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THE USE OF FRACTAL DIMENSIONS IN FILTRATION

S.T.H. Brock and E.S. Tarleton (e.s.tarleton@lboro.ac.uk)
Department of Chemical Engineering, Loughborough University, Loughborough, Leics., LE11 3TU, UK.

ABSTRACT

To enable the fractal characterisation of structures in filtration systems, a computer program has been written to simulate and measure the characteristics of particles growing on a filter surface in two dimensions. Two analysis techniques have been used to give both a roughness factor (using a perimeter fractal dimension) and density factor (using an enclosing circle fractal dimension) for the simulations. These techniques have been used to characterise both the overall structure of the simulated cake and the interstitial spaces between particles. Results have shown a correlation between simulation parameters and fractal dimension.

KEYWORDS

Fractal dimension; Filtration; Simulation.

INTRODUCTION

Much work has been performed in recent years with regard to fractals[1]. Although most has apparently been of little practical use, some work has been performed to investigate the relationship between fractal dimension and the characteristics of particulate systems[2-4]. This area, which is of interest here, has been examined to determine the role of fractal dimension in characterising deadend filtration systems.

The data in this paper show a summary of the results from an ongoing research project examining 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 and thus provide more accurate filtration analysis and scale-up procedures than those currently available. The importance of particle motion to the structure of agglomerates, and hence filter cakes is highlighted.

SIMULATION OF CAKE GROWTH

A number of simulations have previously been performed, using a variety of methods. An example is that of Giona and Patierno[5] who used a Monte Carlo approach to model the build up of a particle structure on a surface. A typical structure was built on a square lattice (on-lattice simulation) and used particles of unit size, that is to say each particle only occupied one square of the lattice. An example of an on-lattice simulation is shown in Figure 1(a). The particle's movement is restricted to adjacent squares in the lattice, i.e. it can only move up, down left or right for any given step. The movement of the particle is governed by a downward probability, with values between 25% (particle is free to move in any of the four possible directions) and 100% (the particle will always move in the downwards direction).

In the current study, cake structures have been formed on a simulated filter surface by particles moving in two dimensions with a given downward and sticking probability. The downward probability is a value determining the likely direction of movement of the particle, whilst the sticking probability is the probability that a particle will stick to another on contact. In the simulation,

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particles are released from a random position at the top of the filter cell and allowed to move within the restrictions of the cell through a number of discrete steps until contact is made with another particle or the base of the cell containing the filter surface.

In contrast to many previous simulations, the model developed by the authors is an off-lattice simulation, that is to say with maximum freedom, a particle is allowed to move anywhere within a 360º radius. An example of an off-lattice simulation is shown in Figure 1(b). The particles used in the simulation are also circular, as opposed to single pixels, which better imitates particles in a filtration system. The motion of particles in the free space of the cell is controlled by the downward probability which is defined at the beginning of the simulation as a number between 0 and 100%. Zero per cent downward probability allows the particle to move in any direction from the current position. One hundred percent downward probability allows the particle to only move vertically downwards. The value of downward probability is infinitely variable between these two extremes, though in practice, intervals of 5% were used for the simulations.

The freedom of movement of a particle is defined by equation (1):

$$F = 360\frac{100 - P}{100} \tag{1}$$

where P is the downward probability and F the freedom of movement in degrees. This means that a particle can move in an arc of $F/2$ degrees either side of the vertically downwards direction. The direction in which a particle moves is defined by equation (2):

$$\theta = \psi\left(F\right) - \frac{F}{2} \tag{2}$$

where θ is the actual direction (degrees from the vertical) in which the particle moves and $\psi(F)$ simply gives a random value between zero and F itself. The downward probability is fixed for the entire simulation, but the direction for a particle is re-calculated after each successive step as the simulation progresses.

When a particle hits a wall of the cell, a new direction is calculated until the particle moves in a direction away from the wall. In this way a particle will move around the cell until contact is made with the base or another particle. When a particle touches the floor of the cell containing the filter medium, its position is instantly fixed and recorded by the program. If, however, a particle contacts another particle already at the surface of the growing cake, the sticking probability must be considered. This is another simulation parameter that is fixed at the start of the program, and calculated for each particle collision. As the failing particle contacts another, a random number between 0 and 1 (i.e. 0 and 100%) is generated. If the number is less than or equal to the sticking probability then the particle will remain at rest where it lands. If, the random value is greater than the sticking probability, however, the landing particle will roll over the particle(s) in the cake, as indicated in Figure 2.

A particle is considered to rest if it has two points of contact, or contact with the filter medium. Figure 2(a) shows the rolling mechanism if the falling particle (2) lands on top of another particle (1) and rolls to the floor unhindered. Figure 2(b) shows the mechanism if the falling particle (3) contacts another (2) after contacting the initial particle (1). Figure 2(c) shows the mechanism if particle (2) has the wall as a point of contact after rolling off particle (1). The falling particle is shown rolling in one particular direction in Figure 2, however, should it land on the other side of a target particle it will obviously roll in the opposite direction.

As well as being able to alter the downward and sticking probabilities, the size of the particles used in the simulation could be set. A size range was specified using a minimum and maximum particle

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radius, and choosing the size of each particle between the two. Coupled with the other probability parameters, this offers a wide scope for varying the simulations.

Using the method described, cakes comprising up to 10^3 particles have been built in a virtual filter cell. Simulations have been performed with varying combinations of downward and sticking probabilities, twenty simulations being generated for each pair of parameters. Using powerful PC's allows a large number of simulations to be carried out and analysed in a short time, enabling a broad picture of cake properties to be built up.

MEASURES OF CAKE PROPERTIES

After a cake structure has been built, it can be analysed using a variety of methods. Both the top surface and the overall structure of the cake can be categorised. The top surface has been analysed using the structured walk method to give a roughness fractal dimension. The overall structure of the cake is characterised by its porosity, which may be measured in two directions, vertically (base to cake surface) and horizontally (wall to wall) to enable a detailed picture of cake structure to be built up.

As well as the overall structure of the cake, the interstitial spaces within the cake may be analysed. Two fractal dimensions can be found for the pore spaces. Firstly a roughness dimension similar to that for the surface, and secondly a density fractal dimension, measured using the enclosing circle technique. The latter shows how the area of the pore space is distributed. Up to 99 pore spaces could be analysed for each set of simulation parameters. Using these methods of analysis, correlations were made between the simulation parameters and cake properties. Each of the analysis techniques was used on all the cakes simulated for each set of parameters and average values taken to represent that particular property for the cakes concerned.

Fractal Dimension

A fractal dimension can be measured for the surface of the cake and the interstitial spaces between the particles within the cake. The former is characterised using the structured walk (roughness fractal dimension) technique and the latter using both the structured walk and enclosing circle (density fractal dimension) techniques.

A structured walk is performed by stepping over the surface of the filter cake using virtual chords of varying lengths. As the steplength decreases, so more of the detail of the cake is shown and the measurable perimeter increases. The relationship between steplength and perimeter is given by equation (3):

$$P = \lambda^{(1-D_S)} \qquad (3)$$

where P is the perimeter measured using a steplength λ. By plotting the perimeter obtained against steplength on a log-log scale, the fractal dimension, D_S can be calculated; the slope of the plot having a value of $1-D_S$. The walk can be carried out in both directions (i.e. left to right and right to left) over the surface of the cake and an average of the two results taken. Good agreement between the two methods was observed in the majority of cases, although the technique can be sensitive to large fissures etc. in the cake structure. A high value for the fractal dimension indicates that the surface of the cake is rougher, as the perimeter increases at a greater rate with decreasing steplength. The structured walk technique applied to the surface of a typical simulated filter cake is shown in Figure 3, with the results of the analysis for a left-to-right structured walk.

Figure 4 shows that the perimeter fractal dimension rises steadily as the sticking probability is increased. As would be expected, at low values of sticking probabilities, the fractal dimension is close to the Euclidean dimension (1.00), but increases as the particles in the simulation become more likely to stick on contact with another particle. These results are also visually noted in the overall structure of the cake. Simulations with a low sticking probability show a smooth surface as the particles roll to rest, whereas large dendritic structures are formed as particles stick together without rolling. This dendrite formation is also seen in the simulations of Giona and Patiemo[5], which shows an increasingly open structure with low downward probability, although as Figure 4 shows, the downward probability has less of an effect on the structure than sticking probability. This open structure has also been seen in previous work involving the growth of agglomerates onto a seed particle[6], which showed that as the motion of the particles is changed from a straight line (ballistic) to random walk (diffusive) the structure of agglomerates built is more open (less densely packed), with a higher perimeter fractal dimension.

The structured walk was also used for analysing the interstitial spaces between particles in the simulated cakes. The technique required a pore space to be isolated by the computer program, and a subsequent structured walk around the outside of the space. In a similar way to the surface analysis, the fractal dimension was found by plotting the perimeter obtained against steplength used. The resulting dimension gives the roughness factor for the space. The structured walk fractal dimension for pore spaces was found to vary between 1.15 and 1.20.

The enclosing circle fractal dimension was also used to characterise the interstitial spaces. This method gives a value for the density fractal dimension, which is a description of the distribution of area of the pore space around its centre of gravity. As its name suggests, the method requires parts of the pore space to be enclosed by circles. These circles have their centre at the centre of gravity of the pore space and radiate outwards towards the outer edge of the pore space. The amount of space occupied by the pore space (measured in pixels) is plotted against the radius of the circle (measured in pixels) enclosing that space, again on a log-log plot, where the fractal dimension is given by equation (4):

$$a = r^{D_E} \tag{4}$$

where a is the pore area enclosed by a circle of radius r. A log-log plot yields a slope of fractal dimension, D_E. Figure 5 shows the enclosing circle technique, with the method for determining the fractal dimension.

Porosity

The porosity of the cake was measured using three different methods, the second of which gave an overall picture of the structure for comparison between the simulation parameters.

Method 1: Cumulative vertical porosity. This technique involves taking slices of the cake from the base of the filter cell up to the top surface of the cake. The porosity is measured as the fraction of the slice occupied by voids for each height of slice.

Method 2: Vertical porosity profile. This technique analyses the porosity of the cake in the same way as the cumulative method, however, the porosity is measured for each small slice, rather than the height of all the slices together. Once all the slices have been analysed, an average is taken to give the porosity of the cake. It is this method that has been used to characterise the overall cake structure.

Method 3: Horizontal porosity profile. This technique uses horizontal slices across the cake, from the left hand wall across to the right to enable phenomena such as the wall effect to be observed. This effect has been studied by others, such as Chan and Ng[7].

The vertical and horizontal methods are shown for the same cake in Figure 6. Figure 6 also shows a typical result for a vertical porosity profile. It should be noted that while the vertical profile is measured across the entire width of cell to show the porosity at that particular height, the horizontal profile only measures from the base of the filter cell up to the highest particle in the slice concerned, not the highest particle in the cake as a whole. This gives a truer value for the porosity at that point.

Figure 7 shows how the porosity of the cake structure increases with increasing sticking probability. Again this is expected as the cake structure becomes more open as the individual particles stick to one another. The minimum value for the porosity agrees well with literature values for theoretical minimum porosity[8]. The porosity increases from approximately 0.25 at 0% sticking probability to a maximum of approximately 0.70 as the sticking probability is increased to 100%. Again, a lesser effect is seen as the downward probability is increased, although the trend is more visible than that for the perimeter fractal dimension. As the downward probability is increased, so the structure of the cake becomes more compact and the porosity therefore decreases.

The methods of fractal and porosity analysis described here have been used to characterise a large number of simulated cakes with varying simulation parameters. The parameters investigated here were the downward and sticking probabilities of particles in the system. The results of these analyses are shown in Figures 4 and 7. The downward probability was seen to have less effect on the cake properties than the sticking probability, therefore the sticking probability was varied in 5% increments, whereas the downward probability was varied in 25% increments. The results show that as the sticking probability is increased, both the surface roughness fractal dimension and the porosity if the cake increase. The opposite is true of their relationship with downward probability, i.e. both the surface roughness fractal dimension and porosity of the cake decrease with increasing downward probability (for the same sticking probability).

CONCLUSIONS

The simulation parameters investigated to date have a quantifiable effect on the structure of the filter cakes built. Increasing the downward probability or decreasing the sticking probability makes the structure of a cake more porous, with larger dendrites forming. This will increase both the porosity and surface fractal dimension of the cake. The porosities measured for the simulations fall into the range of porosities calculated from experimental work with calcium carbonate and talc suspensions, indicating that it should be possible to match the simulation parameters with physical constants for the systems concerned. The next stage of experimental work is to sample real filter cakes and analyse their internal structure using various fractal dimensions and compare these to three dimensional simulations.

NOMENCLATURE

a	pore area (pixels)
D_E	fractal dimension, enclosing circle
D_S	fractal dimension, structured walk
F	freedom of movement (º)
P	perimeter (pixels)
R	radius of circle (pixels)
λ	steplength of structured walk (pixels)
θ	direction of movement (º)

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TABLES AND FIGURES

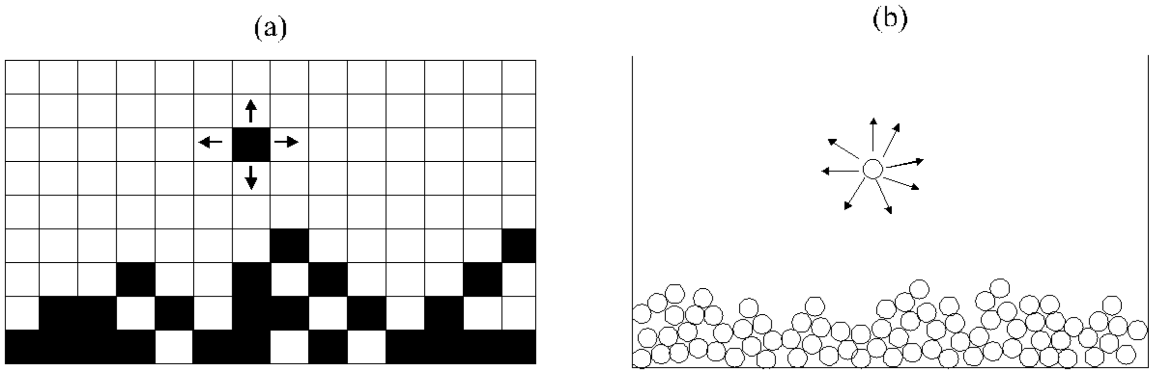

Figure 1: Typical on-lattice (a) and off-lattice (b) simulations.

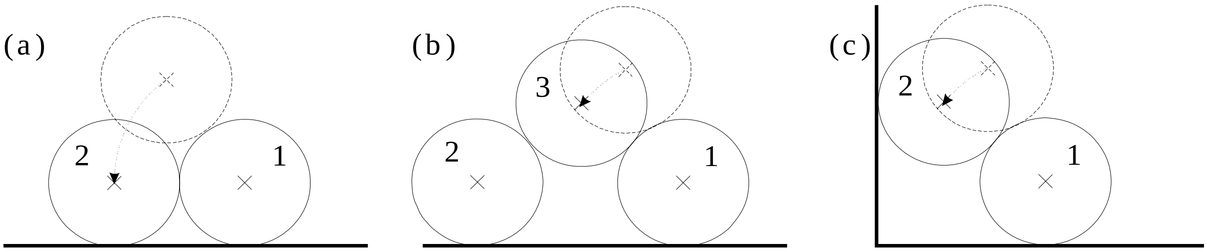

Figure 2: Particles rolling to rest at the base of the filter cell.

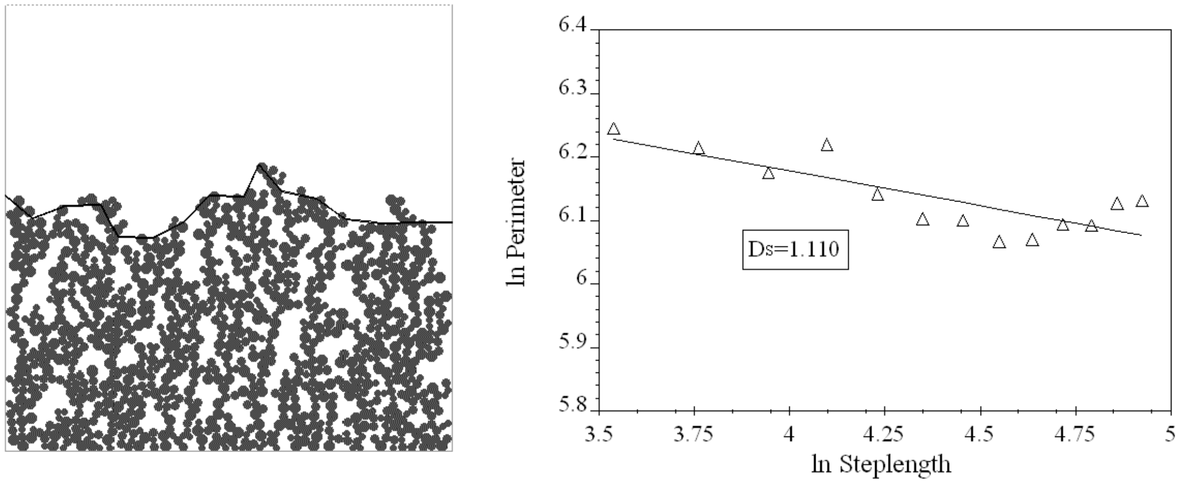

Figure 3: Structured walk technique for the surface analysis of a simulated filter cake.

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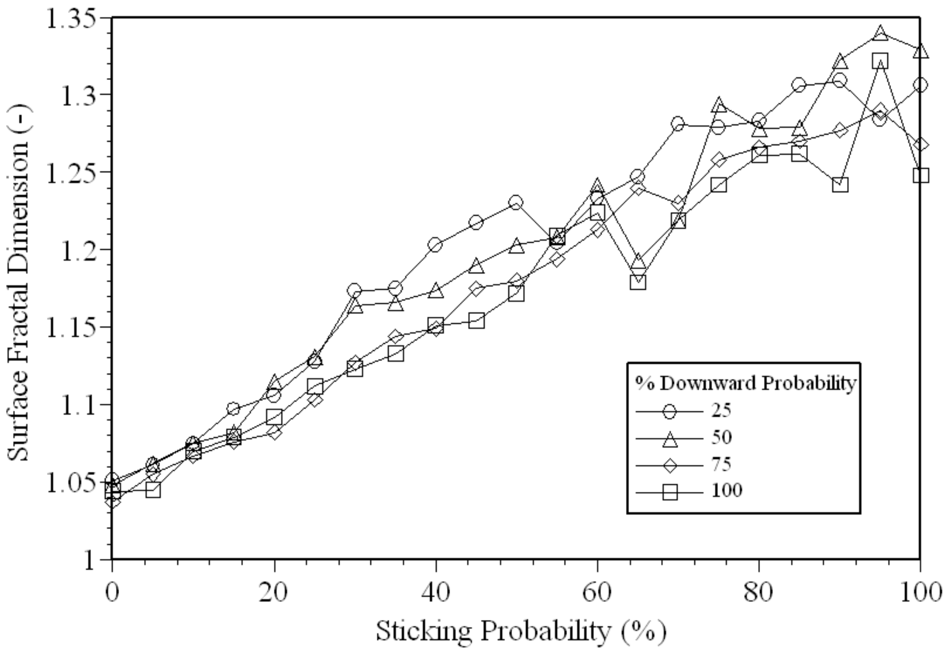

Figure 4: Structured walk analysis of simulated filter cakes.

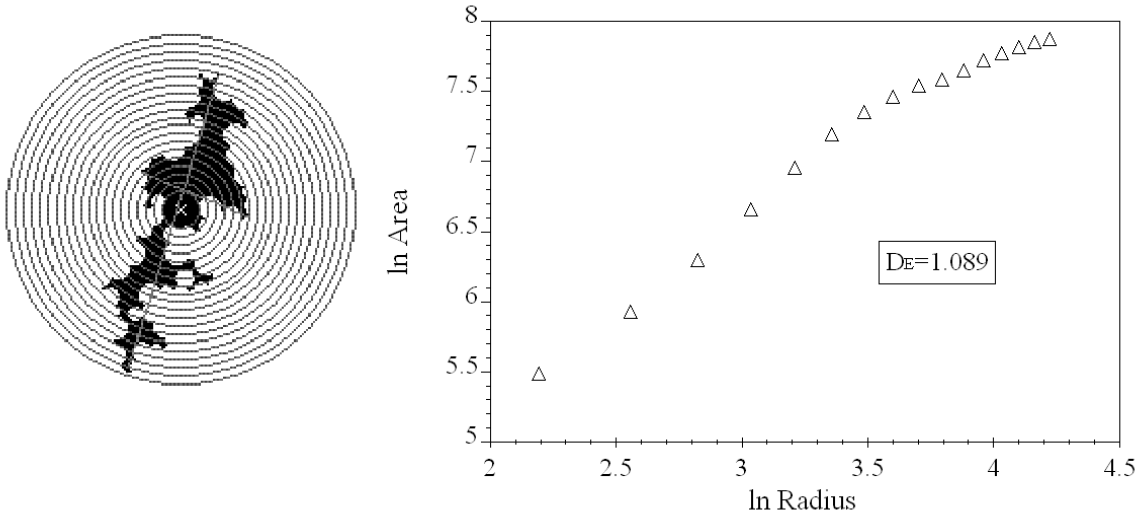

Figure 5: Enclosing circle technique for the analysis of an individual pore space.

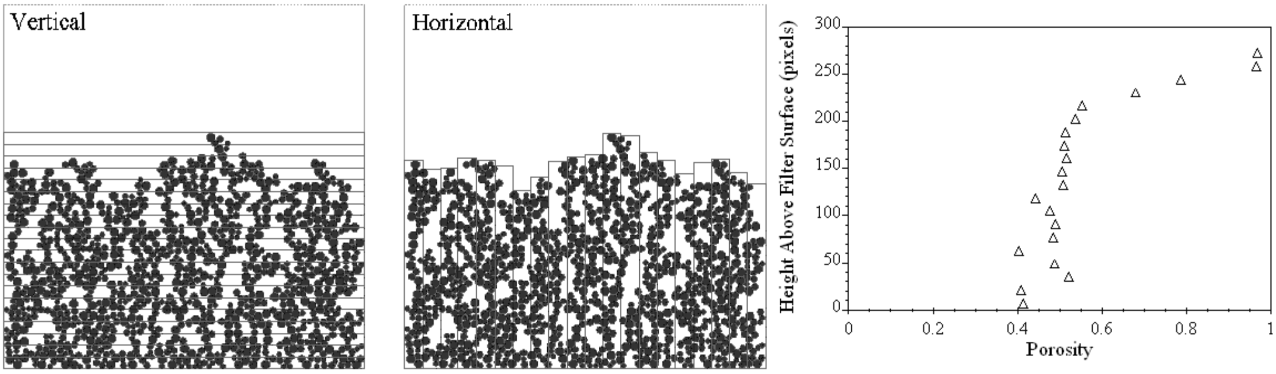

Figure 6: Porosity measurement showing vertical and horizontal methods.

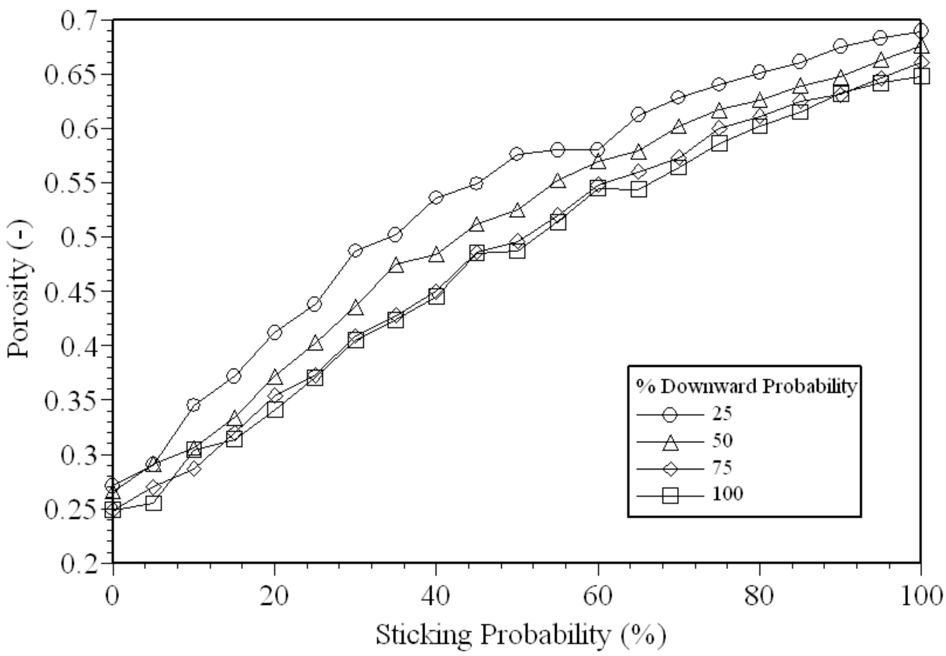

Figure 7: Porosity analysis of simulated filter cakes.

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