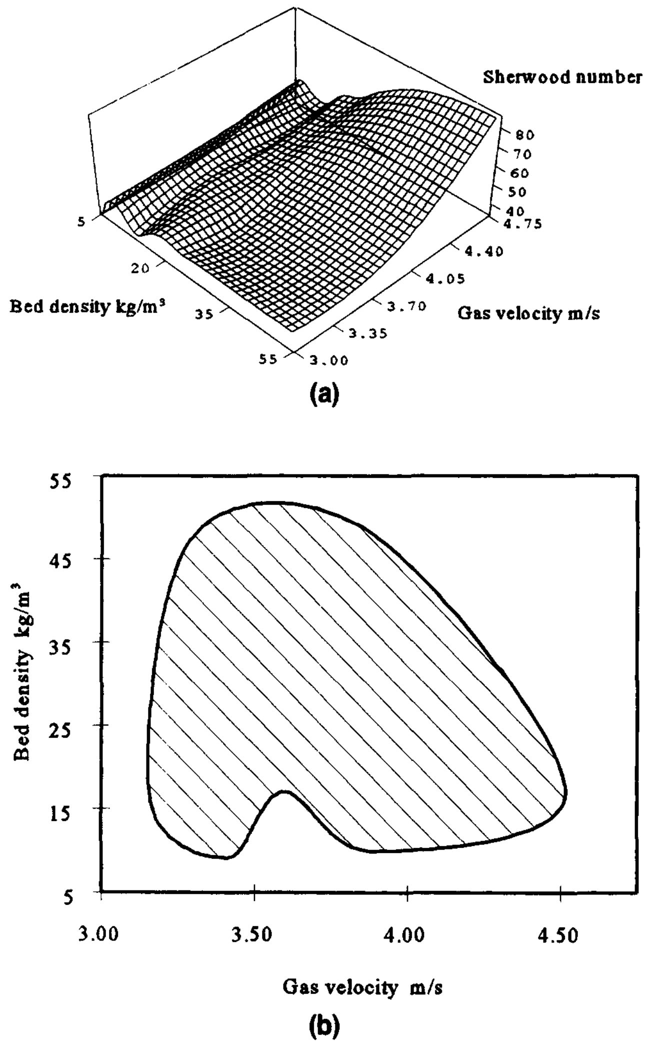


Figure 4. Parametric variation of the calculated Sherwood number for: (a) bed particle size 54 μm and coefficient $K = 3$; (b) shaded area that represents the training domain in the gas-velocity bed-density plane for the same bed particle size.

of Halder and Basu are needed for a wide range of flow conditions so that the network can be better trained.

Conclusions

Existing heuristic models for the mass transfer from a coarse particle to the bulk of a fast bed of fines have been analyzed. It has been found that the hydrodynamic behavior of a large particle under fast-fluidized bed conditions is dominated by particle–particle collisions. It is, however, unclear how to supply the rigorous treatment of particulate flows over a coarse particle that could lend insight into the complexity of this problem and strategies for overcoming it. The back-propagation, feed-forward artificial neural network is therefore proposed for dealing with this system. The primary benefit of this neural network is that a more accurate correlation can be obtained using much fewer computational resources

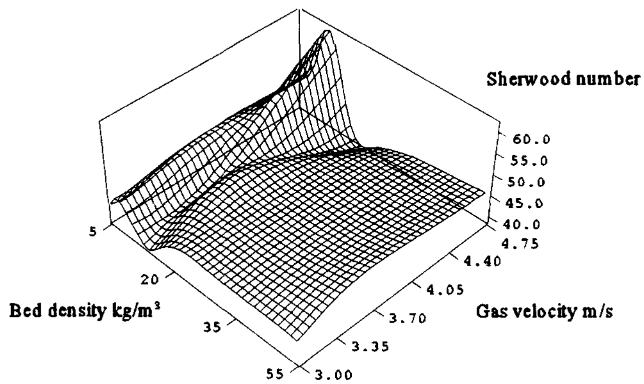


Figure 5. Parametric variation of the calculated Sherwood number for bed particle size 54 μm and coefficient $K = 10$.

compared to the currently used heuristic models. Although the success of a neural network is limited by the size of data set, this work demonstrates that the present network design can positively impact generalization. However, the small size of the training data set could lead to large extrapolation errors. In the future, this approach will be used to investigate mass-transfer parameters in fluidized beds for which more experimental results are available.

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