

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)

$$\frac{a_d}{a_s} = F_{eff} \frac{29.12(Wb_1 F r_{b_1})^{0.17} S^{0.188}}{Re_b^{1.2} Sc^{0.33} (1 - 0.93 \cos \gamma) (\sin \theta)^{0.33}} \quad (1)$$

Mass-transfer coefficients (k_L, k_G)

$$k_L = 2.0 [(D_L C_L U_{L0} / \nu) (S+5)]^{0.5} \quad (2)$$

$$k_G S i D_{G0} = 0.054 [U_{G0} + U_{L0} / \nu C_L S (W_1)]^{0.5} \nu^{0.2} D_{G0}^{0.75} \quad (3)$$

* To whom correspondence should be addressed. University of Texas at Austin, PRC-CEER, 28150 Sumat Rd (R7130), Austin, TX 78758. Phone: (512) 475 6889. 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

$$\text{HETP} = (U_{G0} / k_G a_d + U_{L0} / k_L a_d) [\ln \lambda / (\lambda - 1)] \quad (4)$$

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

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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 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 **Ludwig's Applied Process Design for Chemical and Petrochemical Plants** A. Kayode Coker, 2010-07-19 The Fourth Edition of Applied Process

Design for Chemical and Petrochemical Plants Volume 2 builds upon the late Ernest E Ludwig's classic chemical engineering process design manual. Volume Two focuses on distillation and packed towers and presents the methods and fundamentals of plant design along with supplemental mechanical and related data nomographs, data charts, and heuristics. The Fourth Edition is significantly expanded and updated with new topics that ensure readers can analyze problems and find practical design methods and solutions to accomplish their process design objectives. A true application-driven book providing clarity and easy access to essential process plant data and design information. Covers a complete range of basic day-to-day petrochemical operation topics. Extensively revised with new material on distillation process performance, complex mixture fractionating, gas processing, dehydration, hydrocarbon absorption and stripping, enhanced distillation types.

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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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 **Distillation and Absorption '92** ,1992

Packed Tower Design and Applications Ralph F. Strigle,1994 **Directory of Graduate Research** American Chemical Society. Committee on Professional Training,2005 Faculties publications and doctoral theses in departments or divisions of chemistry chemical engineering biochemistry and pharmaceutical and or medicinal chemistry at universities in the United States and Canada Chemical Engineering Progress ,2000 Packed Columns American Institute of Chemical Engineers. Equipment Testing Procedures Committee,1990 *Distillation and Other Industrial Separations* Gail Nalven,1997 A compendium of 31 recent articles selected for their usefulness to process industry practitioners and for their practical emphasis 18 articles are on distillation and 13 on other separations technologies e g adsorption centrifugation and membranes as well as phase separators cyclones elect **World Congress III of Chemical Engineering** ,1986

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