

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 (1990) 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_d)

$$\frac{a_d}{a_s} = F_{\text{eff}} \frac{29.12(W_b V_f r_{\text{eff}})^{0.17} S^{0.188}}{Re_L^{0.2} Sc^{0.23} (1 - 0.93 \cos \gamma) (\sin \theta)^{0.2}} \quad (1)$$

Mass-transfer coefficients (k_L, k_G)

$$k_L = 2.0 [(D_L C_L U_{\text{eff}}) / (\nu + S)]^{0.33} \quad (2)$$

$$k_G S i D_{\text{eff}} = 0.054 [U_{\text{eff}} + U_{\text{eff}} / \nu S (\nu + S)]^{0.33} \nu^{0.2} D_{\text{eff}}^{0.2} \quad (3)$$

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HETP

$$\text{HETP} = (U_{\text{eff}} / k_L a_d + \lambda U_{\text{eff}} / k_G a_d) [\ln \lambda / (\lambda - 1)] \quad (4)$$

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-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 B5M-400	400	45	not perforated
Montz B5M-400-60	400	60	not perforated

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Table of Contents Hetp And Pressure Drop Prediction For Structured Packing

1. Understanding the eBook Hetp And Pressure Drop Prediction For Structured Packing
 - The Rise of Digital Reading Hetp And Pressure Drop Prediction For Structured Packing
 - Advantages of eBooks Over Traditional Books
2. Identifying Hetp And Pressure Drop Prediction For Structured Packing
 - Exploring Different Genres
 - Considering Fiction vs. Non-Fiction
 - Determining Your Reading Goals
3. Choosing the Right eBook Platform
 - Popular eBook Platforms
 - Features to Look for in an Hetp And Pressure Drop Prediction For Structured Packing
 - User-Friendly Interface
4. Exploring eBook Recommendations from Hetp And Pressure Drop Prediction For Structured Packing
 - Personalized Recommendations
 - Hetp And Pressure Drop Prediction For Structured Packing User Reviews and Ratings
 - Hetp And Pressure Drop Prediction For Structured Packing and Bestseller Lists

5. Accessing Hetp And Pressure Drop Prediction For Structured Packing Free and Paid eBooks
 - Hetp And Pressure Drop Prediction For Structured Packing Public Domain eBooks
 - Hetp And Pressure Drop Prediction For Structured Packing eBook Subscription Services
 - Hetp And Pressure Drop Prediction For Structured Packing Budget-Friendly Options
6. Navigating Hetp And Pressure Drop Prediction For Structured Packing eBook Formats
 - ePub, PDF, MOBI, and More
 - Hetp And Pressure Drop Prediction For Structured Packing Compatibility with Devices
 - Hetp And Pressure Drop Prediction For Structured Packing Enhanced eBook Features
7. Enhancing Your Reading Experience
 - Adjustable Fonts and Text Sizes of Hetp And Pressure Drop Prediction For Structured Packing
 - Highlighting and Note-Taking Hetp And Pressure Drop Prediction For Structured Packing
 - Interactive Elements Hetp And Pressure Drop Prediction For Structured Packing
8. Staying Engaged with Hetp And Pressure Drop Prediction For Structured Packing
 - Joining Online Reading Communities
 - Participating in Virtual Book Clubs
 - Following Authors and Publishers Hetp And Pressure Drop Prediction For Structured Packing
9. Balancing eBooks and Physical Books Hetp And Pressure Drop Prediction For Structured Packing
 - Benefits of a Digital Library
 - Creating a Diverse Reading Collection Hetp And Pressure Drop Prediction For Structured Packing
10. Overcoming Reading Challenges
 - Dealing with Digital Eye Strain
 - Minimizing Distractions
 - Managing Screen Time
11. Cultivating a Reading Routine Hetp And Pressure Drop Prediction For Structured Packing
 - Setting Reading Goals Hetp And Pressure Drop Prediction For Structured Packing
 - Carving Out Dedicated Reading Time
12. Sourcing Reliable Information of Hetp And Pressure Drop Prediction For Structured Packing
 - Fact-Checking eBook Content of Hetp And Pressure Drop Prediction For Structured Packing
 - Distinguishing Credible Sources
13. Promoting Lifelong Learning

- Utilizing eBooks for Skill Development
 - Exploring Educational eBooks
14. Embracing eBook Trends
- Integration of Multimedia Elements
 - Interactive and Gamified eBooks

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