Neural Network Modeling of Structured Packing Height Equivalent to a Theoretical Plate

Gregory S. Pollock and R. Bruce Eldridge*

Separations Research Program (Mail Code R7100), The University of Texas at Austin, Austin, Texas 78758

The height equivalent to a theoretical plate (HETP) of nine types of structured packing was successfully modeled using a neural network. The network was trained on data similar to that used to develop semiempirical mass-transfer models. The HETP was then predicted using the trained network. The neural network model yields a very accurate prediction of experimentally determined HETP values, and it is more accurate than a traditional semiempirical model. Using the neural network, it is also possible to rank the relative importance of input variables in determining the HETP. In particular, this work shows that the roughness of the structured packing surface is a very important input parameter.

Introduction

The height equivalent to a theoretical plate (HETP) is a key parameter for describing mass-transfer efficiency in structured packing. Column designers use the HETP to calculate the height of packing necessary to achieve a given separation. The HETP depends on the geometry of the packing, the physical properties of the chemical system, and the operating conditions of the column.

In a previous paper, Whaley et al.[1] first examined the applicability of neural network technology to modeling HETP. Their data contained only four types of packing, all from the same manufacturer and with the same specific surface area. This paper provides a similar treatment of neural network modeling of HETP over a considerably larger scope of data, including nine packings from three manufacturers and more than 600 data points. This enhanced packing database provides a more complete evaluation of the neural network approach. It also allows a detailed investigation of the parameters which impact the performance of structured packing in distillation service. The data were collected on a cyclohexane/*n*-heptane system at the University of Texas Separations Research Program. A listing of all tested packings is presented as Table 1.

Neural Network Model

A neural network model is essentially a curve fit in multidimensional space, with the number of dimensions equal to the number of input variables for the model. Details of the fundamentals of neural networks are available elsewhere.[2] For purposes of the present study, the network was trained for 50 cycles (or epochs) using the conjugate gradient algorithm. The number of hidden nodes and the training time were both optimized by cross validation, or training on different sections of the data set in turn and averaging the results. Initially, the model used 15 input variables to describe the physical properties of the system and the structural properties of the packing. The input variables, which are the same for traditional semiempirical models, are listed in Table 2.

* To whom correspondence should be addressed. Phone: (512) 471-7067. Fax: (512) 471-1720. E-mail: rbeldr@che.utexas.edu.

Table 1. Packing Characteristics

name	specific area (1/m)	crimp angle (deg)	surface	no. of points
Koch Flexipac 2	223	45	not perforated	121
Montz B1-250	244	45	not perforated	29
Montz B1-250.60	244	60	not perforated	31
Montz B1-400	394	45	not perforated	42
Montz B1-400.60	394	60	not perforated	29
Montz BSH-400	378	45	perforated	60
Montz BSH-400.60	382	60	perforated	129
Norton Intalox 1T	312	47	perforated	4
Norton Intalox 2T	214	46	perforated	157

The data were divided into training and testing sets, to evaluate the network with fresh data that was not used to train the network. The training set was also randomized and normalized to similar magnitudes, to keep the network from initially biasing toward certain groups of points or input variables. A parity plot of model-predicted HETP vs the experimentally measured value for all points in the testing set appears as Figure 1.

It is well-known that when the vapor velocity exceeds a threshold value, the hydraulics in the column change drastically, and the column is considered to be "flooding". Columns are not operated above the flooding velocity because of poor mass-transfer rates and high pressure drop. Because data taken under flooding conditions generally cannot be modeled accurately, any data points that exhibited an order of magnitude increase in pressure drop with a slight increase in velocity were discarded from the training and testing sets. Training and testing only on data below the flood point resulted in a more accurate model, as shown by the parity plot in Figure 2.

Comparison with Physical Models

The performance of the neural network was compared with the performance of an accepted traditional model, the Rocha−Bravo−Fair model.[3,4] Our comparison shows that the neural network model predicts HETP for this data set better than the Rocha−Bravo−Fair model, a semiempirical model based on the two-film theory of mass transfer. The root-mean-square (RMS) error for the Rocha−Bravo−Fair model is 7.53, compared to a

10.1021/ie9908128 CCC: $19.00
Published on Web 04/13/2000

Table 2. Input Variables

variable	units	variable	units	variable	units
vapor velocity	m/s	vapor viscosity	kg/m·h	slope of eq. line	
liquid velocity	m/s	liquid viscosity	kg/m·h	specific area	m^2/m^3
vapor density	kg/m^3	vapor diffusivity	m^2/h	void fraction	
liquid density	kg/m^3	liquid diffusivity	m^2/h	perforation	
surface tension	dyn/cm	relative volatility		crimp angle	deg

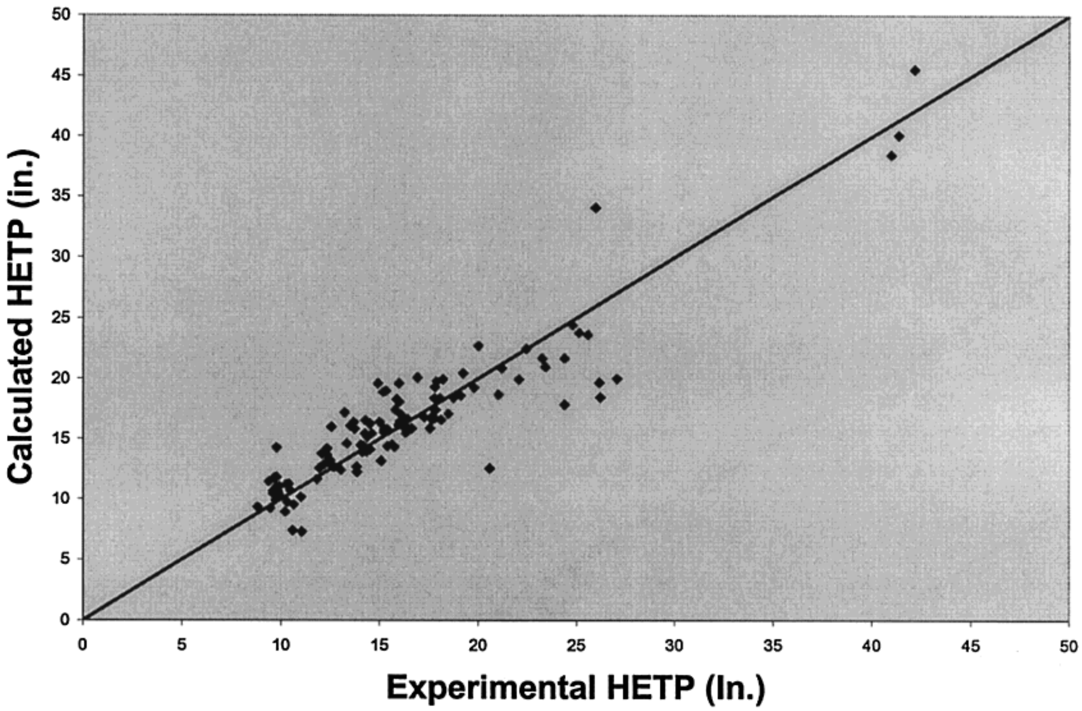

Figure 1. Parity plot for test data set (without any training data).

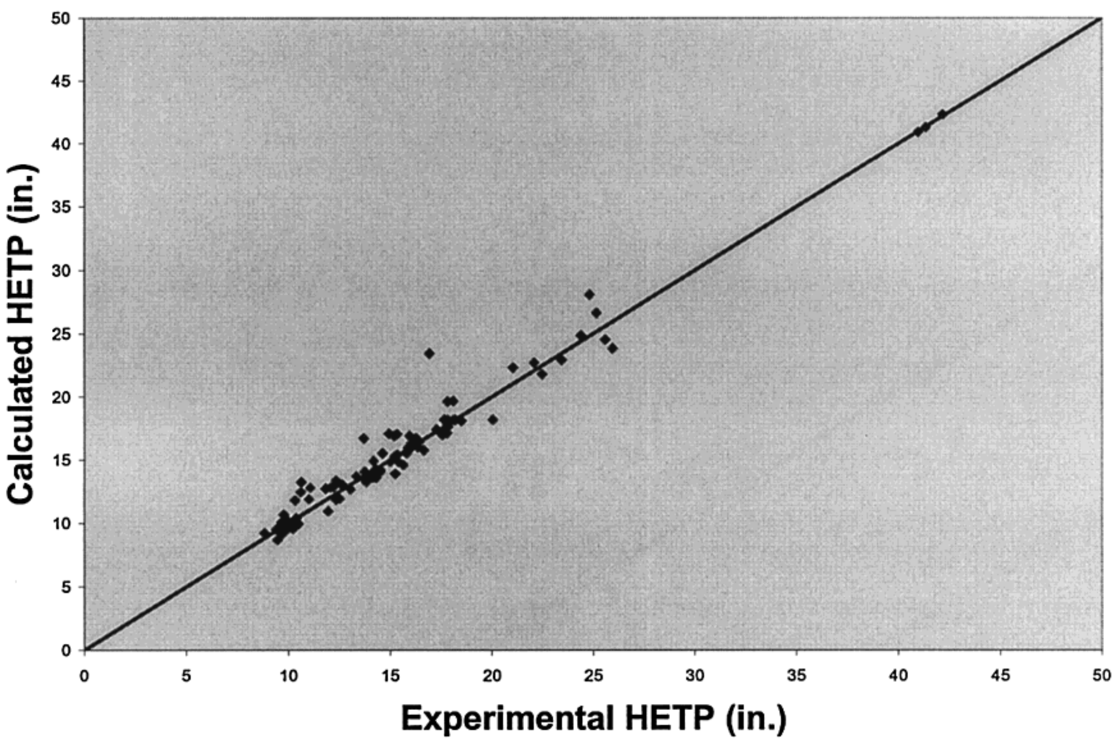

Figure 2. Parity plot for test data below flooding velocity (without any training data).

rms error of 1.15 for the neural network model. Both errors were calculated with data below flooding conditions. As demonstrated in Figure 3, the Rocha–Bravo–Fair model consistently underpredicts the HETP for most of the data collected for this study. One disadvantage of the purely empirical neural network model is that it is less accurate when trying to predict HETP for a type of packing significantly different from the packing

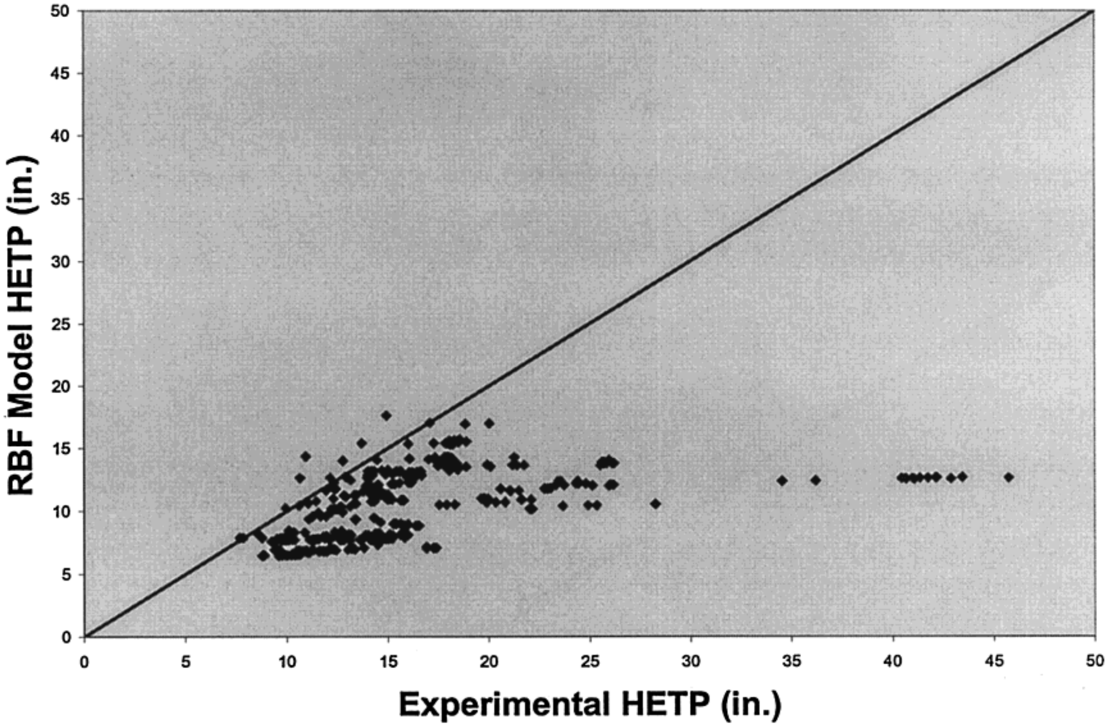

Figure 3. Parity plot for the Rocha–Bravo–Fair model.

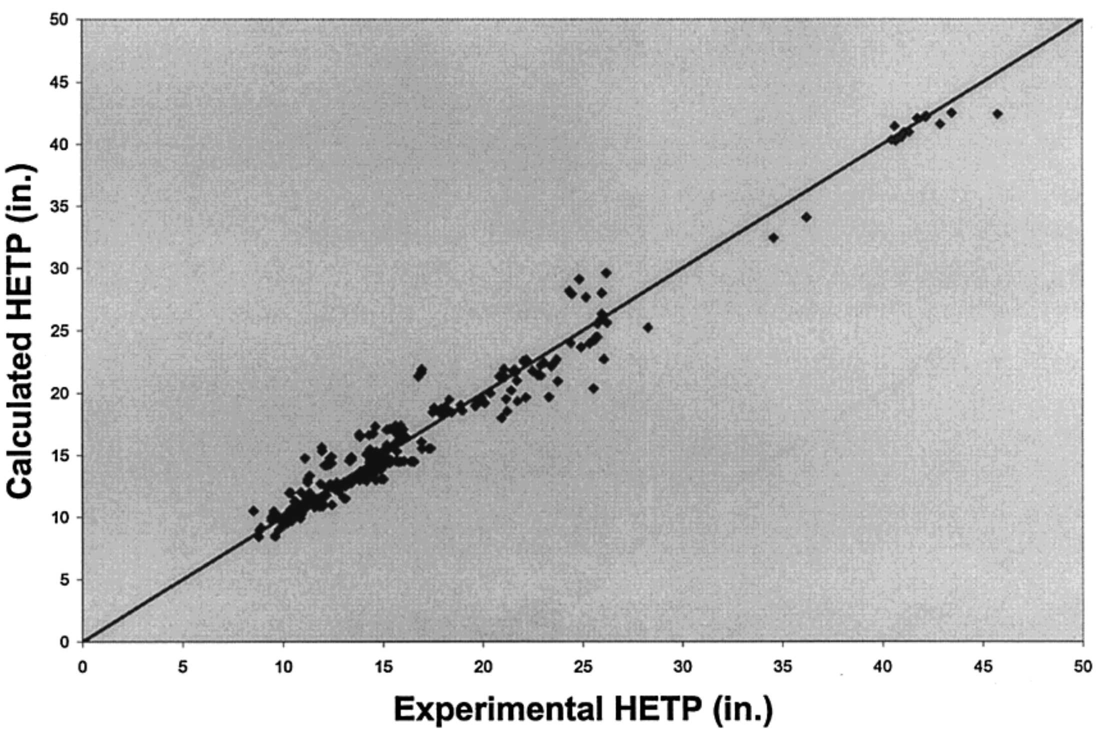

Figure 4. Parity plot for rough packing trained with a surface parameter (rms = 1.25).

used to train the network. This theoretical flaw was experimentally confirmed by training the network without any data for a specific type of packing and then testing on data for that packing, with usually unsatisfactory results. However, the neural network model clearly maintains a better fit as long as the training set characterizes the system of interest.

Surface Effects

It has long been known that the surface of structural packing has a large effect on the HETP of the system. This correlation is quite evident when attempting to describe HETP using a neural network model. To demonstrate this, the packings used in this study were divided into two classes—"smooth" and "rough"—and the data were fit three different ways with respect to this designation. First, the network was trained on both smooth and rough packing, and a parameter was used to distinguish between the two types of packing. A parity plot for this model with a surface parameter appears as Figure 4. The network was again trained on smooth and rough packing, but no parameter was

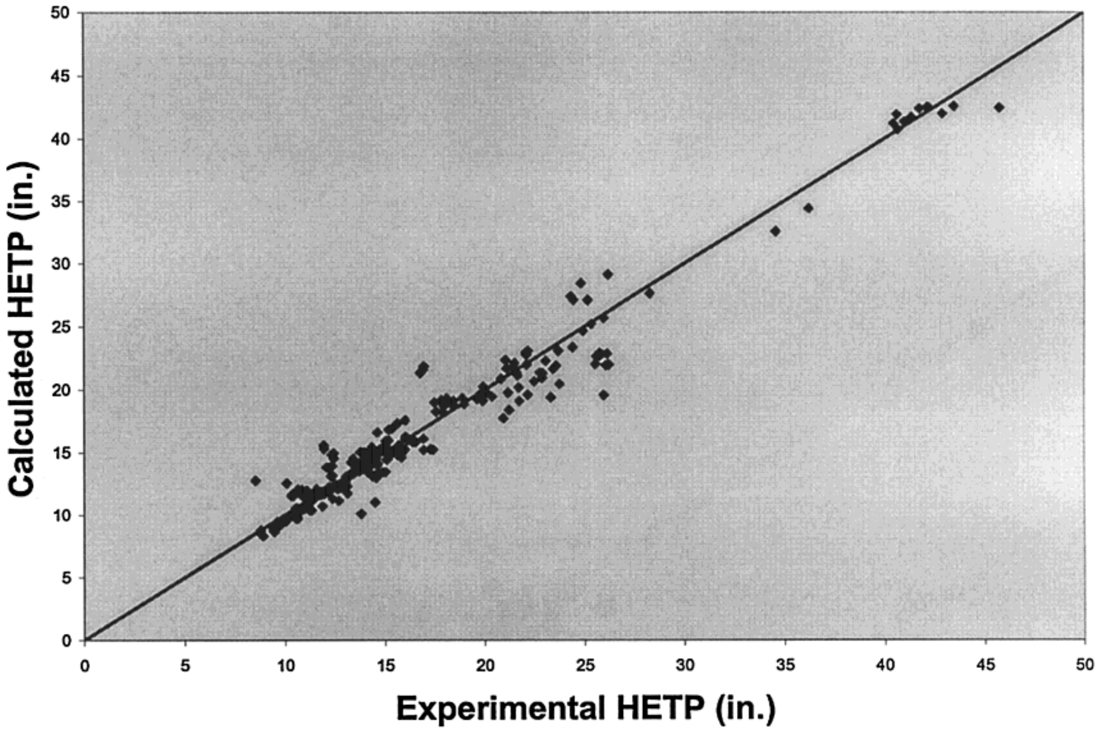

Figure 5. Parity plot for rough packing trained without a surface parameter (rms = 1.33).

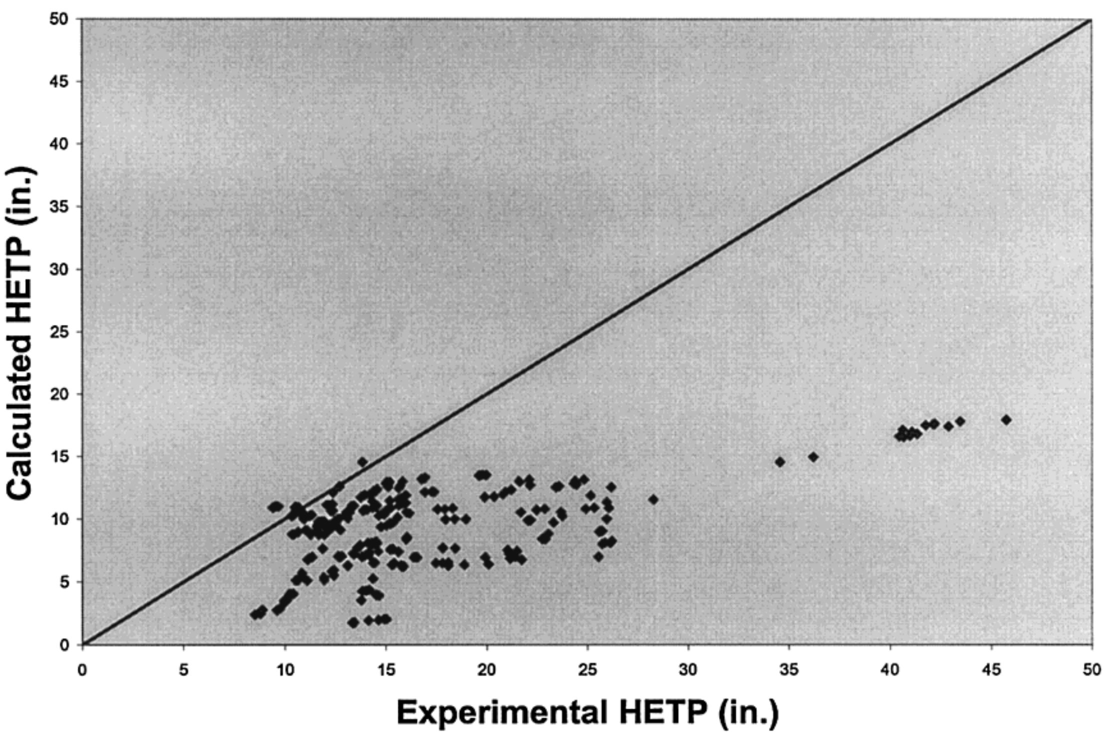

Figure 6. Parity plot for rough packing trained on smooth packing (rms = 7.36).

used to distinguish between the two types of packing. The accuracy of this model suffered slightly, with the rms error increasing from 1.25 to 1.33. A parity plot for the model without a surface parameter appears as Figure 5. Finally, the network was trained on only smooth packing and then tested on only rough packing. A parity plot for this model appears as Figure 6. Clearly, the quality of the curve fit decreases sharply from Figures 4 to 6, indicating that the effect of surface roughness cannot be ignored when creating a model for HETP.

Sensitivity Analysis

In work by Bode and Whaley, the input variables for predicting HETP were narrowed to the seven most critical by using the finite difference method to perform a sensitivity analysis. This exercise was repeated for our larger data set and yielded a different set of critical inputs. Although Bode and Whaley highlighted the sensitivity of their network toward the corrugation angle, that phenomenon was not noted for this network, primarily because our data set contained a wider

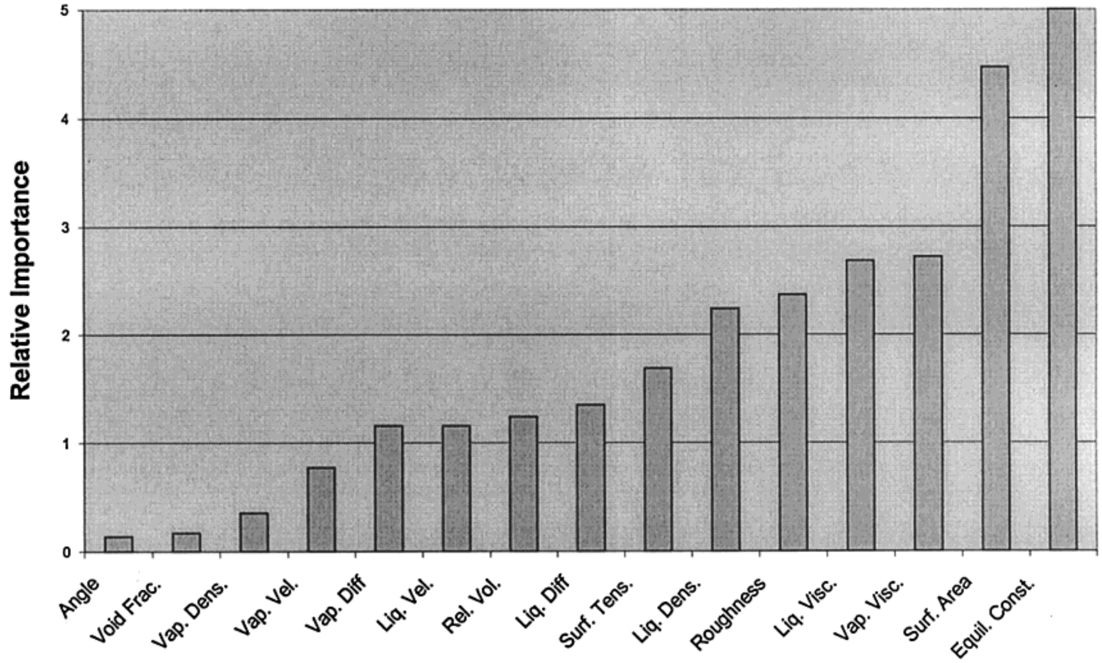

Figure 7. Relative importance of input variables.

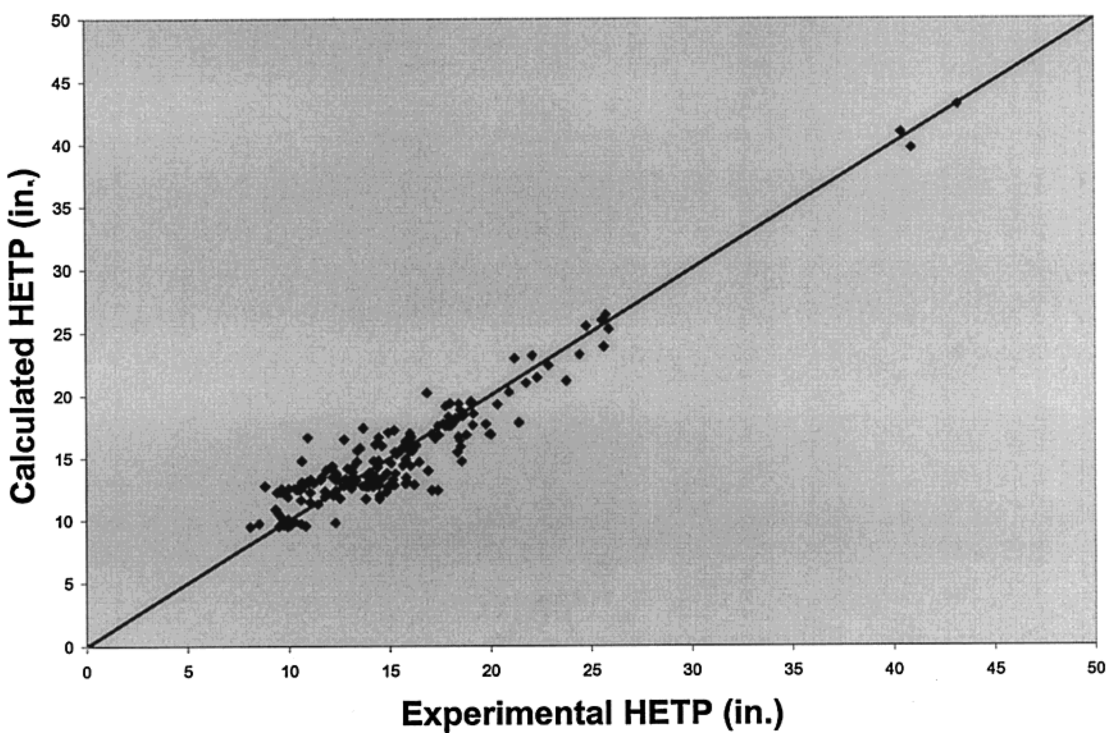

Figure 8. Parity plot for a network retrained with the top six input variables.

variation among other packing parameters such as specific area. With the larger data set, the network became more complicated, and the sensitivity of the network toward each variable was harder to interpret. However, the network did consistently show a significantly higher sensitivity toward the following six variables, as shown in Figure 7: liquid density, liquid viscosity, vapor viscosity, equilibrium constant (operating pressure), specific area, and roughness factor of the packing. The neural network was retrained using only these six inputs, and a parity plot for this network appears in Figure 8. Although the fit is not as tight as that with all 15 variables, it represents a simpler model for which the data may be more easily obtained. The sensitivity analysis highlights what appear to be the most critical factors in determining HETP, although some skepticism is warranted considering their change with the larger data set.

Conclusions and Future Work

This work illustrates that a neural network can be used to predict HETP in distillation columns with structured packing. With a large enough set of training data, the neural network appears to extrapolate to similar packing types outside the set. The neural network performs substantially better than the traditional Rocha–Bravo–Fair model, although both have problems in the flooding regime. A sensitivity analysis yielded the six most important network input variables from the original 15 variables. A simplified model based on these six inputs still predicted HETP with reasonable accuracy. The neural network also highlighted the importance of the surface roughness in the determination of HETP. It is vitally important to include data from packing with a similar surface in the training set to obtain an accurate prediction of HETP.

The comparative performance on other chemical and packing combinations, especially on an industrial scale, needs to be evaluated to determine the overall performance and applicability. Although network performance for types of packing within the training set are positive, the limits of applicability from one packing type to another need to be examined further. Finally, more sensitivity analysis may help refine physical models and improve the understanding of this important step in the design of distillation columns.

Acknowledgment

The NetLab package from Aston University was used for most of the simulations reported. The authors thank the Separations Research Program for both their data supply and financial support.

Literature Cited

(1) Whaley, A. K.; Bode, C. A.; Ghosh, J.; Eldridge, R. B. HETP and Pressure Drop Prediction for Structured Packing Distillation Columns Using a Neural Network Model. *Ind. Eng. Chem. Res.* **1999**, 38 (4), 1736−1739.

(2) Mehrotra, K.; Mohan, C. K.; Ranka, S. *Elements of Artificial Neural Networks*; MIT Press: Cambridge, MA, 1997.

(3) Rocha, J. A.; Bravo, J. L.; Fair, J. R. Distillation Columns Containing Structured Packings: A Comprehensive Model for their Performance. 1. Hydraulic Models. *Ind. Eng. Chem. Res.* **1993**, *32* (4), 641−651.

(4) Rocha, J. A.; Bravo, J. L.; Fair, J. R. Distillation Columns Containing Structured Packings: A Comprehensive Model for their Performance. 2. Mass Transfer Model. *Ind. Eng. Chem. Res.* **1996**, *35* (5), 1660−1667.

Received for review November 11, 1999
Revised manuscript received February 29, 2000
Accepted March 16, 2000

IE9908128