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FRACTAL DIMENSIONS OF COMPUTER SIMULATED AGGLOMERATES

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ABSTRACT

As a step towards classifying the fractal nature of filter cakes, particle agglomerates have been grown onto seed particles using a new computer simulation. The agglomeration process was controlled by varying the amount of diffusion influence in the growth mechanism. The perimeter and density fractal dimensions of simulated agglomerates comprising up to 800 particles were measured using three different automated techniques. The perimeter dimension was found to increase markedly with larger diffusion influence, whilst the density of the structure, measured using the enclosing circles and radius of gyration methods, decreased as the level of diffusion increased. The importance of these results to the characterisation of cake filtration processes is discussed.

KEYWORDS

Fractals; Filtration; Structure

INTRODUCTION

Much work has been performed in recent years with regard to fractals¹. Although the majority has apparently been of little practical use, some work has been performed to investigate the relationships between fractal dimension and the characteristics of particulate systems²⁻⁴. This is of particular interest here as the cakes formed during so called 'dead-end' filtration may be thought of as growing particle agglomerates on a filter surface.

The data in this paper show a summary of the results from an ongoing research project which examines the relationship between fractal dimension and the filtration characteristics of suspensions and filter cakes. The work performed aims to identify better methods of characterising cake structure to provide more accurate filtration analysis and scale-up procedures than are currently available. The data provided in this paper highlights the importance of particle motion to the structure of agglomerates, and hence filter cakes.

COMPUTER MODEL DEVELOPMENT AND AGGLOMERATE ANALYSIS

Although the computer program used to create agglomerates is not described in detail here, it essentially comprised a set of modular routines capable of defining, growing and analysing agglomerates for set numbers of particles with given size distributions. Each of the 15 modules in the program was constructed and tested prior to insertion in the main program, and the main program was further tested with relatively small agglomerates of large particles to ensure correct growth and analysis. Agglomerate growth was simulated in both two and three dimensional space using up to 800 circular or spherical particles where the degree of diffusion influence was varied over the range 0% (i.e. pure ballistic motion) to 100% diffusion in 5% increments. Attachment of particles was determined from geometric considerations whilst the variable diffusion was achieved by allowing particles to move through the control space in either a pre-described or random

direction dependent on the proportion of diffusion influence. An example of a 2-D agglomerate with 50% diffusion is shown in Figure 1.

The 2-D agglomerate structures were analysed by three different techniques. The first, the structured walk, may be likened to measuring the agglomerate perimeter with a pair of 'dividers' at sequentially varied steplengths.

The gradient measured from a log-log plot of steplength (λ) against measured perimeter (*P*), known as a 'Richardson plot', yields the (structural) perimeter fractal dimension (D_p) as given by eqn. (1)³

$$P = \lambda^{(1-D_p)} \tag{1}$$

With the enclosing circle analysis technique, the area (*A*) of the particles contained within progressively larger circles is measured and a density fractal dimension (D_d) determined from the gradient of the mass (*M*)-length (*I*) relationship according to

Agglomerates were also analysed using a radius of gyration (R_g) technique where

$$R_g = \sqrt{\frac{I_g}{A}} \tag{3}$$

and I_g is the second moment of area for the agglomerate. A series of radius of gyrations are calculated by progressively increasing the number of particles counted in the agglomerate up to the maximum number of particles. The radius of gyration is plotted against the number of particles on a log-log scale and the density fractal dimension is given by the reciprocal of the slope of the resultant straight line.

The 3-D agglomerates were analysed by 2-D projections in the case of structured walk and by substituting volume for area in the cases of enclosing circle and radius of gyration.

RESULTS

 $M \sim I^{D_d}$

In order to examine the influence of diffusion on agglomerate/cake growth, a total of 840 simulations have been performed in both 2-D and 3-D using the computer program described. For the 2-D case agglomerates containing up to 800 circular particles were grown with varying degrees of diffusion influence between 0 and 100% (i.e. a total of 420 simulations). Due to the statistical nature of agglomerate growth it was necessary to impose error levels to identify wholly representative results, and for the current purpose, structured walk analyses were considered valid when $r^2 < 0.10$, enclosing circle analyses when $r^2 < 0.02$ and radius of gyration analyses when $r^2 < 0.002$. Thus, each of points on Figures 2-4 represents an average of the results within the respective error limits.

When the structured walk technique was used to analyse the range of simulated agglomerates a change in the perimeter fractal dimension was observed. A gradual variation was seen at lower diffusion levels with a steeper variation becoming apparent at approximately 70% diffusion (see

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(2)

Figure 2). The fractal dimension increased from 1.25 to 1.45 for the agglomerates analysed, with the more rapid change corresponding to a fractal dimension of 1.27. The changes in agglomerate structure were also visually apparent with agglomerates built using lower levels of diffusion appearing more dense.

The enclosing circle analysis gave numerical values to the observed changes in particle density within the structures. Figure 3 shows that the density fractal dimension decreased from a maximum value close to the Euclidean dimension of 2.00 to 1.75 as the level of diffusion influence increased from 0% to 100%. A change in gradient on the plot was again observed at approximately 70% diffusion and a density fractal dimension of 1.94.

In Figure 4 the radius of gyration analysis shows similar trends to the enclosing circle data presented in Figure 3. The density fractal dimension is again seen to decrease from a value close to the Euclidean dimension to 1.74 with varying diffusion influence, the steeper change in gradient again occurring at approximately 70% diffusion and a density fractal dimension of 1.91.

Although no data for 3-D simulations are presented in this paper, the general trends observed for 2-D simulations and analyses were repeated for corresponding 3-D simulations involving spheres, rather than circles. The sharp changes in fractal dimension seen at levels of diffusion approaching 70% were not repeated as more gradual changes in the fractal dimensions were recorded. The 3-D data will be the subject of a future paper.

CONCLUSIONS

The results presented in this paper are a product of the first year in a planned three year research program aimed at examining and characterising the fractal nature of filter cakes. The results obtained to date in both 2-D and 3-D have shown how the degree of diffusion influence can alter measured fractal dimensions, with steeper changes being observed in the region of 70% diffusion for 2-D. The next stage of the project requires comparison of the computer simulated agglomerates with 'real' agglomerates obtained from the sampling of filter cakes from a well controlled filtration system. Ultimately it is hoped that the fractal techniques outlined here will offer a better way of characterising cake structure and filtration characteristics. Currently porosity and resistance measurements are gathered and correlated against pressure to characterise the compressibility of filtration systems and provide scale-up parameters. It is known that even small changes in measured porosity can significantly alter filtration rates⁵ and it may prove beneficial to use another, more accurate, descriptor of cake structure such as the fractal dimension.

NOMENCLATURE

- A area (m^2)
- D_d density fractal dimension (-)
- *D_p* perimeter fractal dimension (-)
- I_g second moment of area (m⁴)
- I length (m)
- M mass (kg)
- *P* perimeter length (m)
- *r* linear regression correlation coefficient (-)
- R_g radius of gyration (m)
- λ steplength (m)

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Figure 1: Example of agglomerate simulation with 50% diffusion.



Figure 2: Structured walk analysis for 2-D simulations.

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Figure 3: Enclosing circle analysis for 2-D simulations.



Figure 4: Radius of gyration analysis for 2-D simulations.