

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)

$$\frac{a_d}{a_s} = F_{\text{eff}} \frac{29.12(W_b V_f r_{\text{eff}})^{0.17} S^{0.188}}{R_{\text{eff}}^{1.2} C_{\text{eff}}^{0.25} (1 - 0.93 \cos \gamma)^{0.25} \sin^2 \theta} \quad (1)$$

Mass-transfer coefficients (k_L, k_G)

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

$$k_G S i D_{\text{eff}} = 0.054 [U_{\text{eff}} + U_{\text{eff}} \sqrt{R_{\text{eff}} S (v_{\text{eff}})^{0.5}}]^{0.75} D_{\text{eff}}^{0.25} \quad (3)$$

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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 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

Heat And Pressure Drop Prediction For Structured Packing

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Hetp And Pressure Drop Prediction For Structured Packing:

Distillation and Absorption 2006 Eva Sørensen,2006 This work contains the proceedings of the Distillation and Absorption conference which happens every 5 years This collection of 100 contributions spanning 23 countries showcase the newest and best distillation and absorption technologies which cover a broad range of fundamental and applied aspects of the technology To address these aspects the contributions have been put into seven themes modelling and simulation steady state dynamic and CFD energy efficiency and sustainability equipment design and operation integrated hybrid and novel processes process troubleshooting and handling operational problems control and operation and basic data Petroleum Refining Design and Applications Handbook, Volume 3 A. Kayode Coker,2022-06-21 PETROLEUM REFINING The third volume of a multi volume set of the most comprehensive and up to date coverage of the advances of petroleum refining designs and applications written by one of the world s most well known process engineers this is a must have for any chemical process or petroleum engineer This volume continues the most up to date and comprehensive coverage of the most significant and recent changes to petroleum refining presenting the state of the art to the engineer scientist or student This book provides the design of process equipment such as vessels for the separation of two phase and three phase fluids using Excel spreadsheets and extensive process safety investigations of refinery incidents distillation distillation sequencing and dividing wall columns It also covers multicomponent distillation packed towers liquid liquid extraction using UniSim design software and process safety incidents involving these equipment items and pertinent industrial case studies Useful as a textbook this is also an excellent handy go to reference for the veteran engineer a volume no chemical or process engineering library should be without Written by one of the world s foremost authorities this book sets the standard for the industry and is an integral part of the petroleum refining renaissance It is truly a must have for any practicing engineer or student in this area This groundbreaking new volume Assists engineers in rapidly analyzing problems and finding effective design methods and select mechanical specifications Provides improved design manuals to methods and proven fundamentals of process design with related data and charts Covers a complete range of basic day to day petroleum refining operations topics with new materials on significant industry changes Includes extensive Excel spreadsheets for the design of process vessels for mechanical separation of two phase and three phase fluids Provides UniSim based case studies for enabling simulation of key processes outlined in the book Helps achieve optimum operations and process conditions and shows how to translate design fundamentals into mechanical equipment specifications Has a related website that includes computer applications along with spreadsheets and concise applied process design flow charts and process data sheets Provides various case studies of process safety incidents in refineries and means of mitigating these from investigations by the US Chemical Safety Board Includes a vast Glossary of Petroleum and Technical Terminology Encyclopedia of Chemical Processing and Design, Volume 69 (Supplement 1) Rayford Anthony,2001-12-12 This 69th volume presents information on circulating fluidized bed

reactors and looks at subjects ranging from basic concepts and hydrodynamics to structure properties and applications of polyolefines produced by single site catalyst technology

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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

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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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