

A Numerical Case Study of Packed Columns

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Abstract

This paper presents results concerning the validation of a recently developed packing algorithm. The basic ethos of this algorithm, known as DigiPac, is to use three-dimensional methods to digitise particle shapes, and to use this digital information directly in computations of how particles pack together without further conversion or the need for modelling. A variety of simulations of packed columns, comprising mono, binary and ternary mixtures of spherical particles, together with shell-side containers, have been undertaken and the results compared to existing experimental data with good agreement being found. 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 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

Particulate beds are commonly encountered in chemical and allied engineering fields, with the application of packed bed systems covering a wide range of areas including heterogeneous catalysis, solids handling, heat recovery, absorption, filtration and distillation. The design and performance prediction of such systems depends greatly on mathematical models that describe the behaviour of fluid flow, heat and mass transfer, and the pressure drop of the fluid through the bed. The models themselves are to a great extent dependant on accurate experimental data describing transport parameters such as effective thermal conductivity coefficients, wall heat transfer coefficients and dispersion coefficients. In turn, these parameters are sensitive to the structural properties of packed beds, namely the global and local voidages. The significance and magnitude of bed voidage is influenced by a number of factors, including the geometry of the particles and container, the method of particle loading and the treatment of the packing matrix during and after deposition. To design effective models of fixed-bed systems a variety of problems must therefore be addressed. Amongst those that merit investigation, the present study assesses the ability of DigiPac to predict the global and local voidage of beds containing mixed-sized particles. These systems occur by design, and in situations when particle breakage occurs, for example, during catalyst dumping.

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Despite the fact that a great deal of work has been undertaken on packed columns (e.g., McGreavy et al., 1986), where attempts have been made to quantify the structural properties of packed beds, this work generally results in empirical correlations which are of limited value due to their restricted range of applicability. Therefore, as yet there is still no definitive method with which to predict the mean and local voidages of a bed which is comprised of various mixtures of regular or irregular shaped particles.

This paper presents the results of a novel approach to predicting the structure of such beds. The key to this approach is that a digital method is used which avoids many of the difficulties associated with traditional approaches to bed design. The key innovation is the digitisation of the particles and packing space which allows particles of any shape to be packed into containers of arbitrary geometry.

2. Overview of the DigiPac Algorithm

DigiPac is a computer-based tool that uses a novel solution for packing objects using digital means, as opposed to the vector approach used by many other traditional packing models. It is capable of packing particles of any shape, from simple geometrical ones to complex arbitrary shapes, into containers of any geometry.

The basis of the algorithm is to map the particles, the container and particle movement on to a grid. Therefore a single particle is just a coherent collection of pixels (two-dimensional) or voxels (three-dimensional) that moves randomly, one grid cell at a time, within the specified boundaries of the container.

In two dimensions there are 8 possible directions (4 orthogonal and 4 diagonal) that a particle can move in, all initially with equal probability. In three dimensions there are 26 possible directions (6 orthogonal and 20 diagonal). In order to encourage particles to settle having undergone movement, the upward component of a move is only accepted by the algorithm with a so-called rebound probability. This results in a directional and diffusive particle motion, which aids the particles in effectively exploring every available packing space.

Since particles reside and move on a grid just one step at a time, collision and overlap detection is a simple matter of determining whether more than one object occupies the same site(s) at any one time.

For the packing of arbitrary shaped particles, DigiPac has several advantages over traditional methods:

- The computational cost depends on the number of pixels/voxels, not the particle shapes,
- The algorithm can be implemented and run on standard PC's – there is no need for costly workstations,
- It is not limited to mathematically or computationally manageable shapes,
- The detection of collisions and overlaps of particles or particles with walls is simple.

A more comprehensive description of the DigiPac algorithm has been given elsewhere (Jia and Williams, 2001; Gopinathan et al., 2003).

3. Results and Discussion

To date, much of the work on the structural properties of particulate bed systems has involved beds of mono-sized spheres, and to a lesser extent binary mixtures of spherical particles (McGreary, 1961; Abe et al., 1979; Moallemi, 1989; Roshani, 1990; Summers, 1994; Ismail, 2000). There is a marked lack of work on ternary mixtures and their effect upon the structural properties of packed beds, although Ismail (2000) did consider such beds.

In industry, mixed-sized packings can be used by design, but are also frequently encountered in situations where stratification due to inefficient packing caused by the presence of the surrounding tube wall occurs, and where breakage occurs during the loading of catalyst pellets. In practice, therefore, it is rare to find mono-size packing in industry. Particulate bed systems effectively always comprise two or more sizes, and work on ternary mixtures is therefore of obvious value to industry.

Previous work on the global properties of beds packed with multi-sized spherical particles (McGreary, 1961; Abe et al, 1979; Summers, 1994) has demonstrated that smaller particles tend to fill the gaps between larger particles. This is demonstrated in Figure 1, where experimentally derived global voidages of beds packed with mono, binary and ternary mixtures of spherical particles are displayed, together with predictions carried out using the DigiPac algorithm. The measured and predicted global voidage is displayed for a range of tube-to-particle diameter ratios and as can be observed, the simulations agree qualitatively and quantitatively with the global voidage values of the experiments which they reproduce.

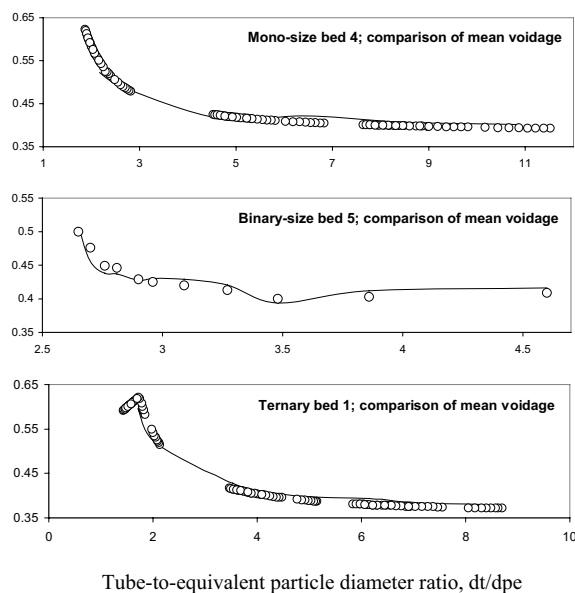


Figure 1. Comparison of predicted (line) and measured (symbol) bulk voidage values of mono, binary and ternary mixed beds using a range of tube-to-equivalent particle diameter ratios.

The claim made by earlier researchers that smaller particles fill the gaps between larger particles is supported by the present results. From Figure 1, it can be seen that the minimum bulk voidages attained for each bed type proportionally decrease in relation to the number of particle sizes. Mono-size beds have an overall minimum porosity value of 39.4% (DigiPac = 40.1%) at a tube-to-particle diameter ratio of 11 compared to binary beds which demonstrate a minimum of 39.3% (DigiPac = 39.7%). In turn, the ternary beds have a lower value of 37.2% (DigiPac = 37.9%) at a tube-to-equivalent particle diameter ratio of 8.4. These results show that DigiPac is capable of predicting not only the minimum porosity values of beds, but also the aspect ratios at which they occur. However, it must be noted that the global voidage furnishes no information about the local properties of a bed. Plug flow is commonly assumed in mono-sized particle beds, i.e. the bed has uniform properties throughout. While this may be the case at the centre of relatively large packed beds, it is certainly not so in the vicinity of the walls. As a result of large void spaces near the wall, flow channels are large in this area, offering less resistance to flow than at the bed centre. Considerable flow mal-distribution therefore exists, and an examination of local voidage distribution is required.

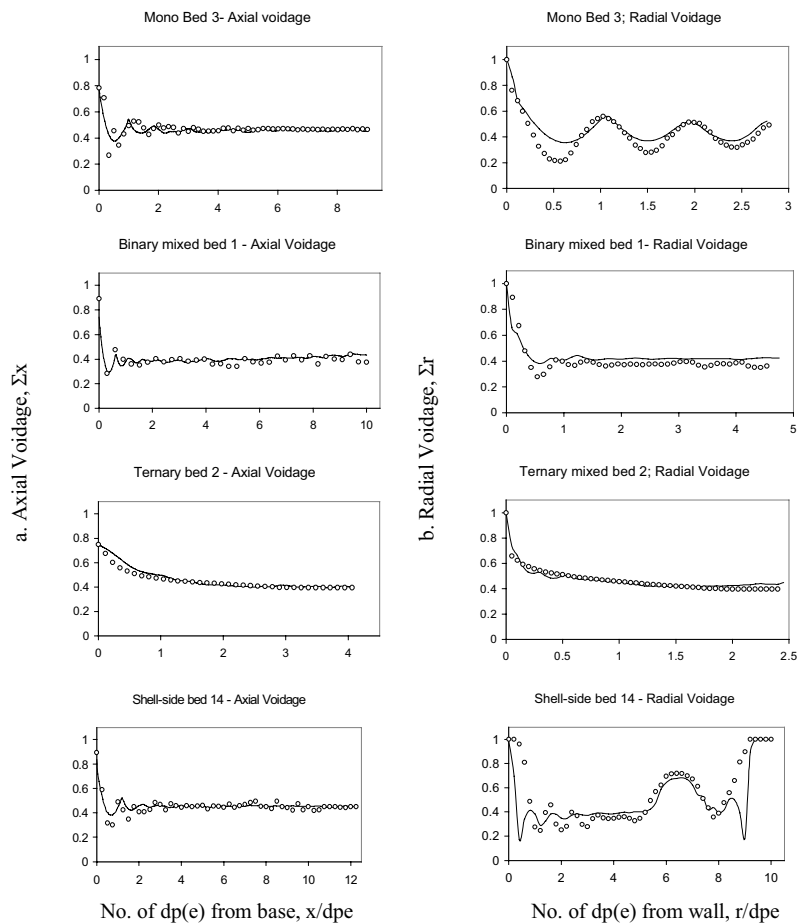


Figure 2. Comparison of predicted (line) and measured (symbol) local voidage values, a) axial and b) radial, for mono, binary, ternary and a shell-side packed beds.

Earlier researches established that a damped cyclic variation of bed voidage in the radial direction takes place in beds packed with mono-sized particles as one moves from the bed wall to its centre. This phenomenon, known as the wall effect, typically extends 6 to 10 particle diameters into the bed before it becomes negligible. It is therefore an important factor in beds with low tube-to-particle diameter ratios. This observation is seen in the results of Figure 2 where the local voidage predictions of a mono-bed are compared to the experimental results. In this bed, which has a relatively low aspect ratio, dt/dpe , of 5.8, wall effects are observed to extend throughout the bed for both experiment and simulation results. In the axial direction, however, end effects are only seen to extend for 3 particle diameters into the bed from the base of the container.

Summers (1994) examined the local voidage distribution of beds comprising a binary mixture of spherical particles. Figure 2 shows that in terms of both experiment and prediction, axial voidage has a similar profile to that of mono-sized beds, with end effects again extending for 3 particle diameters into the bed. However, when compared to the mono-bed results, the radial voidage is more uniform, having a value of 1.0 at the wall and then exhibiting a damped oscillation for a distance of 2 particle diameters into the bed. This is once again reproduced with a good degree of accuracy in the DigiPac simulations. The binary bed used in this comparison had an aspect ratio of 9.8.

Ismail (2000) investigated the packing of ternary mixtures of spherical particles. The results for a ternary bed show the qualitative and quantitative agreement of the DigiPac simulation with the experiment in terms of axial and radial voidage variation. The graph showing axial voidage indicates a very high value of 75% at the inlet of the bed, which decreases exponentially until a constant value of 40% is reached, which is lower than the values recorded in the mono and binary beds. However, most noticeable when compared to the mono and binary results is the fact that the experimental radial voidage is completely uniform. This phenomenon is reproduced in the DigiPac simulation. This suggests that the smaller particles are infilling the pore spaces between larger particles, thereby reducing the voidage of the bed and dampening the oscillations which were seen so prominently in both the mono and binary radial directions. The effects of the bed ends are also observed to extend to a distance of around $L/dpe = 3.0$, while the wall effects extend for 1 particle diameter into the bed.

Also displayed in Figure 2 are axial and radial voidage results for a shell-side bed (Ahmad, 2000). This bed contains an array of pipes, in this case seven, running in the axial direction. The aim here is to demonstrate that DigiPac has the ability to accurately simulate more complex situations than have been investigated previously.

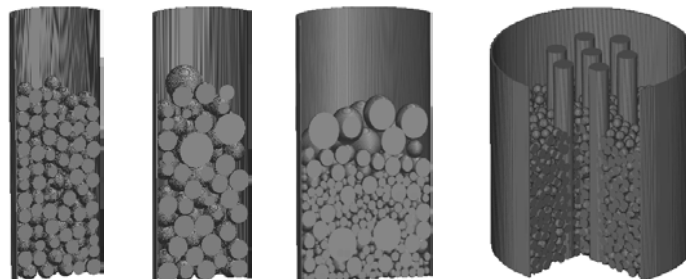


Figure 3. Cross-sectional images of mono, binary and ternary packed beds, and a shell side bed.

The use of shell-side beds is truer to an industrial environment, wherein particles not only have to pack into a container but also have to arrange around a series of objects, in this case pipes, used for heat transfer purposes. Again, as with mono, binary and ternary packed columns, a range of aspect ratios were investigated as well as different number combinations of pipes. The local voidage results (Figure 2) from the bed displayed here shows that DigiPac is able to reproduce with a reasonable degree of accuracy the results obtained experimentally. In terms of axial voidage, end effects extend for 3 particle diameters, with a small amount of oscillation near the base of the bed. The radial voidage, however, is necessarily more complicated due to the array of pipes in the container which gives rise to much more voidage fluctuation. However, what is clear is that DigiPac reproduces the results, particularly in the centre of the bed, with a good degree of accuracy, both qualitatively and quantitatively.

Lastly, Figure 3 shows cross-sectional images produced by DigiPac for all the beds examined. It may be noted that, as well as producing quantitatively reliable results for these beds, these qualitative images are also of value to the design process.

4. Conclusions

A new approach to simulating the packing of particles in packed columns using digital techniques has been introduced and demonstrated to provide results that agree well with available experimental data. In addition to mono and binary packed beds, which have been extensively investigated, attempts to reproduce the packing structure of ternary beds have been successful. An initial study into shell-side packed beds has also produced promising results, whereby the predicted local voidage is close to the experimentally derived results. In conclusion, the digital techniques utilised by DigiPac provide a powerful modelling capability for packed bed systems that have the potential to be of value to the improved design of a wide range of unit operations. Further work will concentrate more closely on shell-side packed beds and the packing of non-spherical particles, in addition to lattice Boltzmann modelling of flow through the resulting bed structures.

5. References

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