

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

Amanda K. Whaley,[†] Christopher A. Bode,[†] Joydeep Ghosh,[‡] and R. Bruce Eldridge^{*,§}

Department of Chemical Engineering, Department of Electrical and Computer Engineering, and The Separations Research Program, The University of Texas at Austin, Austin, Texas 78712

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)

$$\frac{a_d}{a_s} = F_{eff} \frac{29.12(Wb_p F r_{p_s})^{0.17} S^{0.188}}{Re_p^{0.2} Sc^{0.33} (1 - 0.93 \cos \gamma) (\sin \theta)^{0.33}} \quad (1)$$

Mass-transfer coefficients (k_L, k_G)

$$k_L = 2.0 [(D_L C_p U_{Lp})^{0.5} (v+S)]^{0.33} \quad (2)$$

$$k_G S i D_{Gc} = 0.054 (U_{Gp} + U_{Lp})^{0.5} S^{0.33} (v_p)^{0.33} D_{Gp}^{0.33} \quad (3)$$

* To whom correspondence should be addressed. University of Texas at Austin, PRC-CEER, 28150 Sumat Rd (RT1301), Austin, TX 78758. Phone: (512) 475 6885. Fax: (512) 471 1739. E-mail: whaley@che.utexas.edu.

[†] Department of Chemical Engineering.

[‡] Department of Electrical and Computer Engineering.

[§] The Separations Research Program.

HETP

$$\text{HETP} = (U_{Gp}^2 Re_p a_s + 2U_{Gp}^2 Re_p a_s) [\ln \lambda / (\lambda - 1)] \quad (4)$$

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 B3-400	400	45	perforated
Montz B3-400-60	400	60	perforated
Montz B5M-400	400	45	not perforated
Montz B5M-400-60	400	60	not perforated

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Mass Transfer in Chemical Engineering Processes Jozef Markoš, 2011-11-04. This book offers several solutions or approaches in solving mass transfer problems for different practical chemical engineering applications: measurements of the diffusion coefficients, estimation of the mass transfer coefficients, mass transfer limitation in separation processes like drying, extractions, absorption, membrane processes, mass transfer in the microbial fuel cell design and problems of the mass transfer coupled with the heterogeneous combustion. I believe this book can provide its readers with interesting ideas and inspirations or direct solutions of their particular problems.

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Process Engineering Norman P. Lieberman, 2017-04-11 This is not your average technical book Using a humorous and easy to understand approach to solving common process engineering problems this unique volume is the go to guide for any veteran or novice engineer in the plant office or classroom Textbooks are often too theoretical to help the average process engineer solve everyday problems in the plant and generic handbooks are often out of date and not comprehensive This guide focuses on the most common problems that every engineer faces and how to solve them The characters walk the reader through every problem and solution step by step through dialogues that literally occur every day in process plants around the world With over half a century of experience and many books videos and seminars to his credit Norm Lieberman is well known all over the world and has helped countless companies and engineers through issues with equipment processes and training This is the first time that this knowledge has appeared in a format like this quite unlike anything ever published before in books on process engineering This is a must have for any engineer working in process engineering

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Distillation Design Henry Z. Kister,1992-02-22 Providing coverage of design principles for distillation processes this text contains a presentation of process and equipment design procedures It also highlights limitations of some design methods and offers guidance on how to overcome them **Perry's Chemical Engineers' Handbook, 9th Edition** Don W. Green,Marylee Z. Southard,2018-07-13 Up to Date Coverage of All Chemical Engineering Topics from the Fundamentals to the State of the Art Now in its 85th Anniversary Edition this industry standard resource has equipped generations of engineers and chemists with vital information data and insights Thoroughly revised to reflect the latest technological advances and processes Perry s Chemical Engineers Handbook Ninth Edition provides unsurpassed coverage of every aspect of chemical engineering You will get comprehensive details on chemical processes reactor modeling biological processes biochemical and membrane separation process and chemical plant safety and much more This fully updated edition covers Unit Conversion Factors and Symbols Physical and Chemical Data including Prediction and Correlation of Physical Properties Mathematics including Differential and Integral Calculus Statistics Optimization Thermodynamics Heat and Mass Transfer Fluid and Particle Dynamics Reaction Kinetics Process Control and Instrumentation Process Economics Transport and Storage of Fluids Heat Transfer Operations and Equipment Psychrometry Evaporative Cooling and Solids Drying Distillation Gas Absorption and Gas Liquid System Design Liquid Liquid Extraction Operations and Equipment Adsorption and Ion Exchange Gas Solid Operations and Equipment Liquid Solid Operations and Equipment Solid Solid Operations and Equipment Chemical Reactors Bio based Reactions and Processing Waste Management including Air Wastewater and Solid Waste Management Process Safety including Inherently Safer Design Energy Resources Conversion and Utilization Materials of Construction **Encyclopedia of Chemical Processing and Design** ,1976 Distillation and Absorption '92 ,1992

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