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)

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

Mass-transfer coefficients (k_L, k_G)

$$k_L = 2.0[(D_L C_E U_{Le})/(\pi S)]^{0.5} \quad (2)$$

$$k_G S/D_G = 0.054[(U_{Ge} + U_{Le})\rho_G S/\mu_G]^{0.8}(\mu_G/D_G\rho_G)^{0.33} \quad (3)$$

HETP

$$HETP = [(U_{Gs}/k_G a_e) + \lambda(U_{Ls}/k_L a_e)][\ln\lambda/(\lambda - 1)] \quad (4)$$

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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Don W. Green,Marylee Z. Southard

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