

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)

$$\frac{a_d}{a_s} = F_{\text{eff}} \frac{29.12(W_b V_f r_{\text{eff}})^{0.17} S^{0.188}}{R_{\text{eff}}^{1.2} C_{\text{eff}}^{0.25} (1 - 0.93 \cos \gamma)^{0.5} \sin \theta} \quad (1)$$

Mass-transfer coefficients (k_L, k_G)

$$k_L = 2.0 [(D_L C_L U_{\text{eff}})^{0.5} (v+S)]^{0.75} \quad (2)$$

$$k_G S i D_{\text{eff}} = 0.054 [U_{\text{eff}} + U_{\text{eff}} \sqrt{C_L S (v+S)}]^{0.75} \sqrt{D_{\text{eff}}} \quad (3)$$

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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 ²)	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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Handbook of Downstream Processing E. Goldberg, 2012-12-06. The last two decades have seen a phenomenal growth of the field of genetic or biochemical engineering and have witnessed the development and ultimately marketing of a variety of products typically through the manipulation and growth of different types of microorganisms, followed by the recovery and purification of the associated products. The engineers and biotechnologists who are involved in the full-scale process design of such facilities must be familiar with the variety of unit operations and equipment and the applicable regulatory requirements. This book describes current commercial practice and will be useful to those engineers working in this field in the design, construction, and operation of pharmaceutical and biotechnology plants. It will be of help to the chemical or pharmaceutical engineer who is developing a plant design and who faces issues such as: Should the process be batch or continuous or a combination of batch and continuous? How should the optimum process design be developed? Should one employ a new revolutionary separation which could be potentially difficult to validate or use accepted technology which involves less risk? Should the process be run with ingredients formulated from water for injection, deionized water, or even filtered tap water? Should any of the separations be run in cold rooms or in glycol-jacketed lines to minimize microbial growth where sterilization is not possible? Should the process equipment and lines be designed to be sterilized in place, cleaned in place, or should every piece be broken down, cleaned, and autoclaved after every turn?

Separation Process Principles J. D. Seader, Ernest J. Henley, D. Keith Roper, 2023-03-21. Separation Process Principles with Applications Using Process Simulator 4th Edition is the most comprehensive and up-to-date treatment of the major separation operations in the chemical industry. The 4th edition focuses on using process simulators to design separation processes and prepares readers for professional practice.

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