Available online at www.sciencedirect.com
SCIENCE DIRECT
Computers and Chemical Engineering 30 (2006) 1178–1188
Computers & Chemical Engineering
www.elsevier.com/locate/compchemeng

An investigation of packed columns using a digital packing algorithm

R. Caulkin *, M. Fairweather, X. Jia, N. Gopinathan, R.A. Williams

Institute of Particle Science and Engineering, School of Process, Environmental and Materials Engineering, University of Leeds, Leeds LS2 9JT, UK

Received 9 May 2005; received in revised form 13 February 2006; accepted 27 February 2006
Available online 18 April 2006

Abstract

This paper presents results concerning the validation of a recently developed packing algorithm. The basic ethos of this algorithm is to digitise particle shapes, and to use the digitised shapes to generate digital packing structures. A variety of simulations of packed columns, comprising mono, binary and ternary mixtures of spherical particles, have been undertaken and the results compared to existing experimental data with good agreement. The ultimate aim of this work is to develop the packing algorithm as a design tool for use in optimising the performance of packed bed systems and, as a first step, to enable the characterisation of any particle population and prediction of particle behaviour in packing, segregation and mixing.

Keywords: Particle packing; Packed columns; Segregation; Mixing

1. Introduction

Despite the fact that numerous experimental studies have been undertaken on the subject of packed columns, as yet there is no definitive method with which to predict the mean and local voidage of a bed which is comprised of mixed shape (regular or irregular) particles or in a column of complex internal geometry. The effect that the relative size and volume content of the mixture have on the voidage still requires careful examination.

Particulate beds are commonly encountered in chemical and allied engineering fields, with packed bed systems being employed in a wide range of disciplines including heterogeneous catalytic reactions, solids handling, heat recovery, absorption and distillation. The design and performance prediction of such systems depends heavily on models describing the behaviour of fluid flow, heat and mass transfer, and the pressure drop of the fluid through the bed. The models themselves are generally dependant on accurate experimental data describing transport parameters such as effective thermal conductivity coefficients, the wall heat transfer coefficient and effective dispersion coefficients. These parameters in turn are sensitive to the structural properties of packed beds, namely the global and local voidage.

The bed voidage is influenced by a number of factors which include the type of particles employed, the container, the method of deposition of the particles and the treatment of the packing that is employed in preparing the bed after deposition. To effectively design and produce fixed-bed reactor models, a variety of problems need to be addressed. Amongst those that merit investigation, the present study looks at the sensitivity of global and local voidage to mixed-sized beds. These systems arise in situations such as bed stratification and particle breakage, which occurs during catalyst dumping.

The aim of this case study is to present a comprehensive validation of a recently developed packing algorithm against the experimental data available. The basic ethos of the packing algorithm is of using three-dimensional methods of characterising particulate products and the direct use of such digital information for computation, without conversion into any geometrical models. A variety of simulations of packed columns, comprising mono, binary and ternary mixtures of particles, are reported and results compared to existing experimental data. The structural arrangement of the bed ends, and the way in which they contribute to the global characteristics, is also examined. The overall aim is to eventually develop the packing algorithm to be capable of quickly and accurately designing fixed-bed reactors with optimal system performance, and to introduce new concepts to enable prediction of their behaviour in packing, segregation and mixing.

* Corresponding author.
E-mail address: pre9rc@leeds.ac.uk (R. Caulkin).

0098-1354/$ – see front matter © 2006 Elsevier Ltd. All rights reserved.
doi:10.1016/j.compchemeng.2006.02.019

Nomenclature

A	percentage of large particles by weight
B	percentage of medium particles by weight
C	percentage of small particles by weight
d_p	particle diameter
d_{pe}	equivalent particle diameter
d_t	cylindrical tube diameter
d_t/d_p	tube-to-particle diameter ratio (aspect ratio)
d_t/d_{pe}	tube-to-equivalent particle diameter ratio
L/d_t	bed length-to-diameter ratio
$r/d_{p(e)}$	radial distance from container wall
S_l	surface area of large sphere
S_m	surface area of medium sphere
S_p	surface area of particles
S_s	surface area of small sphere
V_l	volume of large sphere
V_m	volume of medium sphere
V_p	volume of particles
V_s	volume of small sphere
$x/d_{p(e)}$	axial distance from base of container

Greek symbols

$\sum_{mean}$	mean/global voidage
$\sum_r$	local radial voidage
$\sum_x$	local axial voidage

2. Experimental techniques

All the experimental results discussed below were obtained from the PhD studies of Moallemi (1989), Summers (1994) and Ismail (2000). The results of Ismail are also reported in two open literature publications (2002a, 2002b). The experimental techniques used by all three researchers are very closely related as all the work was undertaken in the same Department at the University of Leeds. Therefore, the following description of how the experimental data were acquired relates to the work of all the studies.

In order to obtain local voidage data for all the mixtures used (mono, binary and ternary spheres), lead particles were poured into cylindrical moulds and filled with dyed liquid epoxy resin, taking care to fill all the interstices. For global data collection, glass spheres were simply poured into the relevant container, and the total voidage recorded by filling the pores with measured volumes of water.

All the cylindrical containers, which represent the packed beds containing the various packings, were constructed using grey PVC which is inexpensive and easily machined. Also, the resin mixture readily adheres to the PVC mould and the softness of the PVC material enables a tube of specific diameter to be cut with ease. The cylindrical containers were made by boring into solid PVC plastic rod until the desired inner diameter of the tube was reached.

The height of all the containers used was 100 mm. The packing material, however, was only stacked into the bed up to a height of approximately 60 mm. The extra height of the container was to enable the chuck on the lathe to grip the container securely. The 60 mm packing height was ample for 50 1 mm cuts of the bed to be made. The accuracy of all bed dimensions is ±0.05 mm.

Lead spheres were used due to the softness, availability and low cost of the material. This is an advantage when increments of the bed are shaved off on the lathe, as the bed can be easily rotated without blunting the machine tool. Another advantage is that lead can be polished and a strong contrast can therefore be obtained between the particles and resin which influences the reliability of the data derived from digital images of the slices.

In order to gain good adhesion between the particles and the resin, the outer coating of the particles was removed beforehand by placing the particles in a container of sand and gently rotating. This increased the surface roughness of the particles, and thus enabled a stronger bond between the particles and the resin to be formed.

For bonding purposes, Ampreg 20 resin was used which is one of a new generation of laminating resins. The resin combines good mechanical properties, low viscosity and generous working times, which make it ideal for this application. Ampreg 20 resin and Ampreg 20 hardener were combined in a 4:1 ratio by weight in batches of 150 g. The resin mixture was dyed by addition of Oxford Blue Colour prior to use in order to increase the contrast between the lead particles and the resin.

The lead spheres used in the experiments were introduced into the cylindrical containers a handful at a time, with gentle tapping of the container after each addition. When each layer was formed, one particle thick, the resin mixture was poured slowly and uniformly over the particles, taking care to fill any gaps between the particles, ensuring that the sides of the bed were filled by the resin and that no air pockets remained. The following layers of particles were then introduced into the bed. This procedure was repeated until the bed was packed to a height of approximately 60 mm. This procedure aimed to simulate a poured randomly packed bed.

After solidification, each bed was periodically turned in a lathe. To expose the first layer of lead particles which were touching the bed end (i.e. at the base of the container), an initial cut was made using the lathe to remove the base of the packed bed. The bed cross-section was then wet with water and polished using silicon carbide paper to improve contrast between the packed particles and resin mixture.

A digital image was then captured and saved on an optical disk. On completion of archiving the first image, the procedure was repeated to a total of 50 times, with 1 mm being machined off axially each time. The same number of images was obtained for each bed investigated. The accuracy of the lathe means that axial cuts were performed to within ±0.001 mm.

By magnifying the images of the consecutive cross-sections of the test samples to the maximum capacity of the VDU screen employed, the highest possible resolution was achieved (8 bit image of 512 × 512 pixels). The images were then captured and stored on an optical disk so that each stored image could be retrieved for subsequent analysis using the colour-contrast method.