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NETWORK FLOW MODEL FOR MICROFILTRATION

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The flow of particles suspended in fluids and transported through different geometries is a process with numerous applications. Realistic filters have randomly-interconnected channel space with complex flow path. However, in micro-fluidic systems, channel space may resemble two-dimensional (2D) tessellation. Here we adopt the network flow concept to analyze 2D micro-filters and study the filter efficiency and the clogging time.

Keywords: clogging time, filter efficiency, microfilter

1. INTRODUCTION

The geometrical and statistical properties of networks are the focous of research efforts in the fields of computer science, mathematical biology, statistical physics and technology. A lot of systems operate as a two-dimensional network and numerous devices are constructed in a planar fashion. Examples are grids of processors, radar arrays, wireless sensor networks, as well as a wide range of micromechanical devices. Especially, the microfluidic systems are built with the use of methods borrowed from the semiconductor industry [1]. Such methods generally employ the fabrication of highly ordered microscale structures. Molecular filtration using nanofilters is an important engineering problem, with very diverse applications ranging from chemical processing to biological applications. Biochemical analysis of aqueous solutions involves the flow of particles of different shapes suspended in fluids and transported through different geometries. A filtrate particle flowing through the pore space may be trapped by the geometric constraint or other adhesive mechanisms. Realistic filters have randomly-interconnected channel space with complex flow path. However, in microfluidic systems, channel space may resemble two-dimensional tessellation [1], [5], [11]. Here, the term “channel” refers to a conduit of any desirable shape through which liquids may be directed and the term “microfluidic” refers to the structure wherein one or more dimensions is less than 10^{-5} m. The problem we consider is the clogging process of a hypothetical microfilter with the channel space built up according to a given two dimensional tessellation. The objective of our investigation is to determine the role played by the network geometry in this process provided that the flow of liquid and suspended molecules is laminar.

2. TECHNOLOGICAL ASPECTS

Physical and technological constituents of network employed in mass transport cover waste range of size scale from huge oil installations with macroscopic pipes to nano-fabricated channels transporting countable sets of molecules [1]. Such nano-scale transport primarily exists in the world of biology where the nanofluidic channels present in living organisms deliver nutrients into cells and evacuate waste from cells. A class of artificially fabricated systems can even organize particles’ transport in a network-like manner with no material-channel-structure inside it, as is the case of systems sorting in an optical lattice [16] or the Maragoni flows induced in thin liquid films for the purpose of microfluidic manipulations. In this latter case such devices as channels, filters or pumps are completely virtual. They have no physical structure and do their job by localized variation in surface tension due to the presence of heat sources suspended above the liquid surface [3].

In this contribution, we pay special attention to microfluidic devices. They are constructed in a planar fashion [5] and typically comprise at least two flat substrate layers that are mated together to define the channel networks. Channel intersections may exist in a number of formats, including cross intersections, “T” intersections, or other structures whereby two channels are in fluid communication [11]. Due to the small dimension of channels the flow of the fluid through a microfluidic channel is characterized by the Reynolds number of the order less than 10. In this regime the flow is predominantly laminar and thus molecules can be transported in a relatively predictable manner through the microchannel.

3. TWO DIMENSIONAL MICRONETWORKS

Numerous channel arrangements forming networks are encountered in technology. Apart from random arrangements an important class of networks, with dedicated channel architecture, is employed in microelectronic and microfluidic devices. Especially, the ordered-channel-space networks are interesting from the theoretical point of view and also because of their applicability in filters.

3.1. Network geometry

These ordered networks have channel spaces built around the lattices known in the literature as Archimedean and the Laves lattices [9]. For a given Archimedean lattice all its nodes play the same role thus, from the mathematical point of view, all the Archimedean lattices are the infinite transitive planar graphs. They divide the plane into regions, called faces, that are regular polygons. There exist exactly 11 Archimedean lattices. Three of them: the triangular, square and hexagonal lattices are built with only one type of face (see Fig. 1) whereas the remaining eight lattices need more than one type of face. The former lattices belong to the regular tessellations of the plane and the latter ones are called semiregular lattices.

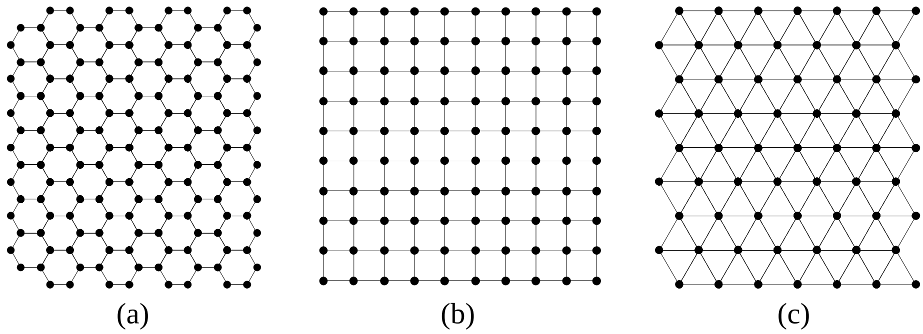

Fig. 1. Regular Archimedean lattices: (a) hexagonal, (b) square and (c) triangular.

Another important group of lattices contains dual lattices of the Archimedean ones. The given lattice *G* can be mapped onto its dual lattice *DG* in such a way that the center of every face of *G* is a vertex in *DG*, and two vertices in *DG* are adjacent only if the corresponding faces in *G* share an edge. The square lattice is self-dual, and the triangular and hexagonal lattices are mutual duals. The dual lattices of the semiregular lattices form the family called Laves lattices. Finally, there are 19 possible regular arrangements of channel spaces.

The lattices are labeled according to the way they are drawn [9]. Starting from a given vertex, the consecutive faces are listed by the number of edges in the face, e.g. a square lattice is labeled as (4, 4, 4, 4) or equivalently as (4^4). Consequently, the triangular and hexagonal lattices are (3^6) and (6^3), respectively. Other, frequently encountered lattices are (3, 6, 3, 6) – called Kagomé lattice and its dual *D*(3, 6, 3, 6) - known as Necker Cube lattice. In some ways these 5 lattices serve as an ensemble representative to study conduction problems in two dimension. They form pairs of mutually dual lattices and also share some local properties as e.g. the coordination number z being the number of edges with common vertex.

Besides the above mentioned lattices, in this paper we have also analyzed other tiling, namely $(3, 12^2)$, $(4, 8^2)$, $D(4, 8^2)$, $(3^3, 4^2)$, and $D(3^3, 4^2)$. Some of these lattices are presented in Fig. 1.

3.2. Percolation phase transition

Percolation theory is a mathematical concept which merges connectivity and transport in complex networks. It deals with the connectivity regarded as the possibility to find an accessible route between terminal nodes of a given network. The physical side of percolation relies on the possibility to pass an amount of transported medium through this accessible route.

Percolation theory was invented in order to explain the fluid behaviour in a porous material with randomly clogged channels [4]. Consider a network with two terminals, source and sink, and assume that only fraction of the channels is accessible to transport. If this part of conducting channel is spanned between the source and the sink then the network is in the conducting phase with nonzero conductibility [6]. If the fraction of channels, available for a medium flow, is not sufficient to connect these two reservoirs the flow conductance vanishes and the network becomes locked. This threshold fraction of working channels for which the network enters the non-conducting phase is called the percolation threshold and this phase change is known as the percolation transition. If, instead of blocked channels, we consider the non-transporting nodes of the lattice then we deal with the so-called site percolation. Here we are mainly interested in the case of non-transporting channels so we will evoke the bond percolation transition at the bond percolation threshold (Table 1).

Table 1. Bond percolation thresholds for networks analysed in this work.

Lattice	Bond percolation threshold p_c
(3^6) triangular	0.3473
(4^4) square	0.5000
(6^3) hexagonal	0.6527
(3, 6, 3, 6)	0.5244
D(3, 6, 3, 6)	0.4756
$(4, 8^2)$	0.6768
$D(4, 8^2)$	0.2322
$(3^3, 4^2)$	0.4196
$D(3^3, 4^2)$	0.5831
$(3, 12^2)$	0.7404

4. EFFICIENCY OF LIQUID TRANSFER THROUGH ARCHIMEDEAN AND LAVES LATTICES

The problem we consider is the conductibility of the networks with Archimedean and Laves channel-network geometries. We focus our analysis on the filter efficiency represented by a drop in filter permeability [7], [10]. Assume that a hypothetic flow of particles transported by fluid is operated by the network whose channels are arranged according to the edges of a given lattice. We apply the network flow language. In this framework, all channels are characterized by their capacitances *C*. These capacitances are quenched random variables governed by a uniform probability distribution defined in the range [0, 1] to assure $C = 0$ for the clogged channel and $C = 1$ for the fully opened channel. We define the filter's effective conductibility as follows

$$\phi(C_1, C_2, \ldots, C_n) = \frac{1}{\Phi_0} \Phi(C_1, C_2, \ldots, C_n) \tag{4.1}$$

where $\Phi(C_1, C_2, \ldots, C_n)$ is the flux transmitted by the filter whose channels have restricted possibilities to maintain the flow and $\Phi_0 = \Phi(C_1 = 1, C_2 = 1, \ldots, C_n = 1)$.

Equation (4.1) permits to compare performance of different lattice geometries in their job as a potential transporting network. We have computed the average values of ϕ for an ample set of values of length (L_X) and width (L_Y) of some of our 10 networks. As an example, in Fig. 2 we present ϕ for the square lattice.

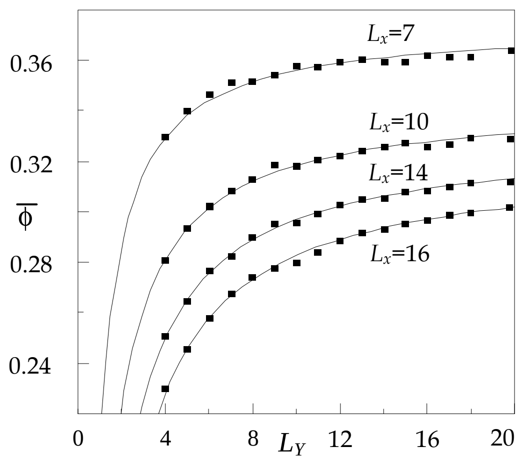

Fig. 2. Average filter's effective conductibility, defined by (4.1), computed for different values of length (L_X) and width (L_Y) of the square lattice. The lines are drawn using (4.2) and they are only visual guides.

We have found that for all lattices ϕ has the following form:

$$\phi(L_X, L_Y) = \left(a_1 + a_2 / L_X^{\delta}\right)\tan^{-1}\left[\psi(L_X)\cdot L_Y\right] \tag{4.2}$$

where: a_1, a_2, δ are the parameters and ψ is the function, all dependent on the lattice symmetry. For sufficiently long and wide network (4.2) is characterized by the value of a_1. This one-parameter characteristic permits us to estimate how two-dimensional networks are resistant against to clogging. For the square, Kagomé and hexagonal lattices a_1 takes the values: 0.237, 0.1722 and 0.1604, respectively. Thus, the square lattice is much more robust then e.g., Kagomé lattice even that both these lattices share the same value of the coordination number $z = 4$, and so their local channel arrangements are similar.

5. SIZE-EXCLUSION FILTERING

Network models play an important role in microscopic description of flows observed in daily experiments. Among the applications worth to mention is the control of ground water contaminant transport and production from oil reservoirs. These, so-called large scale phenomenas, involve an ample volume of liquid. On the other hand there are micro- or even nano-scale flows through highly integrated microfluidic devices [11]. In this work we are concerned mainly with these micro-flows problems.

Size-exclusion filtration is a process for cleaning a fluid from undesirable molecules by passing it through a medium in order to mechanically arrest the harmful molecules [7], [10], [17]. The connectivity of the medium is modelled by a network model. We consider a hypothetic flow of particles transported by fluid through the network of channels arranged according to the positions of the edges of the chosen lattice. All channels are characterized by their radii r which are quenched random variables governed by a given probability distribution. This distribution will be specified later. In order to analyze the filter clogging process we employ a cellular automata model with the following rules [14, 15]:

- Fluid and a particle of a radius R enter the filter and flow inside it due to an external pressure gradient.
- The particle can move through the channel without difficulty if $r > R$, otherwise it would be trapped inside a channel and this channel becomes inaccessible for other particles.
- At an end-node of the channel, the particle has to choose a channel out of the accessible channels for movement.
- If at this node there is no accessible channel to flow the particle is retained in the channel. Otherwise, if the radius of the chosen channel $r' > R$ the particle moves to the next node.

- The movement of the particle is continued until either the particle is captured or leaves the filter.
- Each channel blockage causes a small reduction in the filter permeability and eventually filter becomes clogged.

A minimalist requirements for the filter blockage investigation:

- injected particles are identical spheres with the radius R,
- the channel radius is drawn from a discrete two-point probability distribution function, whereas $P(r > R) = p$ is the only model parameter.

In our minimalist model the channel space is represented by a network of interconnected, wide (W) and narrow (N), cylindrical pipes. Fluid containing suspended particles flows through the filter according to the previously stated rules.

We present the results of the numerical simulations of the above specified filter. Every time step particles enter the filter - one particle per each accessible entry channel and we count the time t required for the filter to clog. For each analyzed geometry and for several values of p from the range $[0.05, p_c]$ we performed 10^3 simulations and then we have built empirical distributions of the clogging time t. Here p_c is the fraction of W channel for which the network lost its filtering capability. It is because of sufficiently high p values that there exist statistically significant number of trajectories formed only by W channels and spanned between input and output of the filter.

Our simulations yield a common observation [2], [8]: the average time required for the filter to clog can be approximated by the following function:

$$\bar{t} \approx \tan\left[\pi p / (2 p_c)\right] \tag{5.1}$$

where the values of p_c are in excellent agreement with the bond percolation thresholds of the analyzed networks (see Table 1). Fig. 3 shows $\bar{t}$ as a function of p for selected lattices, 3 lattices out of 10 lattices we have analyzed.

6. CONCLUSION

In this paper we have discussed transport properties of two-dimensional networks. We heve exploited two extreme pictures: a cellular automata microscopic-like picture and a completely statistical approach to an operating network considered it as the network supporting the flow trough a collection of randomly conducting channels. Even though the cellular automata rules are too simple to capture the detailed interactions in the real system this approach enable us to see how the system becomes damaged. Also the network flow concept is useful to study the interplay between geometry and transport properties of ordered lattices. Its main advantage relays on a very simple

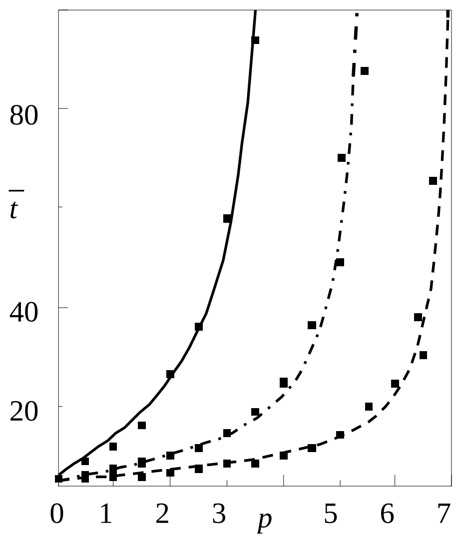

Fig. 3. Average clogging time for regular lattices: solid line, triangular lattice; dashed line, square lattice; dash-dotted line, hexagonal lattice. The line are drawn using (5.1) and they are only visual guides.

representation of the inner structure yet keeping a bridge between the conductibility, the geometry (lattice's symmetry, coordination number) and the statistical global property (bond percolation threshold).

An interesting subclass of transportation problem, not directly discussed in this contribution, concerns the transport in environments that evolve in time [12]. Each pair of neighbouring nodes is connected by a channel, which can be conducting or blocked and the state of the channel changes in time. An example is a network of chemically active channels that capture undesired molecules. Ones the molecules are trapped by channel-binding-centres the channel itself becomes inactive during the chemical reaction needed to convert the molecules. Keeping fixed the portion of conducting channels the evolving environment reorganises their positions. The conductibility of the network in such circumstances differs from that one corresponding to the static partition of gradually clogging channels. Appropriate models of transport in changing environment deal with so-called dynamic (or stirred) percolation [13].

Even that dynamically percolated networks have not been analysed here our efficiency analysis and cellular automata approaches are also applicable in such case. We expect to analyse the effective conductibility of two-dimensional lattices with evolving bond-activities in the near future.

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MODEL SIECIOWY MIKROFILTRACJI

S t r e s z c z e n i e

Mikroukłady filtrujące charakteryzują się dwuwymiarową regularną siecią kanałów. Praca dotyczy wpływu symetrii sieci na wydajność filtrów i ich odporność na zatykanie. Układ filtrujący jest modelowany za pomocą sieci wzajemnie połączonych kanałów, których średnice są dyskretnymi zmiennymi losowymi o zadanych rozkładach prawdopodobieństwa. Średnice kanałów są tak dobrane, że płyn i filtrowane cząstki przepływają swobodnie przez kanały szerokie (*S*), zaś w kanałach wąskich (*W*) cząstki są zatrzymywane. Ruch cząstki trwa do momentu jej zatrzymania w jednym z kanałów lub do momentu opuszczenia filtru. Cząstki są wprowadzane do układu do czasu jego zablokowania. Analizowano sieci kanałów o symetriach reprezentatywnych dla dwuwymiarowych filtrów o strukturach kanałów odpowiadających regularnym i półregularnym podziałom płaszczyzny. Z otrzymanych histogramów czasu blokowania filtru wynika, że dla każdej struktury sieci kanałów wartość oczekiwana czasu blokady ma rozbieżność typu tangens, gdy frakcja kanałów *S* staje się bliska progowi perkolacji wiązań danej sieci. Statystycznie zbiór kanałów *S* zaczyna umożliwiać komunikację między wejściem i wyjściem z układu i układ traci własności filtrujące.