EFFECT OF PACKING ON PERFORMANCE OF TRICKLE BED REACTOR

Thameed Aijaz

DEPARTMENT OF CHEMICAL ENGINEERING

INDIAN INSTITUTE OF TECHNOLOGY DELHI

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Thameed Aijaz

Department of Chemical Engineering

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CERTIFICATE

This is to certify that the thesis entitled '**Effect of Packing on Performance of Trickle Bed Reactor**' submitted by **Mr. Thameed Aijaz** to the Indian Institute of Technology-Delhi for the award of degree of **Doctor of Philosophy (Ph.D.)** is a bona fide record of research work carried out by him under our supervision. The contents of this thesis have not been submitted to any other institutes or university for the award of any degree or diploma.

Professor K. D. P. Nigam
Professor
Department of Chemical Engineering
Indian Institute of Technology Delhi
Hauz Khas, New 110016, India

Professor Shantanu Roy
Institute Chair Professor
Department of Chemical Engineering
Indian Institute of Technology Delhi
Hauz Khas, New 110016, India

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New Delhi

ABSTRACT

Packed beds have particles of different shapes, which are assumed to be equally and uniformly distributed. However, in general, the actual arrangement of packing may not be so: rather, the bed usually contains a "signature" of the way the particles are dumped into the bed. There is considerable interest in "fingerprinting," a packing arrangement that results as a result of both the packing type, size and shape, and method of packing. Moreover, interactions being multiscale in space and time, the complexity of the problem increases, thereby rendering a generalized treatment a challenging endeavour. However, efforts have been put forward to anticipate the overall reactor performance by modeling it and then comparing the predicted results with the available experimental data.

In this work, an attempt has been made to generate beds, with surface abnormalities visually observed in industrial packed bed reactors, using a simulation tool to get a detailed portrayal of particle distribution in the bed. Five types of beds were generated with different packing methods. The voidage information of the simulated packed bed was compared with the experimental data. The bulk voidage for different beds was in the range of 37.3 to 46.3%. Moreover, radial and axial voidage for all the five types were compared and were in good agreement with reported experimental measurements. To analyse bed property at a macroscopic level, Voronoi analysis was performed for two structured packings, Square Packing (SP) and Hexagonal Close Packing (HCP). As HCP and SP are two extremes, peaks for any type of packing will lie between the two. Moreover, different particles shapes (spherical, cylindrical, trilobe, and quadrilobe) were considered, and their effect on packing properties was studied. It was observed that cylindrical particles having an aspect ratio of 1 has bulk voidage of 0.38, and for quadrilobe, the value is 0.43. As the aspect ratio was increased, bulk voidage also increased as more disorder is present in the

bed. A function for estimation of radial voidage for particles of various shapes and aspect ratios was proposed.

In order to evaluate the performance of the Trickle bed reactors (TBR), Compartment Network Model (CNM) was employed where a packed bed is treated as a network of interconnected cells. The CNM, which is a simple model which when coupled with flow information and measurement of local bed porosity, yielded estimation on the performance of a TBR even for an industrial-scale reactor, albeit at a much lower computational cost. Further, detailed cell-wise information can be used to improve the design of TBR for a deeper process where conversion levels are higher. Moreover, the model has an inherent computational advantage over other available models, which solves second-order nonlinear differential equations. Also, evaluating one cell at a time rather than solving the whole bed simultaneously using some iterative scheme makes CNM a valuable diagnostic tool of industrial-scale TBR.

सार

पैक्ड बेड में अलग-अलग आकार के कण होते हैं, जिन्हें समान रूप से और समान रूप से वितरित माना जाता है। हालांकि, सामान्य तौर पर, पैकिंग की वास्तविक व्यवस्था ऐसी नहीं हो सकती है: बल्कि, बिस्तर में आमतौर पर "हस्ताक्षर" होता है जिस तरह से कणों को बिस्तर में डंप किया जाता है। "फिंगरप्रिंटिंग" में काफी रुचि है, एक पैकिंग व्यवस्था जो पैकिंग प्रकार, आकार और आकार और पैकिंग की विधि दोनों के परिणामस्वरूप होती है। इसके अलावा, अंतरिक्ष और समय में बहुस्तरीय होने के कारण, समस्या की जटिलता बढ़ जाती है, जिससे सामान्यीकृत उपचार एक चुनौतीपूर्ण प्रयास बन जाता है। हालांकि, रिएक्टर के समग्र प्रदर्शन का अनुमान लगाने के लिए इसे मॉडलिंग करके और फिर उपलब्ध प्रयोगात्मक डेटा के साथ अनुमानित परिणामों की तुलना करने के लिए प्रयास किए गए हैं।

इस काम में, बेड में कण वितरण का विस्तृत चित्रण प्राप्त करने के लिए सिमुलेशन टूल का उपयोग करते हुए, औद्योगिक पैक्ड बेड रिएक्टरों में सतह की असामान्यताओं के साथ, बेड उत्पन्न करने का प्रयास किया गया है। विभिन्न पैकिंग विधियों से पांच प्रकार के बिस्तर तैयार किए गए। प्रयोगात्मक डेटा के साथ नकली पैक किए गए बिस्तर की शून्य जानकारी की तुलना की गई थी। विभिन्न बिस्तरों के लिए थोक शून्यता ३७.३ से ४६.३% की सीमा में थी। इसके अलावा, सभी पांच प्रकारों के लिए रेडियल और अक्षीय शून्यता की तुलना की गई और रिपोर्ट किए गए प्रयोगात्मक माप के साथ अच्छे समझौते में थे। मैक्रोस्कोपिक स्तर पर बिस्तर की संपत्ति का विश्लेषण करने के लिए, दो संरचित पैकिंग, स्क्वायर पैकिंग (एसपी) और हेक्सागोनल क्लोज पैकिंग (एचसीपी) के लिए वोरोनोई विश्लेषण किया गया था। चूंकि एचसीपी और एसपी दो चरम सीमाएं हैं, किसी भी प्रकार की पैकिंग के लिए चोटियां दोनों के बीच स्थित होंगी। इसके अलावा, विभिन्न कणों के आकार (गोलाकार, बेलनाकार, त्रिलोब और क्वाड्रिलोब) पर विचार किया गया, और पैकिंग गुणों पर उनके प्रभाव का अध्ययन किया गया। यह देखा गया कि 1 के पक्षानुपात वाले बेलनाकार कणों में 0.38 की थोक

शून्यता होती है, और क्वाड्रिलोब के लिए, मान 0.43 होता है। जैसे-जैसे पहलू अनुपात में वृद्धि हुई, बिस्तर में अधिक विकार मौजूद होने के कारण थोक शून्यता भी बढ़ गई। विभिन्न आकार और पहलू अनुपात के कणों के लिए रेडियल शून्यता के आकलन के लिए एक समारोह प्रस्तावित किया गया था।

ट्रिकल बेड रिएक्टर (टीबीआर) के प्रदर्शन का मूल्यांकन करने के लिए, कम्पार्टमेंट नेटवर्क मॉडल (सीएनएम) को नियोजित किया गया था, जहां एक पैक किए गए बिस्तर को इंटरकनेक्टेड कोशिकाओं के नेटवर्क के रूप में माना जाता है। सीएनएम, जो एक सरल मॉडल है, जो प्रवाह की जानकारी और स्थानीय बेड सरंध्रता के माप के साथ मिलकर, एक औद्योगिक पैमाने के रिएक्टर के लिए भी टीबीआर के प्रदर्शन पर अनुमान लगाता है, हालांकि बहुत कम कम्प्यूटेशनल लागत पर। इसके अलावा, विस्तृत सेल-वार जानकारी का उपयोग टीबीआर के डिजाइन को बेहतर बनाने के लिए किया जा सकता है जहां रूपांतरण का स्तर अधिक होता है।इसके अलावा, मॉडल में अन्य उपलब्ध मॉडलों पर एक अंतर्निहित कम्प्यूटेशनल लाभ होता है, जो दूसरे क्रम के गैर-रेखीय अंतर समीकरणों को हल करता है। साथ ही, किसी पुनरावृत्त योजना का उपयोग करके पूरे बिस्तर को एक साथ हल करने के बजाय एक समय में एक सेल का मूल्यांकन करना सीएनएम को औद्योगिक पैमाने पर टीबीआर का एक मूल्यवान निदान उपकरण बनाता है।

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