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Properties of percolating clusters on finite lattices applied to model filtration processes

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Patterns formed by neighboring blocked and blinded (occupied) cells in a filtration process are the same as the clusters formed in a percolation process. New criteria are discussed to detect for which occupation probability an infinitely long cluster occurs. Programs have been written that generate a Voronoi tessellation, create information for the cluster program of a regular triangular lattice, and produce clusters, calculating their fractal dimension.

Keywords: percolation theory, filtration process, lattices, clusters

1. Introduction

Activity in the modelling and simulation of membranes and filtration has increased rapidly in recent years. In particular, percolation theory has played an important part in these investigations.[1,2] *Figure 1* shows a modified Voronoi network as a model for a filter membrane. The Voronoi structure is based upon a Poisson random distribution of centers.

It is tempting to consider the vertices as sites and the cell edges as bonds. However, since particles in the fluid occupy the cells at random the cells should be seen as sites or bonds. The easiest approach is then to consider the cells themselves or their nuclei as sites. The bonds are then the (virtual) lines connecting neighboring sites (nuclei). They are the edges and nodes on the matching Delauney triangulation which are, respectively, the bonds and the sites of the percolation problem (*Figure 2*). Evidence from much experimental data suggests that such a model is very suitable for a number of practical applications.[3,4]

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2. Terminology and notation

Consider a structure (network, tessellation, lattice) consisting of sites (atoms, nodes) and bonds. The bonds can be oriented (directed) or not. The coordination number, z, of a regular structure (i.e., one based upon the regular plane figures) is the number of bonds leaving each site. Two sites are said to be neighboring if they are connected by one bond.

Two distinct types of percolation exist: bond and site. In the former, each bond has a finite probability, p, of being opened or $q = 1 - p$ of being blocked. In site percolation, it is the sites that are opened (or closed) with a fixed probability. In both cases, the "fluid" cannot pass through blocked entities. In Ref. 5 it is demonstrated that every bond percolation problem can be converted into a site problem on another structure, the covering lattice. This lattice can be constructed by placing a site on each bond of the original lattice and drawing a bond between any sites whose corresponding bonds on the original lattice have a common site. Site percolation is thus the more fundamental type of percolation and is the only type to be considered in this paper.

It is stressed that the idea of a fluid is merely used to define the percolation problem in a comprehensible (physical) manner. In order to understand most of the percolation properties, fluid should be interpreted in a a more mathematical sense, such as "there is a

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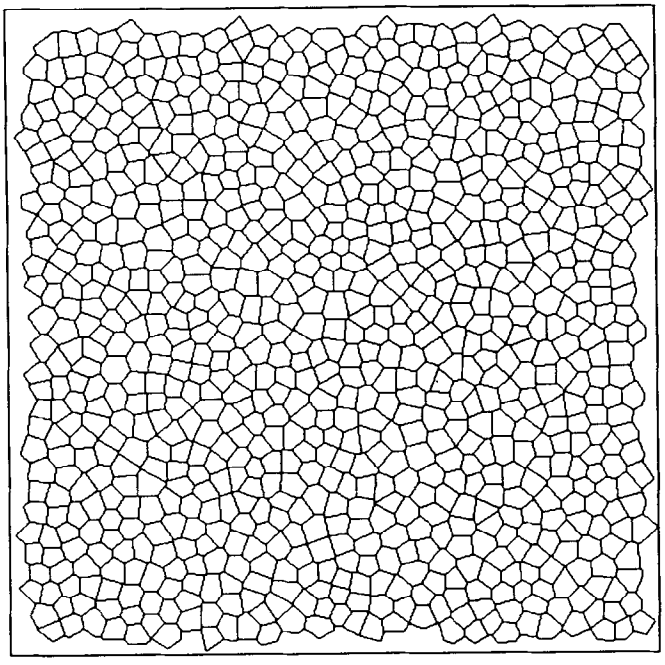

Figure 1. A modified Voronoi network as a model for the filter membrane

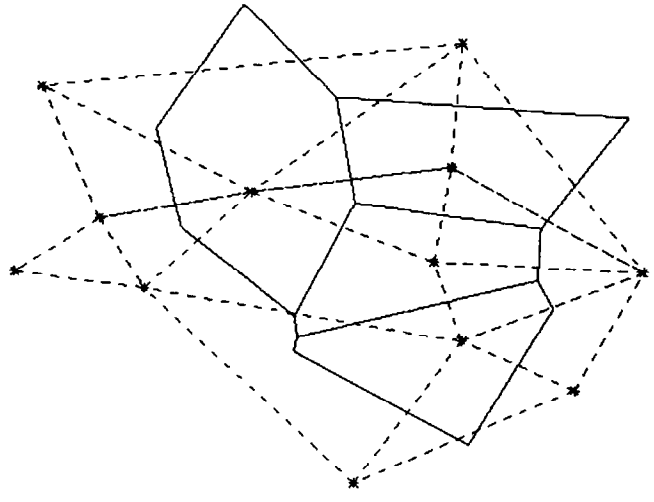

Figure 2. A small Voronoi tessellation (bold) and its Delaunay triangles

connection between ..." In some applications one will call opened sites empty and blocked ones occupied. This is the terminology used for the application described in this paper in order to avoid confusion with the blockage of a pore (see below).

Occupied sites are either isolated from other occupied sites or they form small groups of neighbors. These groups are called clusters. Isolated sites are regarded as clusters of size unity. Generally, we call any cluster consisting of s occupied and connected sites an s-cluster, i.e., a connected component of size s. Simulation is assumed to take place on a finite lattice. In order to generate some statistics about the clusters of independent lattice size it is convenient to divide the number of clusters by the number of lattice sites in the whole lattice. We define $n_s(p)$ to be the average number of s-clusters per site. This is also the total number, E, of s-clusters divided by the number of sites in the structure.

If the probability, p, of being occupied is near zero, then most sites will be isolated with only a few pairs and triplets present. If, on the other hand, p is close to unity, then nearly all opened sites are connected to each other and form a large cluster, the percolating, incipient, or spanning cluster. *Figures 3–5* show the clusters formed by various occupation probabilities. At $p = 0.42$ there is no spanning cluster (*Figure 4*), whereas increasing the occupation probability to $p = 0.52$ causes a spanning cluster to occur (*Figure 5*). Percolation theory deals with the number and properties of these clusters, how they occur, and the way in which the fluid flows through the membrane.

The probability that a site chosen at random belongs to an N-sized cluster (in physical terms that fluid from an arbitrary site will wet $N - 1$ other sites) is denoted by $P_N(p)$. Alternatively, $P_N(p)$ is the fraction of sites (occupied or not) belonging to an N-size cluster. P_N and n_s are related thus

$$P_s(p) = sn_s(p) \tag{1}$$

$P_\infty(p)$ is the probability that a randomly chosen atom wets infinitely many others, or in general terms, the probability that a randomly chosen site belongs to an (the) infinite cluster. It is also the fraction of sites belonging to the infinite cluster. The probability that an arbitrary site belongs to any cluster is therefore equal to the probability p that it is occupied:

$$\sum_s sn_s(p) + P_\infty(p) = p \tag{2}$$

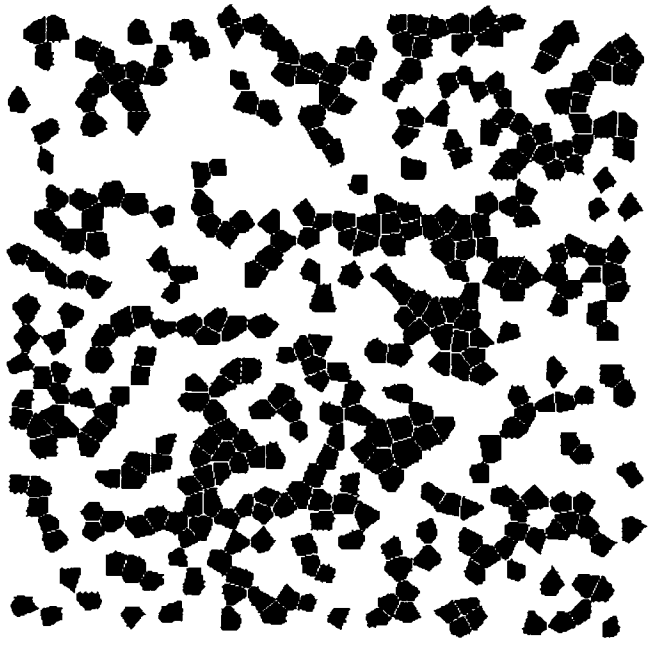

Figure 3. Clusters on a modified Voronoi lattice at $p = 0.30$

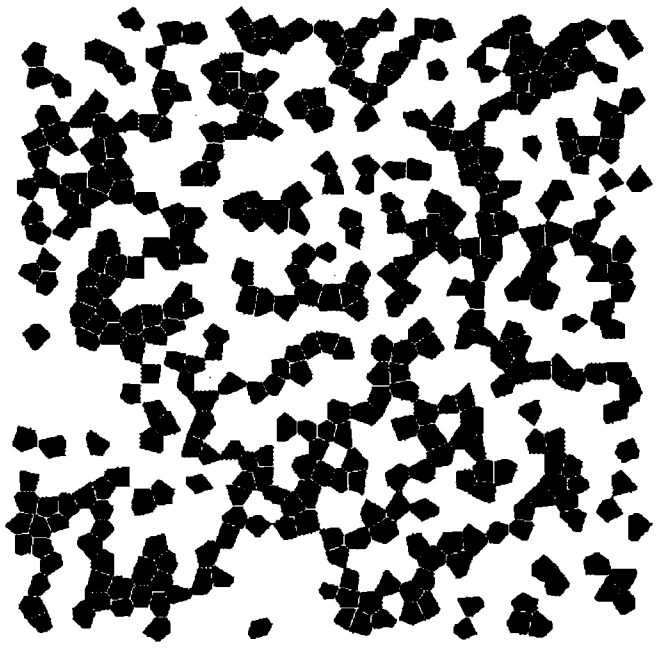

Figure 4. Clusters on a modified Voronoi lattice at $p = 0.42$

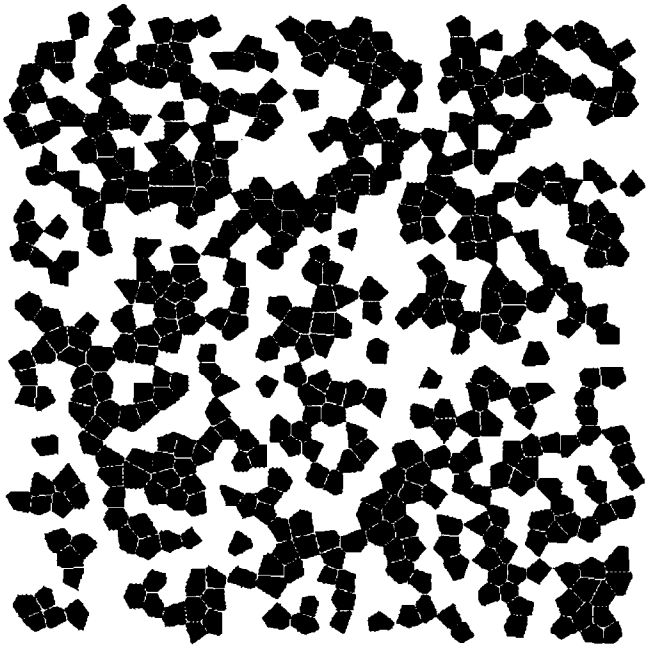

Figure 5. Clusters on a modified Voronoi lattice at $p = 0.52$

The sum is taken over all finite s. The percolation probability, p_c, is then defined as

$$p_c = \sup(p | P_\infty(p) = 0) \tag{3}$$

A real structure is usually finite. To apply percolation to a physical structure with finite dimensions, another definition of percolation is required. A connecting cluster is defined as a cluster that connects two opposite sides of the structure. The percolation probability then becomes:

$$p_c = \frac{n_c}{N}$$

and

$$n_c = \sup(n | \text{no connecting cluster exists}) \tag{4}$$

where N is the number of sites in the membrane, and n is the number being occupied. In Ref. 6, it is shown that the second definition becomes equivalent to the first in the limit $N \to \infty$. p_c is thus a threshold where for the first time an "infinite" percolating cluster occurs.

Critical probabilities, p_c, for a number of lattices, have been estimated by Monte Carlo calculations and from series expansions of the mean cluster size (see Section 5). Exact solutions for p_c have also been obtained for a few two-dimensional lattices. Sykes and Essam[7] calculated the exact critical probability on some two-dimensional lattices by using the idea of a matching lattice. Until now, no report has been made of an exact formula for p_c (site percolation) on a square lattice. In Ref. 8, p_c is obtained by Monte Carlo simulation using a polynomial expression (*Table 1*). Thus, a percolating cluster of infinite size occurs at $p = p_c$. For two-dimensional site percolation problems, Fisher[3] proved that two infinite clusters cannot coexist. A more general proof (in all dimensions) of the uniqueness of the percolating cluster is given by Grimmet.[9]

Finally the average cluster size, $S(p)$, is given by

$$S(p) = \frac{\sum_s s^2 n_s(p)}{\sum_s s n_s(p)} = \frac{\sum_s s P_s(p)}{\sum_s s n_s(p)} \tag{5}$$

where the sums are taken over all finite s. If $S(p)$ were to be calculated over all s (loosely defined as the real mean cluster size) then the average cluster size would become infinite above p_c since there exists an infinite cluster. The average cluster size given by equation (5) increases until reaching a peak at p_c, after which it decreases with increasing p.

3. Percolation on a Voronoi structure

For the percolation considered in this paper the Voronoi lattice has a (percolation) coordination number of 6, i.e., each site is connected on average with six neighboring cells (each cell has an average of 6 edges or 6 neighbors). In this case the triangular lattice has the same percolation coordination number.

Table 1. Percolation probabilities

Lattice type	p_c
Triangular	0.5
Voronoi	0.5
Hexagonal	0.7
Square	0.59275[6]

In the original percolation problem all sites have the same fixed probability p of being occupied. This situation will be simulated by blocking randomly chosen cells of the lattice until $100p\%$ out of the total amount of sites is occupied. (If we choose again an already occupied cell we resume by choosing a new one.) It is believed that owing to the law of large numbers, this is a good realization of the theory. Cluster size data was averaged over several simulation runs.

With regard to the blockage process of the filter, some additional features must be added to the membrane model. A distribution of particles in the feed is considered and the particle size of these is represented by the diameter, D_p. Assume that there is an equal probability of any particle in the fluid (the feed) settling on any pore of the membrane. Thus, take a random pore and select a particle from a normal distribution. With the first and second moments of $f(D_p)$ defined, a particle diameter can be selected using the central limit theorem:

$$D_p = \bar{D}_p + \frac{\sigma}{(N/12)^{1/2}} \sum_{n=1}^{N} \left(r_n - \frac{N}{12} \right) \tag{6}$$

where r_n is a uniformly distributed random number between 0 and 1 (which is normally available in a programming language) and $N \geq 12$. $\bar{D}_p$ is taken as the mean hydraulic diameter (i.e., 4 × area/perimeter) of the membrane cells. This diameter is a close enough approximation to the diameter of the maximum inscribed circle of a pore. By varying the coefficients $\bar{D}_p$ and $\sigma(D_p)$ in the particle distribution function $f(D_p)$, the effect of varying particle sizes on the performance of the membrane can be examined.[3]

Initially, the pore that is chosen to interact with the particle is open. The diameters of the pore and the particles are then compared. If the particle is bigger than the pore the particle will block it. Otherwise it will flow through the membrane. Lim[3] and Chan[4] considered a third case: when $D_{Pore} \leq D_{Particle} \leq 1.1D_{Pore}$ then the pore becomes blinded. The difference between being blinded and blocked is that, for example by means of backflushing, a blocked pore can be reopened (freed of its particle). Only the blockage of cells is considered in this paper.

If a particle arrives at a pore j, which is already blocked, then pores in the immediate neighborhood of j are examined to see if any of these are open. If a neighboring free pore is available, the particle is allowed to pass to this for processing. If all the surrounding pores are sealed, the particle settles onto the surface of the membrane.

The alterations to the standard percolation problem necessary to form a model of the filtration process can be summarized as follows:

(1) A chosen pore can only become occupied if the incoming particle is larger than the pore, and
(2) If a pore is already occupied then its neighbors are investigated.

If a regular lattice is used as a model of the membrane (e.g., a honeycomb structure), the first difference would have no effect on the cluster formation (it will only take more computation time to occupy all the cells). The "modified" blockage process has been applied to a modified Voronoi lattice consisting of 80,000 cells, with σ (cell area) = 0.29 × mean cell area. The average particle diameter $\bar{D}_p$ was chosen to be the averaged hydraulic diameter of the cells. By varying the coefficients $\bar{D}_p$ and σ in the particle distribution function, $f(D_p)$, the effect of varying particle sizes on the performance of the membrance can be examined.[3]

Using the "percolation" detection criterion described in Section 4, it was found that p_c has a higher value than in the standard percolation problem (*Figures 6a and 6b*). The value of p_c increases with the narrowing of the particle size distribution. The particle size dispersion $\sigma(D_p)$ indicated below the horizontal scales in *Figures 6a and 6b* is expressed as a fraction of the mean particle diameter. The higher value of p_c is due to some large unoccupied holes which are necessary to form the infinite cluster from large finite ones. The chance of becoming occupied by a big enough particle decreases with decreasing $\sigma(D_p)$.

This also yields a decrease in the average cluster size (*Figure 7*) particularly above intermediate p ($p > 0.4$), where bigger clusters are formed by the coalescing of smaller ones. It then happens that cells in between two clusters are too large to become occupied.

The second alteration (2) with random occupation causes the clusters to expand more quickly. The chance of an empty cell, neighboring a cluster, becoming occupied is the probability that that cell is chosen, increased by the chance that a neighboring occupied cell is rechosen. Empty sites, away from a cluster, have less chance of being chosen. It is this type of empty site that gives the most contribution to the total perimeter in the structure, and, since they are less likely to become occupied, the total perimeter remains "shorter" (*Figure 7*).

4. Detection of the percolation threshold

Percolation probabilities are exactly known or well approximated on regular and Voronoi lattices. However, by applying a different process to decide whether to occupy a site or not, the percolation threshold may change. In this section some criteria are studied to investigate such changes.

Be definition, at an occupation probability, p_c, an "infinite" cluster is being formed. By calculating the real mean cluster size above the percolation threshold, it is seen that the mean size diverges to infinity for $p > p_c$. However, in equation (5) the sum is calculated over finite cluster sizes. The mean cluster size then has a distinctive peak at p_c.[7] On a finite lattice it is difficult to know when an infinite cluster occurs. Usually that cluster is defined as the first spanning cluster (touching two opposite borders). This assumption is only valid for large lattice sizes and preferably when periodic boundary conditions are used (i.e., occupied sites at the same height on the

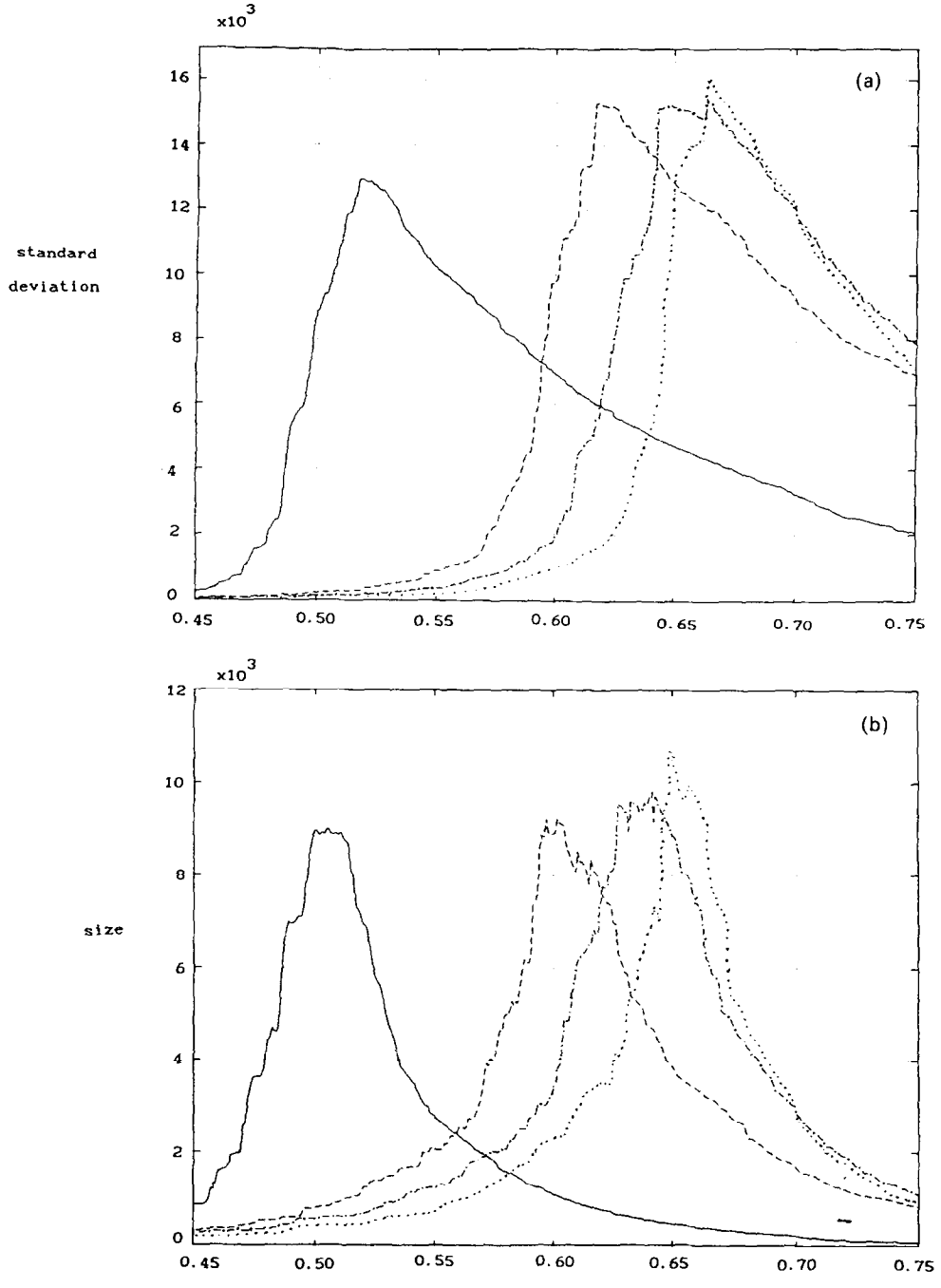

Figure 6. Detecting p_c for different particle distributions. (a) The standard deviation on the mean cluster size calculated over all clusters (80,000 cells) ——, percolation; – – –, Sdev (particle) = 0.4; –·–·–, Sdev (particle) = 0.2; ·····, Sdev (particle) = 0.1. (b) The largest cluster size minus the mean cluster size calculated over all clusters (80,000 cells)

extreme left and right borders of the lattice belong to the same cluster).

Since it cannot be decided exactly whether an "*infinite*" cluster has occurred, it is not possible to calculate the mean cluster size according to equation (5). Thus, the difference between the size of the biggest cluster and the real mean cluster size has been calculated. Ideally, on an infinite lattice, this should diverge to infinity at p_c and then drop to zero, above p_c. *Figure 8* shows the plot of that curve for a Voronoi lattice, a triangular lattice, and a square lattice, for a tessellation of 100,000 sites (the curve is also the average over five runs). As can be observed, there is a distinct peak very near the theoretical value of p_c ($p_c = 0.5$ for the Voronoi and triangular lattice and 0.6 for the square lattice). This criterion was averaged over 5 tessellations. It is then

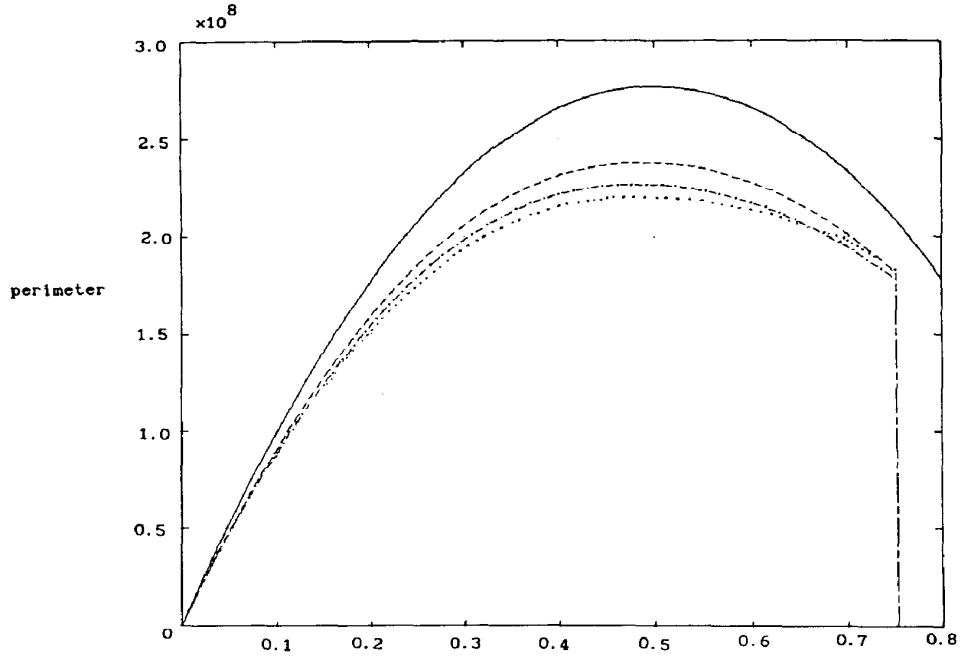

Figure 7. Total cluster perimeter for different particle distributions (the total perimeter in the lattice at increasing p (80,000 cells). ——, percolation; – – –, Sdev (particle) = 0.4; –·–·, Sdev (particle) = 0.2; ·····, Sdev (particle) = 0.1

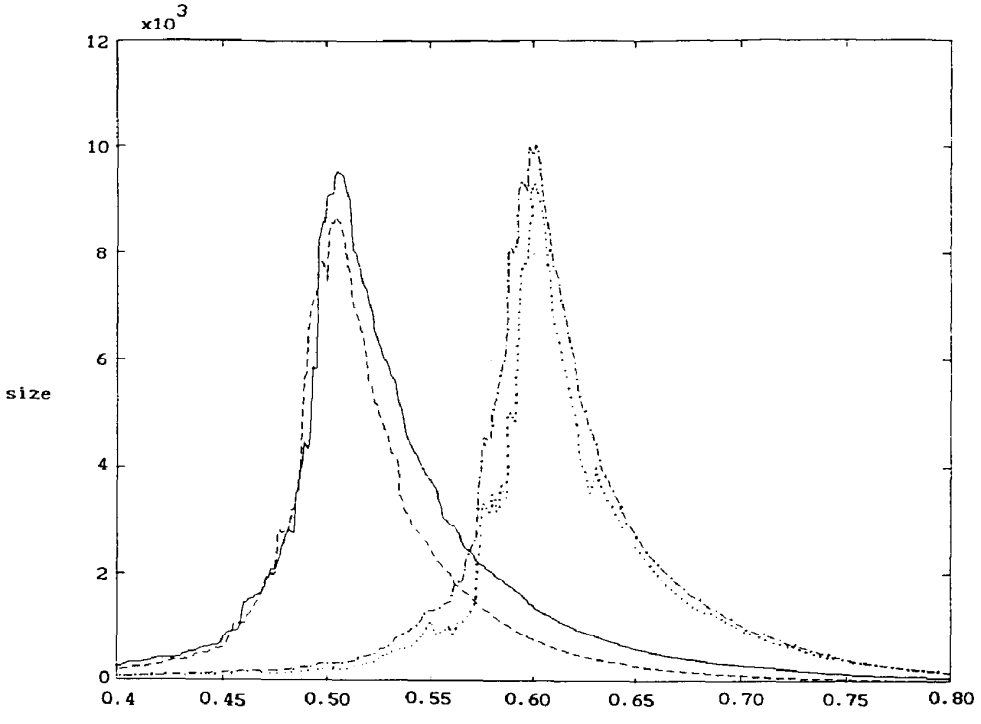

Figure 8. The largest cluster size minus the mean size calculated over all clusters (80,000 cells). ——, Voronoi; – – –, triangular; –·–·, square lattice; ·····, Sdev on square lattice

possible to calculate a standard deviation for the criterion at each p; this is plotted for the square lattice.

Another method of finding the percolation threshold is to look at the behavior of the standard deviation of the mean cluster size for increasing p. *Figure 9* shows the standard deviation for a Voronoi, triangular, and square lattice. Again, bearing in mind the mean cluster size behavior, there should be a peak at p_c. As can be observed, the peak lies near and slightly above, the percolation threshold.

Yet another criterion to find p_c could be to consider

the total perimeter in the network. When only one site is occupied, the total perimeter is that of the particle. When all sites are occupied, the total perimeter is that of the hull around all sites. It is clear that at intermediate occupation probability there is more perimeter in the network than at low or even at full occupation. *Figure 10* shows the plot of the total perimeter in the network. For triangular and Voronoi lattices, this maximum is at $p = 0.5$ and coincides with the percolation threshold p_c. However, when plotting the total perimeter formed by clusters on a square lattice by increasing p, the maximum is

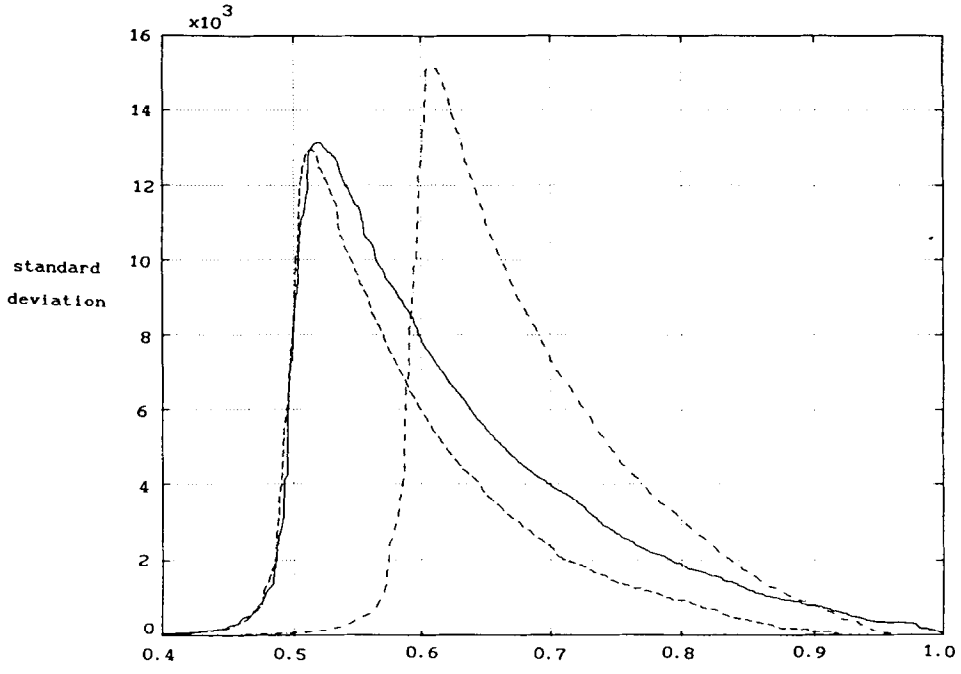

Figure 9. The standard deviation on the mean cluster size calculated over all clusters (80,000 cells). ——, Voronoi lattice; – – –, triangular lattice; –·–·, square lattice

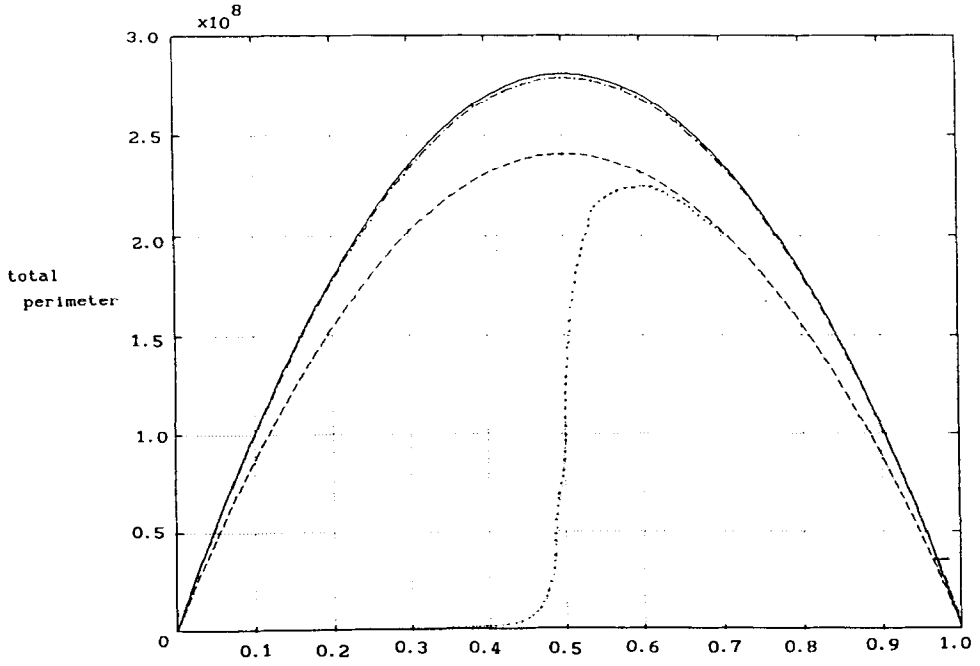

Figure 10. The total perimeter in the lattice. ——, Voronoi lattice; – – –, triangular lattice; –·–·, square lattice; ·····, perimeter of largest cluster

still at about $p = 0.5$, which is not the p_c for a square lattice. The total perimeter is therefore not a good criterion to find p_c.

Finally, *Figures 11* and *12* show the area and perimeter, respectively, of the largest cluster at a certain p. Since at p_c this largest cluster becomes "infinite," its area and perimeter should diverge as well. Although the plot shows the data obtained on a tessellation of 80,000 cells, the transition is not very visible and so it looks more difficult to determine the p_c. The first criterion (largest cluster size minus average cluster size) seems to be the best.

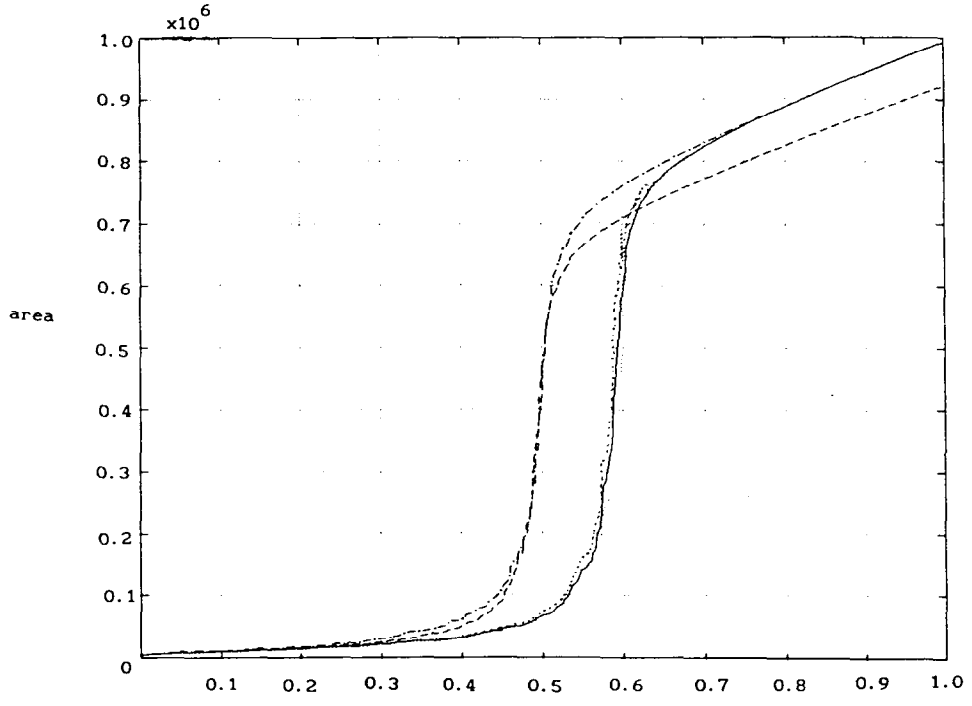

Figure 11. The area of the largest cluster for increasing p. ——, Voronoi lattice; – – –, triangular lattice; –·–·, square lattice; ·····, Sdev on square lattice

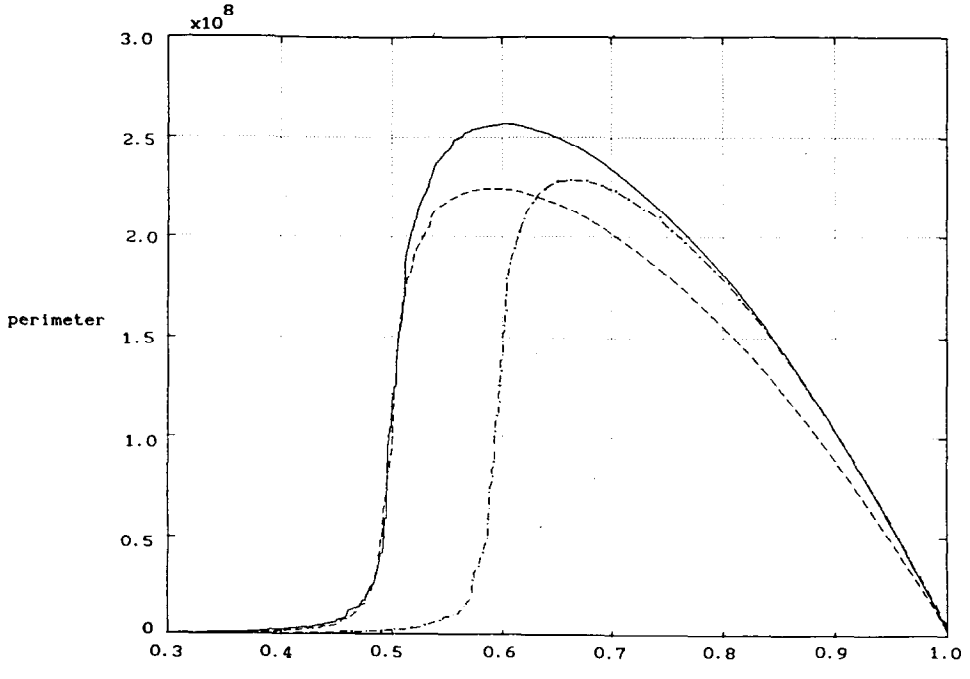

Figure 12. The perimeter of the largest cluster for increasing p (80,000 cells). ——, Voronoi lattice; – – –, triangular lattice; –·–·, square lattice

5. Series expansions

The average number, n_s of "small" clusters on regular lattices can be calculated exactly. Take for example a pair in the square lattice, i.e., a two-size cluster. It consists of two occupied squares surrounded by six empty neighboring squares. Moreover, it can be oriented either horizontally or vertically in the lattice. Thus, the average number of pairs is $n_2 = 2p^2(1-p)^6$ since in percolation each of the squares involved is either occupied (with probability p) or empty (with probability $q = 1 - p$) entirely independently of the other squares. $n_i(p)$ for $i = 1,2,3$ are given below for square and triangular lattices (*Table 2*).[10]

Generally, the number of empty lattice sites that are nearest neighbors to occupied cluster sites is denoted by the perimeter, t, and the number of geometrically different s-sized cluster configurations with perimeter t as g_{st}. Sometimes g_{st} is called the number of lattice animals or polynomios. The number of s-sized clusters can be written exactly as

$$n_s(p) = \sum_t g_{st} p^s (1-p)^t \tag{7}$$

It is easy to calculate at what occupation probability, p, the maximum of a certain cluster number occurs. This maximum is found by setting the p-derivative of n_s equal to zero. On a square lattice, for $s = 1$, one finds $p_{max}(1) = 1/5$, and for $s = 2$, $p_{max}(2) = 1/4$. In both cases the position of the maximum is below the percolation threshold $p_c = 0.59275$ and for the larger cluster the maximum is closer to p_c than for the smaller one. If one determines the position of $p_{max}(s)$ for intermediate s, one can then show that p_{max} extrapolates for $s \to \infty$ to a value very close to p_c. *Figures 13–15* show the probability distribution of clusters of sizes of 1 to 4 calculated from series expansion and from the Monte Carlo simulation used in this work. The calculations apply in this case to a square and triangular lattice. Excellent agreement between these two sets of results are shown.

Table 2. Average number of small clusters

	Square	Triangular
$n_1(p)$	pq^4	pq^6
$n_2(p)$	$2p^2q^6$	$3pq^8$
$n_3(p)$	$p^3(2q^8 + 4q^7)$	$p^3(2q^9 + 9q^{10})$

It appears to be an extremely difficult task to calculate the cluster occurrence on Voronoi lattices by series. One can try to calculate the occurrence of a one-sized cluster by using the approximated distribution function of the cell edges. This leads to a sum of terms like $C_i p(1-p)^i$, with i the cell order and C_i the probability of an i-edged cell. For bigger clusters this would become an incommensurable task. Since the triangular lattice has the same coordination number as the Voronoi lattice, a resemblance between the exact formulas of *Table 2* and the computer data of the Voronoi structure could be hoped for. The resemblance between the data and the exact plot of $n_s(p)$ of triangular lattices is very good below $p = 0.1$. However, above this value the agreement deteriorates (i.e., where the powers of $1 - p$ in the expansion series get more predominant). The exact solution for a triangular lattice is thus not the exact one on a Voronoi lattice.

The real strength of the exact polynomials for $n_s(p)$ lies in the determination of p_c and the critical exponents

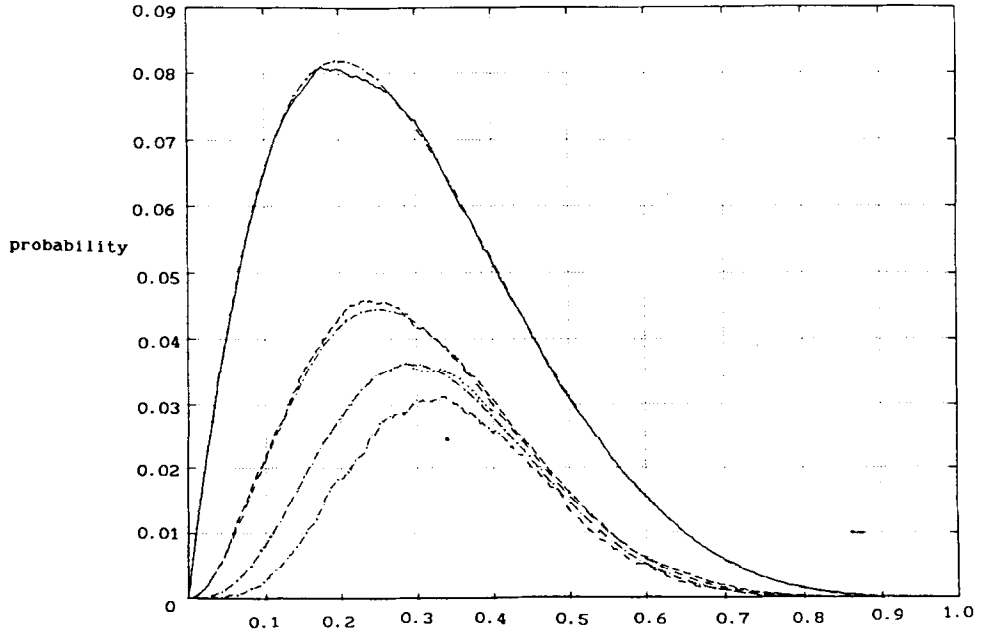

Figure 13. The probability distribution of clusters from series expansion and Monte Carlo simulation—square lattice. ——, 1-size clusters; – – –, 2-size clusters; ·····, 3-size clusters; –·–·, 4-size clusters and the exact probability

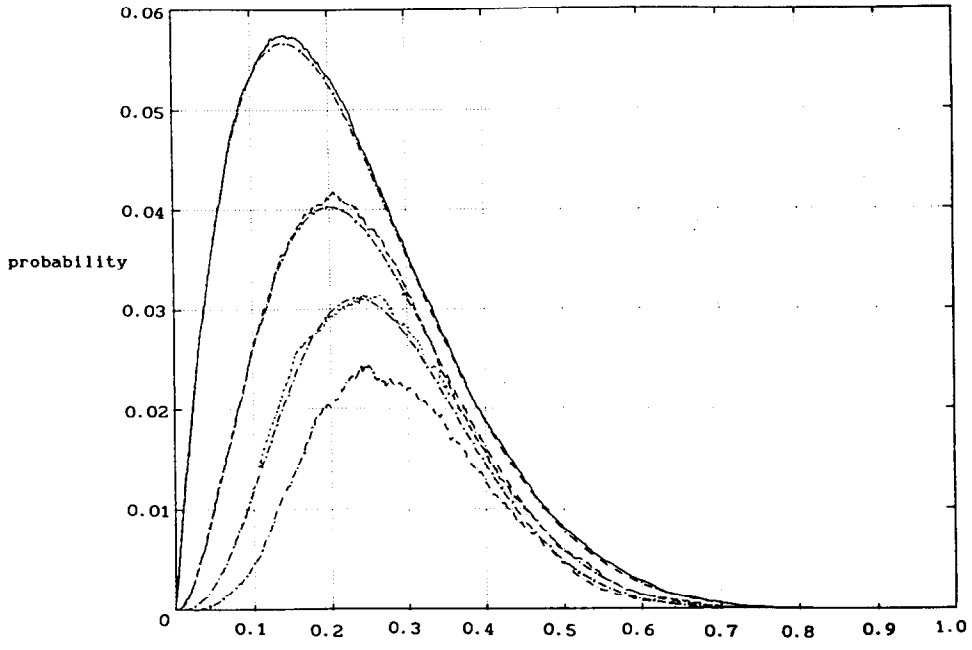

Figure 14. The probability distribution of clusters from series expansion and Monte Carlo simulation—triangular lattice. ——, 1-size clusters; – – –, 2-size clusters; ·····, 3-size clusters; –·–·, 4-size clusters and the exact probability

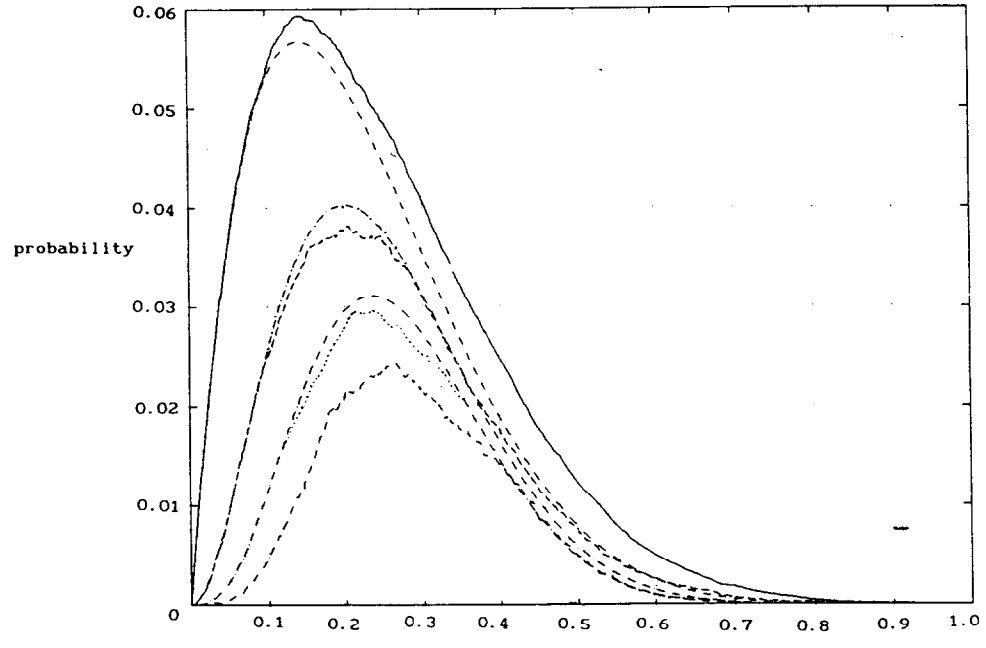

Figure 15. The probability distribution of clusters from series expansion and Monte Carlo simulation—Voronoi lattice. ——, 1-size clusters; – – –, 2-size clusters; ·····, 3-size clusters; –·–·, 4-size clusters and the exact probability

like β, γ, and σ (see Section 6). For this purpose all terms $(1-p)^t$ of $n_s(p)$ are being expanded by the polynomial law and orders the results in powers of p. Thus, we arrive at the power series for the moment M_k of the cluster size

$$M_k = \sum a_i p^i \tag{8}$$

By looking at the radius of convergence of this series, for example $k = 2$, the percolation threshold, p_c (most moments of the cluster size diverge at p_c), is found. However, this determination is inaccurate since only cluster numbers to $s \cong 20$ are known. Suitable extrapolations like the ratio method and Padé approximations gave the percolation threshold and the critical exponent with great accuracy from a limited number of expansion terms.

6. Dimensional invariants

Certain features of the critical probabilities, p_c have been observed to depend only on the dimensionality of the lattice and not on the specific lattice type. Scher and Zallen[11] introduced a dimensional invariant useful for site percolation. The critical volume fraction, v_c, is defined by the ratio of the area of the circles centered on opened sites with a radius half the nearest-neighbor distance to that of the lattice. It then appears that $v_c = 0.45 \pm 0.02$ for two-dimensional regular lattices.

Other better known dimensional invariants are the critical exponents. The behaviour of p close to p_c is called the critical behavior. The major part of percolation theory deals with the peculiar phenomena near that concentration p_c. The theory attempting to describe them is called the scaling theory. This theory was used to describe phase transitions long before the advent of percolation. There is a strong analogy between the two theories which has made it possible to copy the scaling equations. Phase transitions were encountered in various research fields. The scaling exponents in the 1/2 spin Ising model for Ferromagnetism have been very important in the development of percolation theory. In the 1/2 spin model the singular part of some magnetic properties near the critical Curie temperature T_c are observed to behave according to powers of the distance from the critical point, i.e., $T_c - T$. (The local order of magnetic moments increases in range as the temperature is lowered to the transition temperature, T_c, of the material. Below T_c, the magnetic moments are aligned, on the average, throughout the sample and we have a magnet. The magnetization, $m(T)$, vanishes as a power-law $(T_c - T)^\beta$ for many magnetic materials near the critical point). The same happens in the percolation model for some cluster size properties. The correspondence between both theoreies can be summarized as follows:[12]

Mean number of clusters	↔ Zero-field free energy
Percolation probability	↔ Spontaneous magnetisation
Mean size of clusters	↔ Initial susceptibility
Pair connectedness	↔ Correlation function

The scaling equations are supposed to be valid only for p near p_c. Furthermore, they only give information concerning the leading nonanalytic (i.e., singular or critical) part of the quantity involved (e.g., singular or critical) part of the quantity involved (e.g., the mean cluster size). Three of them concern the main moments of the cluster size.

$$n_s(p) \propto s^{-\tau} F[(p - p_c)s^\sigma] \quad \text{and} \quad n_s(p) \propto s^{-\tau} \tag{9}$$

$$\sum_s n_s(p) \propto |p - p_c|^{2-\alpha} \tag{10}$$

$$\sum_s s n_s(p) \propto P(p) \propto (p - p_c)^\beta \tag{11}$$

$$\sum_s s^2 n_s(p) \propto S(p) \propto (p_c - p)^{-\gamma} \tag{12}$$

Equations (10) and (12) are sometimes written as

$$\sum_s s^k n_s(p) = M_k \propto |p - p_c|^{(\tau - 1 - k)/\sigma} \tag{13}$$

The critical exponents α, β, and γ can then be written as combinations of τ and σ

$$2 - \alpha = \frac{\tau - 1}{\sigma}, \qquad \beta = \frac{\tau - 2}{\sigma}, \qquad \gamma = \frac{3 - \tau}{\sigma} \tag{14}$$

Before giving the final scaling equation some further definitions are required. The correlation function or pair connectivity, $g(r)$, is the probability that a site, distance r from an occupied site, belongs to the same cluster. The radius of gyration, R_s, is the average root mean square distance between occupied sites that belong to the same finite cluster. It is given by

$$R_s^2 = \sum_{i=1}^{s} \frac{|\mathbf{r}_i - \mathbf{r}_0|^2}{s} = \sum_{i,j} \frac{|\mathbf{r}_i - \mathbf{r}_j|^2}{2s^2} \tag{15}$$

$\mathbf{r}_0$ is the position of the center of mass of the cluster. The coherence, correlation, or connectivity length, ξ, is the average radius (of gyration) of a typical cluster. This is also the average distance of two sites belonging to the same cluster:

$$\xi^2 = \frac{2\sum_r r^2 g(r)}{\sum_r g(r)} = \frac{2\sum_s R_s^2 s^2 n_s}{\sum_s s^2 n_s} \tag{16}$$

Its scaling law is then

$$\xi(p) \propto |p - p_c|^{-\nu} \tag{17}$$

It has been observed that estimates of the critical values via various techniques (series expansion, Padé approximations, random walk theories, Monte Carlo simulations, renormalization groups) lie very close to the exactly known value of the same kind of scaling equations used in (other) phase transition theories. All presently available evidence strongly suggests that the critical exponents depend only on the dimensionality of the lattice, but not on the lattice structure itself.[1] They should thus also be valid on our Voronoi structure. The "exact" results of the scaling exponents for two-dimensional lattices are the following[1]:

$$\sigma = 36/91 \qquad \tau = 187/91$$
$$\alpha = -2/3 \quad \beta = 5/36 \quad \gamma = 43/18 \quad \nu = 4/3 \tag{18}$$

Scaling exponents give only limited cluster information. Again, they merely describe the behavior of the singular part of cluster moments near (and above) percolation threshold. The reason then why they were mentioned is that they seem to give the exact fractal dimension of both finite and infinite clusters.

7. Creating clusters: a program description

In order to generate clusters on various types of lattices, the program has to have information on the structure of the lattice. This necessary information is given below and

is presented to the cluster program by means of a file:

Total number of cells (n_max)
Number of cells at the border of the lattice (border)
Mean cell area (mean_cell_area)
Mean hydraulic diameter of a cell
a list n_max long of all cell data
x and y coordinate of a cell's nucleus
the number of neighbors of a cell
the area and perimeter of a cell
the number of neighboring cells in anticlockwise order.

A cell corner (i.e., a vertex) can be found by taking the incenter of the triangle through the cell's nucleus and two consecutive neighbors.

The cluster program can handle lattices other than Voronoi structures provided that a cell is specified by its nucleus and the nuclei of neighboring cells. It is therefore necessary to write the cell edges as bisectors of lines through neighboring nuclei. A regular lattice is thus seen as a Voronoi lattice but with more regularly spaced points. This is possible for most regular lattices and was done for the triangular and square lattices.

Cluster data are updated when the occupation probability is increased; this is when a new cell becomes occupied. To explain how this is done it is necessary to describe the data structure of a cluster. Each cluster has: (1) a distinctive number, (2) an area, (3) a perimeter, (4) a size, number of occupied sites belonging to it, and (5) a list containing all cells belonging to it. Each cell has a variable that contains the number of the cluster to which it belongs, or null if it is still empty.

In the standard percolation problem, the decision to occupy a lattice site is strictly random. However, the decision algorithm described in Section 3 was also implemented. When a new cell is then chosen to become occupied, it will surely have to belong to a cluster. Two cases will occur and these are described below, together with the action to be taken:

(1) The cell is surrounded by empty neighbors. A new 1-size cluster has to be created. The new cluster has to have a number. Its area and perimeter become the area and perimeter of the occupied cell.

(2) One or more neighbors of the newly occupied cell are already occupied and thus belong to one or more clusters. The new cell adds to the biggest neighboring cluster. If there were neighbors belonging to different clusters, those clusters would be swallowed by the largest one. The area of the largest cluster is increased by the area of the cell and that of the (possibly already swallowed) other clusters. The perimeter of the largest cluster is increased by that of the cell and that of the other possible clusters minus twice that part of the perimeter of the cell, neighboring to already occupied neighbors or clusters.

In both of the above cases, the following general statistics are updated: (1) the total perimeter in the lattice, (2) the mean cluster size, (3) the standard deviation on the cluster size, and (4) the number of n-sized clusters.

At increasing probability (e.g., steps of 0.01) statistics about the clusters are put into a MATLAB file. These statistics are:

maximum cluster size
area and perimeter of the largest cluster
total perimeter
area and perimeter of clusters (>100 cells)
number of s-sized clusters for s up to 10
mean cluster size
standard deviation on the cluster size.

8. Conclusions

It has been shown how percolation theory can be linked with a filtration process. An algorithm to obtain relevant data and statistics about clusters has been implemented. The program updates the cluster statistics as the occupation probability is increased. With a simple modification the cluster program has been used to simulate the deterioration of a filter membrane.

Changes have been studied of some cluster properties near the percolation threshold on different finite lattices (square, triangular, and Voronoi). These properties are the area and perimeter of the largest cluster, the total perimeter in the lattice, the standard deviation on the mean area, and the size of the largest cluster minus the average cluster size. The last criterion had the most distinctive behavior at the percolation threshold.

Also discussed are the differences between the percolation and filtration processes. In the latter process, the percolation threshold was at a higher blockage probability, there was less perimeter in the network, and the mean cluster size was lower for whatever occupation probability.

References

1 Stauffer, D. *Introduction to Percolation Theory*. Taylor and Francis, London, 1985
2 Wilkinson, E. T. and Davies, G. A. The application of percolation theory to the analysis of sieve blinding. *Chem. Eng. Sci.* 1989, **44**, 459–470
3 Lim, J. H. F. Ph.D. Thesis, University of Manchester, UK, 1990 (restricted until 1996)
4 Chan, K. L. Simulation of the pore structure and performance of certain types of microfiltration. Ph.D. Thesis, University of Manchester, UK, 1988
5 Fisher, M. E. Critical probabilities for cluster size and percolation problems. *J. Math. Phys.* 1961, **2**, 620–627
6 Broadbent, S. R. and Hammersley, J. M. Percolation processes: crystals and mazes. *Camb. Phil. Soc.* 1957, **53**, 629–641
7 Sykes, M. F. and Essam, J. W. Exact critical percolation probabilities for sites and bond problems in two dimensions. *J. Math. Phys.* 1964, **5**, 1117–1127
8 Ziff, R. M. Test of scaling exponents for percolation-cluster perimeters. *Phys. Rev. Lett.* 1986, **56**, 545–548
9 Grimmet, G. *Percolation*. Springer Verlag, New York, 1989
10 Sykes, M. F. and Glen, M. Percolation processes in two dimensions I. Low-density series expansions. *J. Phys. A: Math. Gen.* 1976, **9**, 87–95
11 Schur, H. and Zallen, R. Critical density for percolation processes. *J. Chem. Phys.* 1970, **53**, 3759–3761
12 Essam, J. W. Percolation theory. *Rep. Prog. Phys.* 1980, **43**, 834–912