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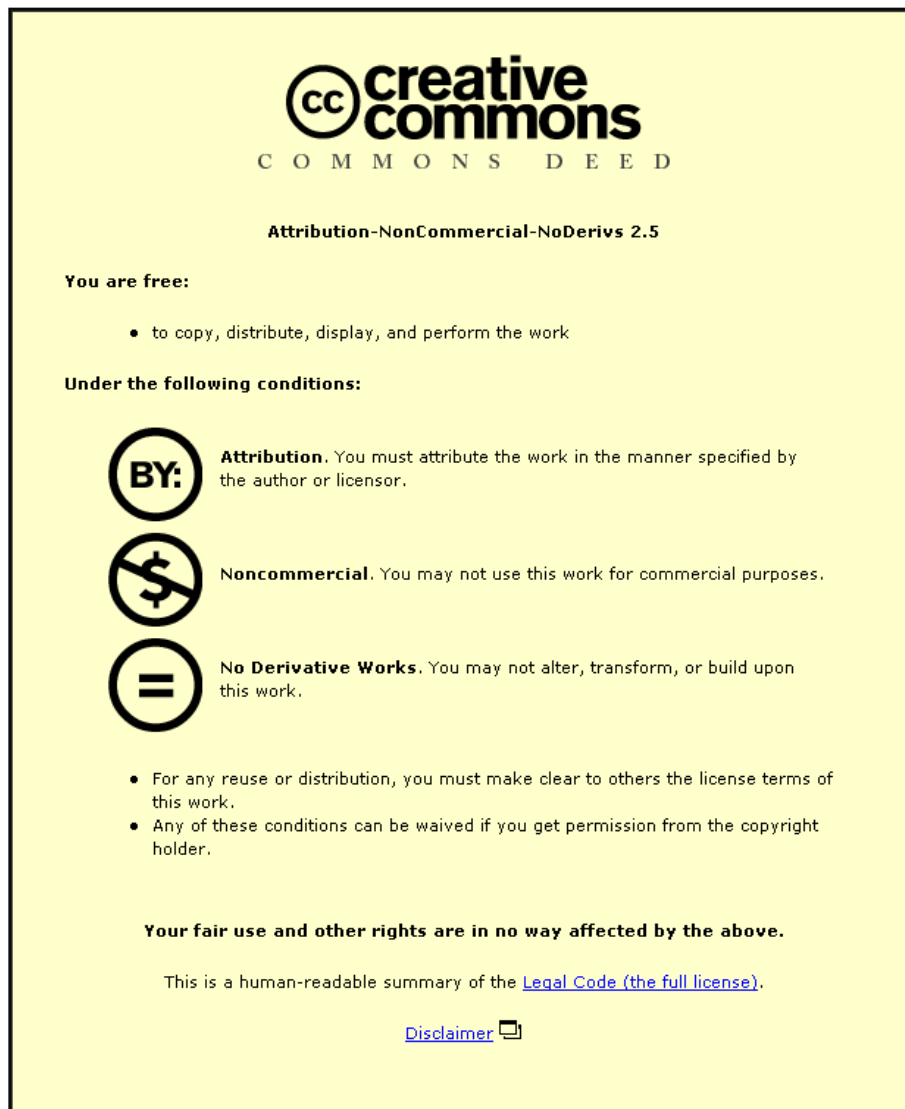
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THE FRACTAL PROPERTIES OF TWO & THREE DIMENSIONAL COMPUTER SIMULATED AGGLOMERATES

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ABSTRACT

As a step towards classifying the fractal nature of filter cakes, particle agglomerates have been grown onto seed particles in both two and three dimensions 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 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.

INTRODUCTION

Much work has been performed in recent years with regard to fractals (Kaye, 1994). 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 systems (Bayles *et al.*, 1987; Schmidt, 1995). The latter 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 aims to identify better methods of characterising cake structure to provide more accurate filtration analysis and scale-up procedures than those currently available.

COMPUTER MODEL DEVELOPMENT AND AGGLOMERATE ANALYSIS

The computer program used to create and analyse agglomerates comprised a set of modular routines capable of defining, growing and analysing agglomerates. Agglomerate growth was simulated in both two and three dimensional space using 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. An example of both 2-D and 3-D agglomerates with 50% diffusion are shown in Figure 1. The 3-D agglomerate shown on the right hand side of Figure 1 has been rendered using 'ray-tracing' software to enable the depth of the structure to be seen more clearly.

In order to examine the influence of diffusion on agglomerate/cake growth, a total of 840 agglomerates were built and analysed in both 2-D and 3-D using the computer program. For 2-D simulations, 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). In the case of the 3-D simulations, the circular particles were substituted by spheres. The perimeter and density fractal dimensions of all the simulated agglomerates were determined using the three different automated techniques of structured walk, enclosing boundary (circle or sphere) and radius of gyration respectively.

The structured walk technique measures the perimeter ruggedness of an agglomerate by measuring the perimeter with a pair of virtual 'dividers' set at progressively varying steplengths. As the steplength is decreased, so more of the detail of the perimeter becomes apparent. The measured perimeter generally shows a log-log relationship with steplength. The enclosing boundary technique involves encompassing an agglomerate with progressively larger circles/spheres and measuring the area/volumes of the particles contained therein. The second density fractal dimension (i.e. radius of gyration) is measured by evaluating the second moment of area/volume of an increasing number of particles within the agglomerate where the seed particle of the agglomerate is the starting point. Both enclosing circle and radius of gyration techniques use logarithmic relationships to calculate the density fractal dimension. 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 the points on Figures 2-4 represents an average of the results within the respective error limits.

RESULTS

Figure 2 shows that when the structured walk technique was used to analyse the simulated agglomerates, a change in the perimeter fractal dimension was observed. For the 2-D agglomerates, a gradual variation was seen at lower diffusion levels with a steeper variation becoming apparent at approximately 70% diffusion. 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 analysis of 3-D structures showed similar trends to 2-D, although the changes in perimeter ruggedness were less pronounced. The results for the 3-D structured walk analysis were obtained by averaging the perimeter fractal dimension for three projections of each agglomerate (arbitrarily defined here as the front, side and top views). The fractal dimension was again seen to change more rapidly around 70% diffusion, but only climbed from 1.19 to a maximum of 1.25, with a fractal dimension of 1.21 corresponding to 70% diffusion.

Figure 3 shows how density fractal dimensions decreased as the level of diffusion influence increased from 0% to 100%. Over this range the enclosing circle fractal dimension reduced from a maximum value close to the Euclidean dimension of 2.00 to 1.75, whilst the radius of gyration analysis showed similar trends, with the density fractal dimension decreasing in this case from 1.94 to 1.74 with varying diffusion influence. Both methods showed a pronounced change in gradient at approximately 70% diffusion corresponding to a density fractal dimension of 1.94 for the enclosing circle method and 1.91 for the radius of gyration technique.

The density analyses of the 3-D structures showed similar trends to the results obtained for 2-D simulations whereby the density fractal dimension decreased with increasing diffusion influence. However, the sharp decrease corresponding to 70% diffusion was not observed. Instead, both the density fractal dimensions decreased in a relatively steady manner. The results of the radius of gyration analyses showed a steeper change in fractal dimension than seen with the enclosing sphere technique. The density fractal dimensions for the latter fell from 3.05 (essentially the Euclidean dimension) to a minimum of 2.50 with an increasing diffusion influence from 0% to 100%. The enclosing sphere procedure, meanwhile, showed only a decrease from 2.72 to 2.46 over the same range. The comparison between the two methods is shown in Figure 4.

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 show 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 by 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 determining filtration characteristics and scale-up parameters.

REFERENCES

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2. G.A. Bayles, G.E. Klinzing and S-H Chiang, 1987, *Part. Sci. & Tech.*, **5**, 371-382.
3. E. Schmidt, 1995, *Filt. and Sep.*, **32**(8), 789-793.

FIGURES AND TABLES

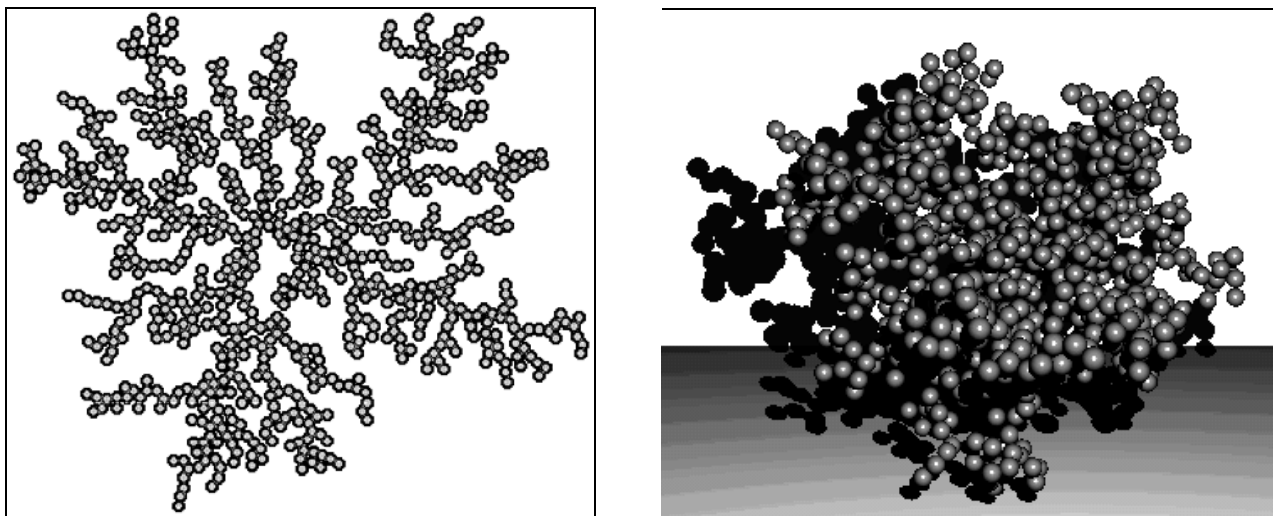


Figure 1: Example of 2-D and 3-D agglomerates with 50% diffusion influence.

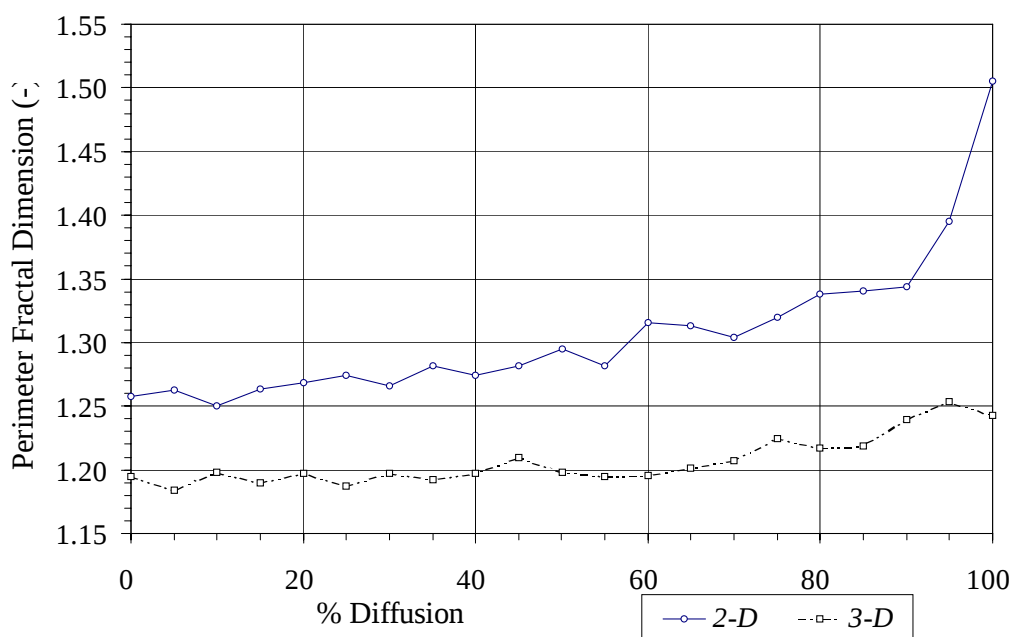


Figure 2: Structured walk analysis for 2-D and 3-D simulations.

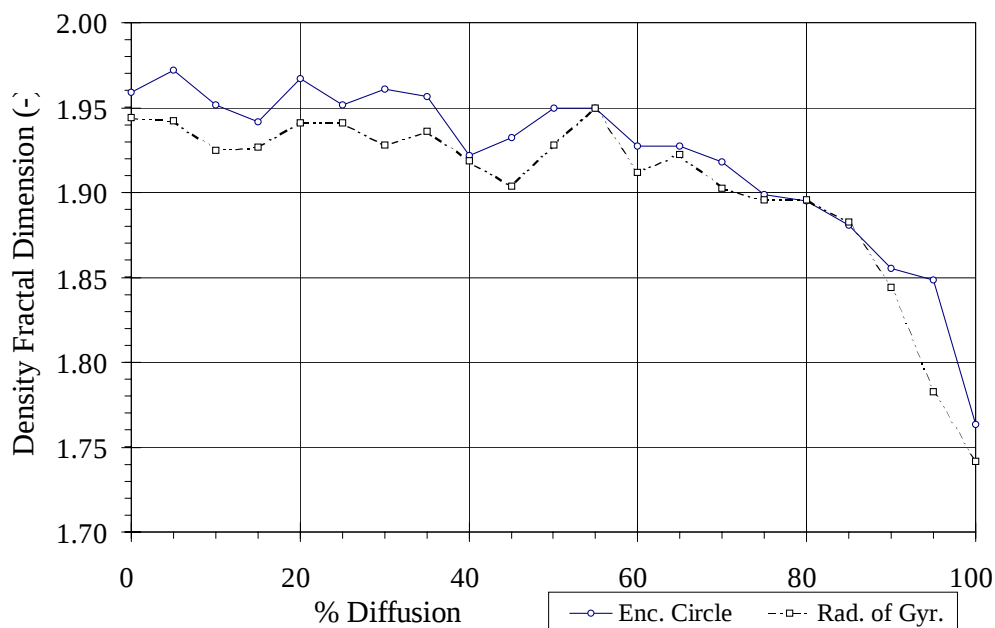


Figure 3: Enclosing circle and radius of gyration analyses for 2-D simulations.

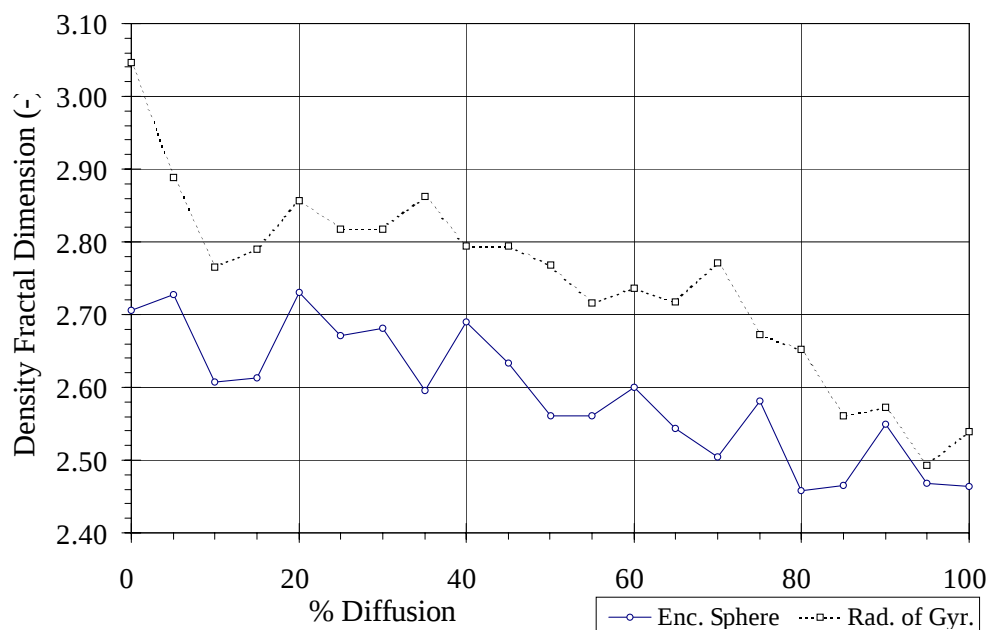


Figure 4: Enclosing sphere and radius of gyration analyses for 3-D simulations.