HETP and Pressure Drop Prediction for Structured Packing Distillation Columns Using a Neural Network Model

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A neural net framework was used to predict the mass-transfer and hydraulic performance of a commercial structured packing operating in distillation service. The results indicated that the approach produced a more accurate prediction than a traditional semiempirical model. The neural net methodology was also used to yield a detailed sensitivity analysis of the operating variables.

Background

The mass-transfer performance of a commercial structured packing is traditionally expressed as a height equivalent to a theoretical plate (HETP). This is the height of packing required to produce a separation identical in composition to that of an ideal device in which the exiting vapor and liquid are in thermodynamic equilibrium. The HETP value is used in combination with the predicted pressure drop performance to fix the design for a commercial packed distillation column.

Various semiempirical models have been proposed to predict structured packing mass-transfer and hydraulic performance. Lockett (1998) conducted a detailed evaluation assessment of various algorithms and concluded that the model of Rocha et al. (1996a,b) provided the most accurate, fundamentally sound, prediction of HETP and pressure drop. Structured packings consist of a system of regularly ordered crimped plates with well-defined flow channels. Semiempirical models used to predict mass-transfer and hydraulic performance take advantage of this degree of uniformity by introducing geometry-dependent parameters. The Rocha−Bravo−Fair model incorporates packing geometry, fluid physical properties, and flow parameters to yield the following predictive expressions:

Effective mass-transfer area (a_e)

$$\frac{a_e}{a_p} = F_{se}\frac{29.12(We_L Fr_L)^{0.15}S^{0.359}}{Re_L{}^{0.2}\epsilon^{0.6}(1 - 0.93\cos\gamma)(\sin\theta)^{0.3}} \tag{1}$$

Mass-transfer coefficients (k_l, k_g)

$$k_l = 2.0\{(D_L C_E U_{Le})/(\pi S)\}^{0.5} \tag{2}$$

$$k_g S/D_G = 0.054\{U_{ge} + U_{Le})\rho_g S/\mu_g\}^{0.8}(\mu_g/D_g\rho_g)^{0.33} \tag{3}$$

HETP

$$\mathrm{HETP} = \{U_{gs}/k_g a_e + \lambda U_{gs}/k_l a_e\}\{\ln\lambda/(\lambda - 1)\} \tag{4}$$

The Rocha−Bravo−Fair model, like all similar semiempirical models, is computationally complex and requires many inputs and intermediate calculations (Rocha et al., 1996a,b). It also relies on experimentally determined factors for each different packing and chemical system. Thus, this application seems suitable for data-driven nonlinear modeling approaches such as certain artificial neural networks. This paper presents a thorough investigation of the suitability of a neural net based approach (MLP) for this problem. A useful side effect of this approach is that the receptive fields of the hidden units can be inspected and a sensitivity analysis can be performed to reevaluate the usefulness of the input parameters used in the traditional model. Traditional models are only strictly valid for chemical systems that have similar properties, and similarly a neural network model is only valid for systems that are reasonably characterized by the training data.

The data set used to train and test the network is a data set that was collected at The Separations Research Program, The University of Texas, as part of a program for testing structured packing (Garcia et al., 1995, 1996). The data set consists of 240 data points for a cyclohexane/*n*-heptane system. The data include HETP and pressure drop values for four different operating pressures (0.33, 1.03, 1.65, and 4.14) and for the four types of Montz structured packings (see Table 1).

The data set includes the physical properties of the mixture for each operating pressure, the packing characteristics, and the experimental HETP and pressure drop values. Initially, the neural network was based on the same 15 inputs (see Table 2) as the traditional model. Subsequent sensitivity analysis led to a substantial reduction in the number of inputs.

Neural Network Model for Predicting HETP

We used an MLP with 10 hidden units, each with a tanh activation function, and one linear output unit to

Table 1. Packing Characteristics

name	specific area (1/m)	crimp angle of packing (deg)	surface treatment
Montz B1-400	400	45	perforated
Montz B1-400.60	400	60	perforated
Montz BSH-400	400	45	not perforated
Montz BSH-400.60	400	60	not perforated

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Table 2. Input Variables

input	units	input	units	input	units
vapor velocity	m/s	vapor density	kg/m^3	slope of equilibrium line	
liquid velocity	m/s	vapor diffusivity	m^2/h	perforation	
liquid diffusivity	m^2/hr	vapor viscosity	kg/(m h)	specific area	1/m
liquid density	kg/m^3	surface tension	dyn/cm	void fraction	
liquid viscosity	kg/(m h)	relative volatility		crimp angle	deg

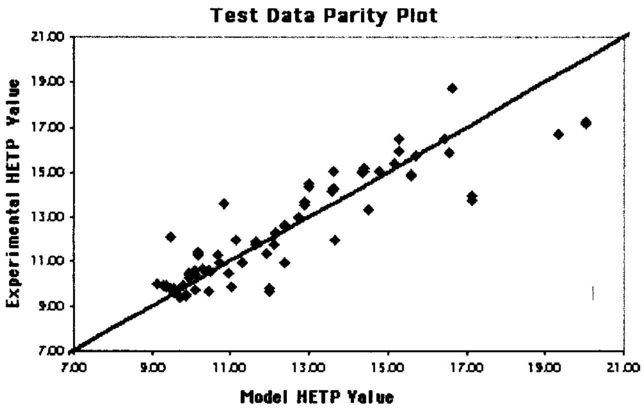


Figure 1.

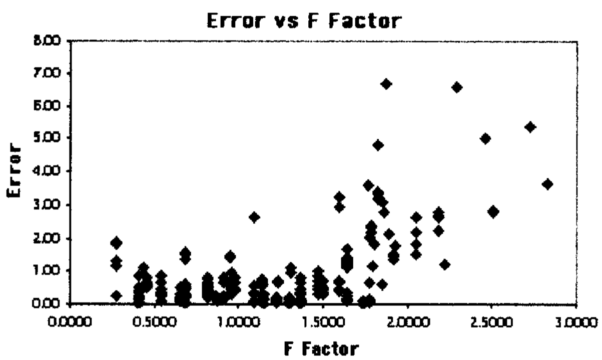
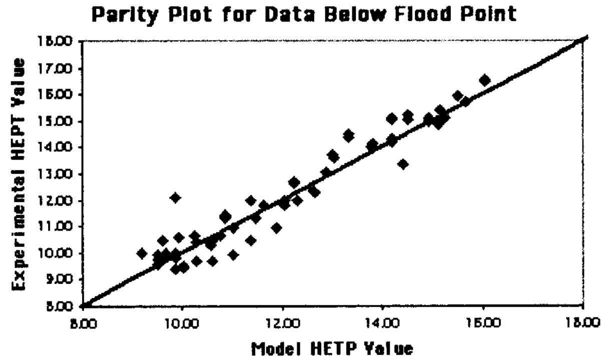


Figure 2.



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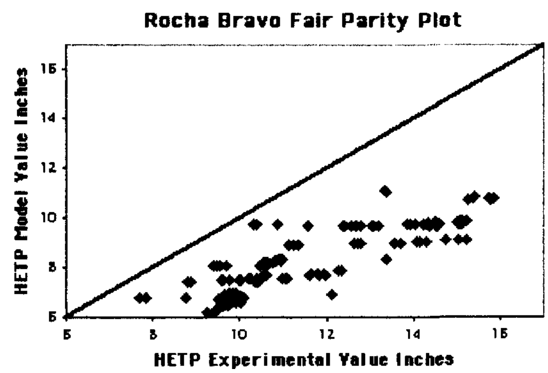

Figure 4.

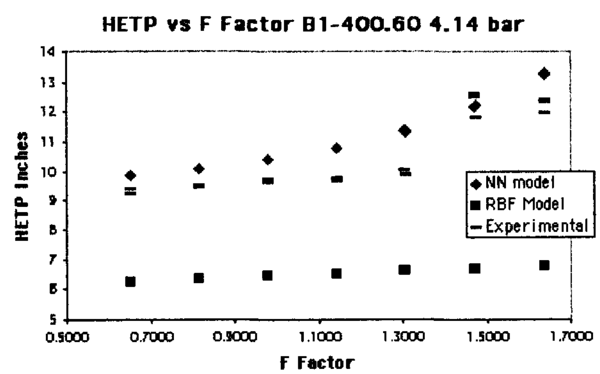

Figure 5.

yield HETP in inches. The network was trained for 30 epochs using the conjugate gradient algorithm. Cross validation was used to determine the network size and number of hidden units. The parity plot for model prediction vs experimental value is shown in Figure 1. From the physics of the system, it is well-known that when the F factor is larger than 1.75, a column is considered to be "flooding". When a column floods, the hydraulics in the tower change considerably and the mass-transfer capability of the system decreases. Because of this poor mass-transfer performance, columns are not operated above the flood point. Therefore, we plotted error vs F factor (Figure 2) and noticed that the error is generally higher for systems with F factors above 1.75. Training and testing only on data with $F < 1.75$ results in a more accurate model (Figure 3).

Comparison with Physical Models

The performance of the neural network was compared to the performance of the traditional model of Rocha–Bravo–Fair model (Rocha et al., 1996a,b). The comparison shows that the MLP predicts the HETP for this data set more accurately than the traditional model does. The root-mean-square (rms) error of the Rocha–Bravo–Fair model is 4.84 compared to a rms error of 1.39 for the neural net model. The parity plot for the Rocha–Bravo–Fair model (Figure 4) indicates that it consistently predicts HETP values that are lower than the experimental values. Also, the Rocha–Bravo–Fair model predicts very little change in the HETP value for different F factor values (different vapor and liquid velocities). This is contrary to the results of the sensitivity analysis for the neural network, which indicates that vapor and liquid velocities are key inputs for the HETP prediction network. To further illustrate the difference in performance of the Rocha–Bravo–Fair model and the neural network model, HETP for each packing/pressure combination was plotted versus F factor. A representative plot is shown in Figure 5. The plot illustrates that the experimental HETP value and neural network model prediction increase with increasing F factor (increasing vapor velocity) and that the Rocha–Bravo–Fair model prediction is lower and relatively flat. The

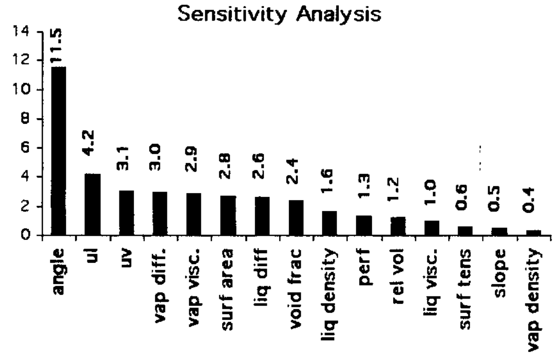

Figure 6.

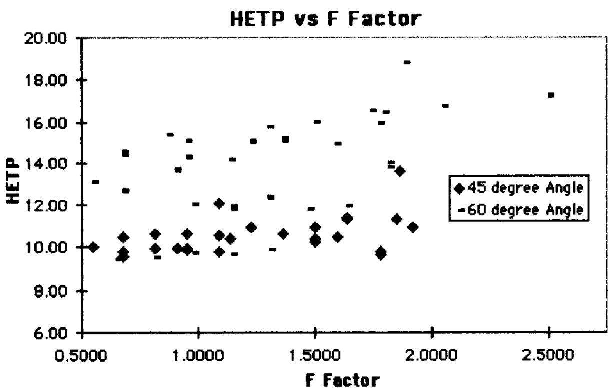

Figure 7.

result was similar for all of the packing and pressure combinations.

Sensitivity Analysis

The next modeling challenge undertaken was to simplify the input space. The impetus for this comes not from a more manageable network but from the actual implementation of the model on experimental data. A model that uses fewer input parameters reduces the amount of data necessary to collect and store. Additionally, the model would have more universal applicability because different researchers and design engineers may possess data for the simplified model while not having a complete data set.

The sensitivity of the output, HETP, to each input was found by using the finite difference method. The average impact of each variable is shown in Figure 6. The results agreed with accepted theoretical models with a few exceptions. The crimp angle proved to have the greatest impact on the HETP prediction. Conventional wisdom says that the crimp angle should be important, but not to the degree shown in the analysis. To examine this result, experimental HETP was plotted against *F* factor for each of the two angles in the data. The results, shown in Figure 7, indicate that a marked difference in the performance of the packing exists for different crimp angles of the packing. The liquid and vapor velocities are also important inputs, ranking second and third in sensitivity values. The Rocha–Bravo–Fair model includes these inputs, but the model is not sensitive to changes in these velocities. The traditional model depends more strongly on the physical properties and therefore predicts basically one HETP value for each packing–pressure combination. The error of the traditional model increases as these velocities increase. This effect is illustrated in Figure 5. The

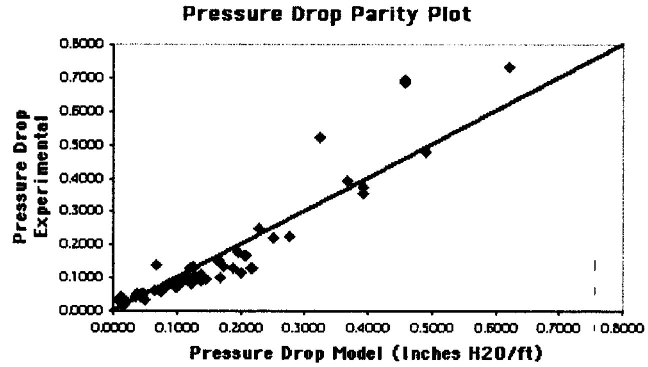

Figure 8.

sensitivity study results were also used to reduce the number of inputs. The model was reduced to the seven inputs with the highest sensitivity values. These inputs include the vapor velocity, the liquid velocity, the vapor diffusivity, the vapor viscosity, the packing surface area, and the liquid diffusivity. This reduced model performed as well as the model with the full input set.

Predicting Pressure Drop

The calculation of column pressure drop in theoretical models is a precursor to the calculation of HETP and is useful in designing a distillation system. The pressure drop was modeled using the same 15 inputs, using an MLP with 10 hidden units, trained for 120 epochs. Cross validation results indicated that the pressure drop network needed to train for longer than the HETP network to obtain satisfactory results. The parity plot for the pressure drop model is pictured in Figure 8.

Again, the results are satisfactory and superior to those obtained by physical models. The use of a single network to predict both pressure drop and HETP is currently being investigated.

Conclusions and Future Work

This work illustrates that MLPs can be used to predict HETP and pressure drop for distillation columns packed with structured packing. The prediction is best if pressure drop and HETP are modeled with two separate networks. Also, the neural network appears to extrapolate well to similar packing types that are not included in the training data set. The neural network performed substantially better than the traditional Rocha–Bravo–Fair model, though both have problems in the flooding regime ($F > 1.75$). A sensitivity analysis was used to select the most important network inputs from the 15 inputs initially used. This analysis was useful and provided insight into the importance of the physical characteristics of the system. The analysis also allowed the inputs to be reduced from 15 to 7 inputs with little difference in model accuracy and also highlighted the importance of the packing crimp angle.

Comparative performance on other chemical and packing combinations should be evaluated to determine the overall performance and applicability. The limits of applicability of models developed for one set of packings to another packing type will be examined in the future. Finally, the sensitivity analysis may point to simpler and improved physical models and an overall better understanding of this important step in the design of distillation columns.

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Nomenclature for the Rocha−Bravo−Fair Model

a_e = effective area (1/m)
a_p = packing surface area (1/m)
F_{se} = Rocha−Bravo−Fair factor for surface enhancement
We_L = Weber number for the liquid
Fr_L = Froude number for the liquid
S = side dimension of corrugation (m)
Re_L = Reynolds number for the liquid
ϵ = void fraction of packing
γ = contact angle (deg)
θ = angle with horizontal for falling film or corrugation channel (deg)
k_L = mass-transfer coefficient, liquid phase (m/s)
k_g = mass-transfer coefficient, gas phase (m/s)
D_L = diffusion coefficient, liquid phase (m^2/s)
D_g = diffusion coefficient, gas phase (m^2/s)
C_E = correction factor for surface renewal
U_{LE} = effective liquid velocity (m/s)
U_{ge} = effective gas velocity (m/s)
ρ_g = gas density (kg/m^3)
μ_g = gas density (kg/m·s)
U_{gs} = superficial gas velocity (m/s)
λ = ratio of slopes, operating line to equilibrium line
HETP = height equivalent to a theoretical plate (m)

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