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Construction of Maximum Tortuosity of Single Fluid Path in Grid-based 2-d System (5×20) and 3-d system (5×20×3) for Certain Value of Porosity

S Viridi[1], FDE Latief[2], SN Khotimah[3]

Physics Department, Faculty of Mathematics and Natural Sciences, Institut Teknologi Bandung, Jalan Ganesha 10, Bandung 40132, Indonesia

[1]dudung@fi.itb.ac.id, [2]fourier@fi.itb.ac.id, [3]nurul@fi.itb.ac.id

Abstract. Tortuosity is an important physical property in porous materials since it describes path length of fluid through the materials, which means how much the loss of kinetic energy. The simplest definition of tortuosity T is λ/L with λ is length of the path and L is the distance between two ends of the path. System is discretized using grid to limit number of possible paths, which could be infinity for continuous system. Porosity of the system is also constrained. Variable T is chosen as macrostates in statistical physics point of view, while all possible paths within this T are the microstates. It is found that some macrostates (more appropriately is its maximum value) have larger thermodynamics probability than the others. It should be a relation between this probability and reported tortuosity.

1. Introduction

Tortuosity is still an interesting parameter in recent years, since it can be implemented in various fields, such in botany for defining root path formation [1], in cardiac cell for studying cytoplasmic diffusivity [2], in battery for investigating ohmic losses [3], and in soil for predicting its value from hydraulic conductivity instead of porosity [4]. Its relations to porosity have been reported in various forms of relation [5, 6]. In this work instead of tortuosity another related term, average tortuosity, is introduced, which is averaged though all possible values within certain value of porosity.

2. Model

Porosity ϕ is fraction of void space V_V in material with total volume V_T [7]

$$\phi = \frac{V_V}{V_T}, \tag{1}$$

hydraulic tortuosity T is [8]

$$T = \frac{\lambda_{avg}}{L}. \tag{2}$$

where λ_{avg} is average length of fluid path and L is the geometrical length of the sample, and specific surface area S is [9]

$$S = \frac{N l_{\mathrm{avg}}}{1-\phi}, \tag{3}$$

with N is number of channels per cross-sectional area and l_{avg} is average peripheral length of each pore, which could be simply circumference of a pore.

A two dimensional model of porous medium is considered, which is relatively similar to [10], where upper and lower plate are assumed to have $\phi = 0$.

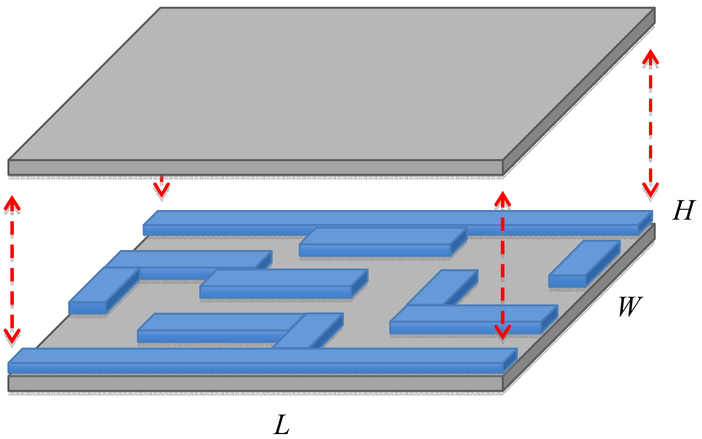

Figure 1. Model of two-dimensional porous medium with length of L and width W.

Part with blue plates in figure 1 represent the material, while the empty spaces represent the void in the porous medium. It can also be shown in two-dimension as given in figure 2. The system is simplified into rectangular grids with size in order of H. Number of grid in L direction is N_L and in W direction is N_W. Total number of grids in the system is

$$N = N_L N_W \tag{4}$$

with

$$N_L = \frac{L}{H}, \tag{5}$$

$$N_W = \frac{W}{H}. \tag{6}$$

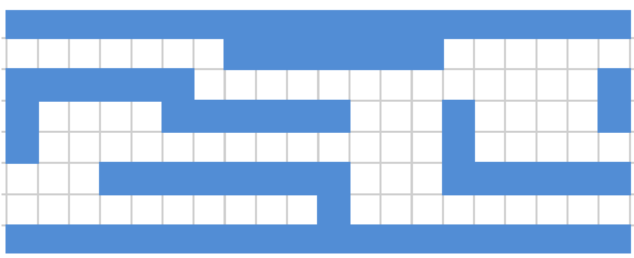

Figure 2. Two-dimension representation of porous medum between upper and lower plates.

Indexing of grids (i, j) begins at the lower left corner (0, 0) and ends at upper right corner (N_L, N_W). Position of grid (i, j) is determined through

$$\left(i\frac{H}{L}, j\frac{H}{W}\right). \tag{7}$$

Grid (i, j) has value 1 for material and 0 for void, which can be represented in the form of

$$G_{ij} = \begin{cases} 0, & \text{for void,} \\ 1, & \text{for matrial.} \end{cases} \tag{8}$$

Using equation (8) porosity of the system is simply

$$\phi = \frac{1}{N} \sum_{j=0}^{N_W} \sum_{i=0}^{N_L} G_{ij} \ . \tag{9}$$

Minimum porosity will be 0, while the maximum will be

$$\phi_{\max} = 1 - \frac{2}{N_W}, \tag{10}$$

since the system must have two side walls with length of N_L and width one grid (or H).

Tabel 1. Configurations in system with size 5×20 and $\phi_{\max}$ = 0.6.

Configuration of void and material grids	ϕ
1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1	0.0
1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 0 1 1 0 1 0 1 0 1 1 0 0 0 0 1 1 1 1 1 1 1 1 0 1 1 1 1 0 0 1 1 1 1 1 1 1 1 0 0 1 1 1 0 1 1 1 0 1 1 0 0 0 1 1 0 1 0 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1	0.2
1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 0 1 0 1 0 0 0 0 0 0 0 0 1 0 0 0 0 0 0 0 1 0 1 1 0 1 0 0 1 0 0 0 0 0 0 1 0 1 0 1 0 1 0 1 0 1 0 0 0 1 0 0 1 1 0 0 0 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1	0.4
1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1	≥ 0.6

In generating certain porosity number of grids representing material is start with value $2N_\mathrm{L}$ until N, which corresponds to porosity $2/N_W$ and 1. A value of certain porosity ϕ will be considered as a macrostate, while all possibilities to construct the state are the microstates. If there are $(N - 2N_L)$ grids and porosity ϕ is the target, then there will be

$$W_\phi = \frac{(N - 2N_L)!}{(N\varphi)!(N - 2N_L - N\varphi)!} \tag{11}$$

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microstates for it. Random process is used to generate the microstates, which is related to values of i and j, but not for the $2N_L$ grids. If f_U is a function to generate number, where $0 \le f_U \le 1$ then

$$k = 1 + \lfloor f_U (I_u - I_l) \rfloor + I_l, , \tag{12}$$

will generate $k = I_l, I_l + 1, .., I_u - 1, I_u$, where I_l and I_u is lower and upper values of desired integer. In the system k will represent i and j. Symbol of floor operation is used in equation (9)

$$\lfloor x \rfloor = \max\{m \in Z \mid m \le x\}, \tag{13}$$

where m is integer. Beside the $2N_L$ grid for materials in order to get a particular value of ϕ

$$N_\phi = \max(0, N - N\phi - 2N_L) \tag{14}$$

random numbers should be generated. Maximum porosity ϕ_{max} is obtained when $N_\phi = 0$ (no random numbers generated) and it will turn equation (14) into equation (11) with help of equation (4). Illustration of system 5×20 is given in table 1, where $\phi_{max} = 0.6$ in this case. Increasing system size can reduce this value, but it is also increasing computation time. If $N \to \infty$ then $\phi_{max} \to 1$.

From table 1 it can be seen that a channel can be constructed if $0.2 \le \boldsymbol{\phi} \le \phi_{max}$, but not always, since for $\boldsymbol{\phi} = 0.2$ it must has $T = 1$ with only one channel. This possibility is not favorable. In this work only perpendicular turns are considered for simplifying the calculation. This will give that the next channel length will be more one grid in length than the channel with $T = 1$, which is given in figure 3.

1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1
1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1
1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1
(a)

1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1
0 0 0 0 0 0 0 0 0 0 **1 1 1 1 1 1 1 1 1 1**
1 1 1 1 1 1 1 1 1 0 0 0 0 0 0 0 0 0 0 0
1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1
1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1
(b)

1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1
0 0 0 0 0 0 0 0 0 0 **1 1 1 1 1 1 1 1 1 1**
1 1 1 1 1 1 1 1 1 0 **1 1 1 1 1 1 1 1 1 1**
1 1 1 1 1 1 1 1 1 0 0 0 0 0 0 0 0 0 0 0
1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1
(c)

1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1
0 0 0 0 0 0 0 **1 1 1 1 1 1 1 1 1 1 1 1 1**
1 1 1 1 1 1 0 0 0 0 0 0 0 **1 1 1 1 1 1 1**
1 1 1 1 1 1 1 1 1 1 1 1 0 0 0 0 0 0 0 0
1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1
(d)

Figure 3. Some examples of single channel with different tortuosity T: (a) 1, (b) 1.05, (c) 1.1, (d) 1.1.

Zeros with red color in figure 3 are the perpendicular turns, where fluid flows could exhibit different fluid friction compare to the straight paths. These types of friction will be adapted from the previous work that in straight line friction will be proportional to velocity, while in the perpendicular turn it will be proportional to square of velocity due to change of coordinate system [11].

3. Results and discussion

For a particular value of porosity ϕ there will be some number of possible configuration or microstates W_ϕ, which is given by equation (11) and number of tortuosity may be varied. What easier to determine is maximum tortuosity T_{max} for a particular value of porosity ϕ as shown in figure 4.

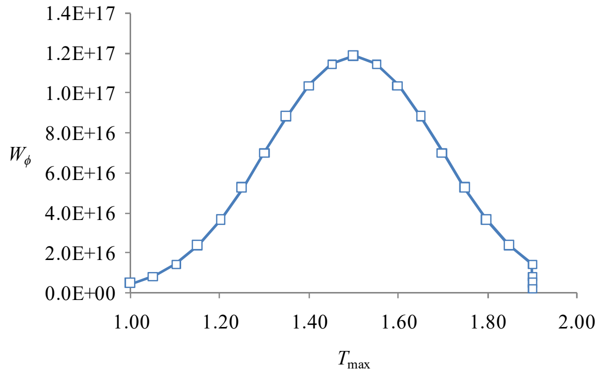

Figure 4. Number of microstates W_ϕ for particular value of maximum tortuosity T_{max}.

It seem that T_{max} = 1.5 (or ϕ = 0.3) gives maximum value of microstates W_ϕ, which can be seen in figure 4 as the peak in the curve. For $\phi \geq 0.38$ value of T_{max} remains at 1.90, where increasing of porosity does not increase value of maximum tortuosity. Several examples of microstates for several value of ϕ, T_{max}, and W_ϕ are given in figure 5. Path with more perpendicular turns give higher value of ϕ and T_{max}, but not always value of W_ϕ.

1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
1	0	0	0	1	0	0	0	1	0	0	0	1	0	0	0	1	0	0	0
1	0	1	0	1	0	1	0	1	0	1	0	1	0	1	0	1	0	1	1
0	0	1	0	0	0	1	0	0	0	1	0	0	0	1	0	0	0	1	1
1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1

1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
0	0	0	0	1	0	0	0	1	1	1	1	1	0	0	0	1	1	1	1
1	1	1	0	1	0	1	0	1	1	1	1	1	0	1	0	1	1	1	1
1	1	1	0	0	0	1	0	0	0	0	0	0	0	1	0	0	0	0	0
1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1

1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
0	0	0	0	0	0	0	0	1	1	1	1	1	0	0	0	0	0	0	0
1	1	1	1	1	1	1	0	1	1	1	1	1	0	1	1	1	1	1	1
1	1	1	1	1	1	1	0	0	0	0	0	0	0	1	1	1	1	1	1
1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1

Figure 5. Examples of configuration with: ϕ = 0.38, T_{max} = 1.9, W_ϕ = 1.41543E+16 (top), ϕ = 0.30, T_{max} = 1.5, W_ϕ = 1.18265E+17 (center), and ϕ = 0.24, T_{max} = 1.2, W_ϕ = 13.60524E+16 (bottom).

Average tortuosity can be calculated from

$$T_{avg} = \frac{1}{W_\phi} \int_1^{T_{max}} m(\mathrm{T}) dT \, , \tag{15}$$

where $m(T)$ is number of microstates for every tortuosity T on a certain value of porosity ϕ. Lower bound of the integral is due to shortest path which gives tortuosity of one, while the upper bound is due to the possible maximum value of tortuosity.

If it is assumed that every value of tortuosity T less than T_{max} has only one microstate on a certain value of porosity ϕ or $m(T) = 1$ then equation (15) will be simplified into

$$T_{avg} \approx \frac{1}{W_\phi} \int_1^{T_{max}} dT = \frac{T_{max} - 1}{W_\phi} \, . \tag{16}$$

Results of equation (16) is presented in figure 6. Values of T_{avg} are quite small since for a certain value of porosity ϕ there is a lot of microstates which do not construct a channel through the system. Minimum value of T_{avg} is found at ϕ about 0.28.

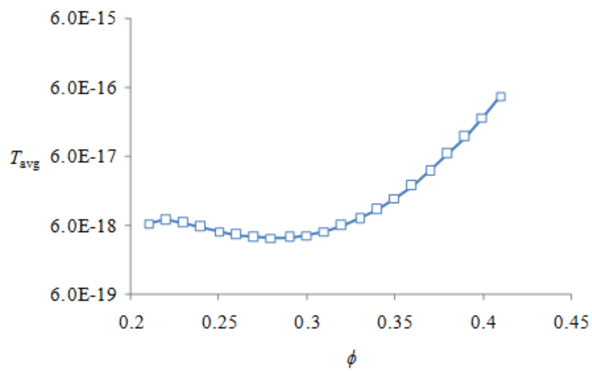

Figure 6. Average tortuosity T_{avg} of certain value of porosity ϕ.

From this point forward let minimum value of porosity ϕ = 0.28 be the focus of this work. For ϕ = 0.28 two u-valleys are required, which is shown in figure 7 with $w_1 = w_2 = 1$, where w_n is width of the n-th u-valley. Another possibility is given in figure 8, where $w_1 = 1$ and $w_2 = 1, .., 12$.

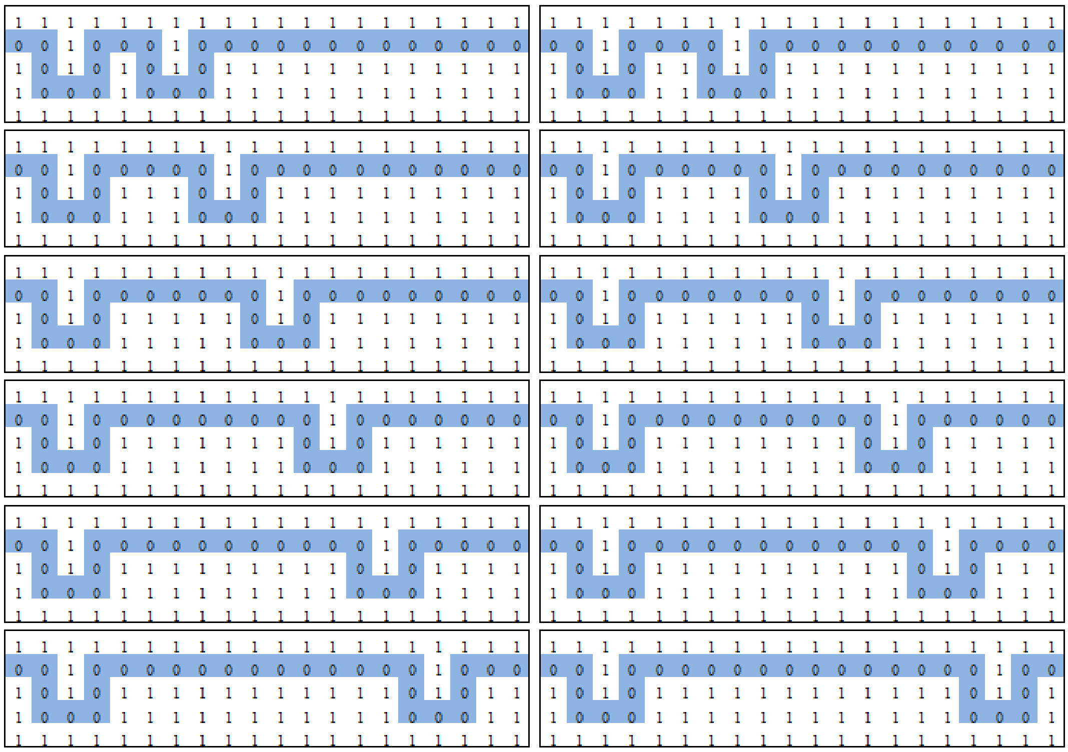

Figure 7. Two u-valleys (ϕ = 0.28 $w_1 = 1$, $w_2 = 1$, $l_{12} = 1$ .. 12) can make 78 microstates by changing position of first u-valley from 1 to 12 (only first 12 is shown).

Distance between the two u-valleys i and j is defined as l_{ij} as shown in figure 7 for l_{12}. For the system value of l_{12} is between 1 and 12, while for longer system with the same width it will be

$$l_{12} \in [1, N_L - 8]. \tag{17}$$

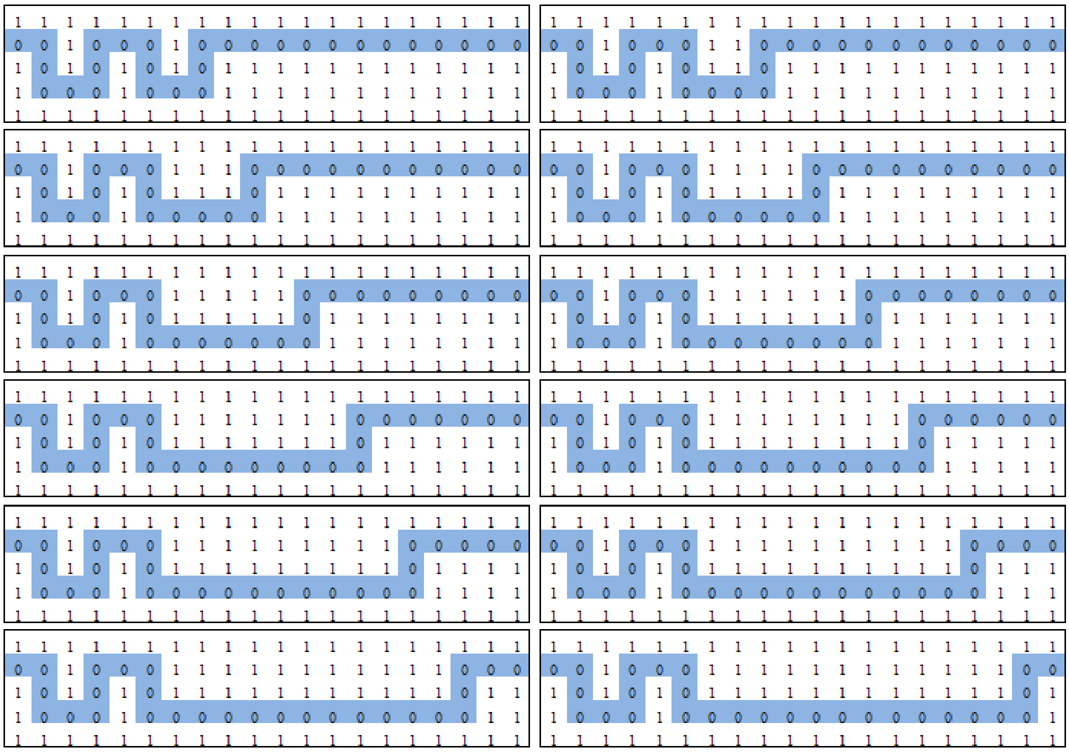

Figure 8. Two u-valleys (ϕ = 0.28 w_1 = 1, w_2 = 1..12, l_{12} = 1) can make 364 microstates by changing position of first u-valley from 1 to 12 (only first 12 is shown).

As in equation (17) for system with longer size but with same width value of w_2 can be summarized as

$$w_{12} \in [1,\, N_L - 8]. \tag{18}$$

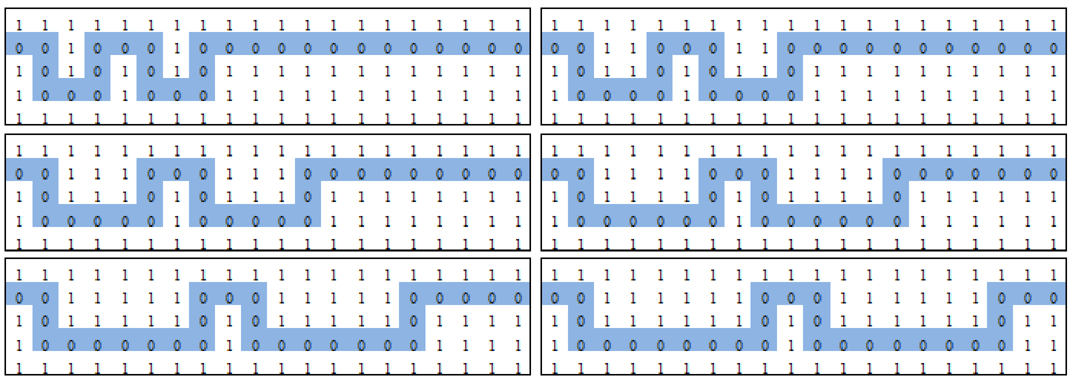

Figure 9. Two u-valleys (ϕ = 0.28 w_1 = 1.. 6, w_2 = 1..6, l_{12} = 1) can make 40 microstates by changing position of second u-valley (only first 6 is shown).

For l_{12} is fixed at one as shown in figure 9 and $w_1 = w_2$ then

$$w_1 = w_2 \in [1,\, \tfrac{1}{2} N_L - 4], \tag{19}$$

where N_L should be even. A more compact relation that can merge equations (17) – (19) is one of the homework for future investigation, also when $N_W > 5$.

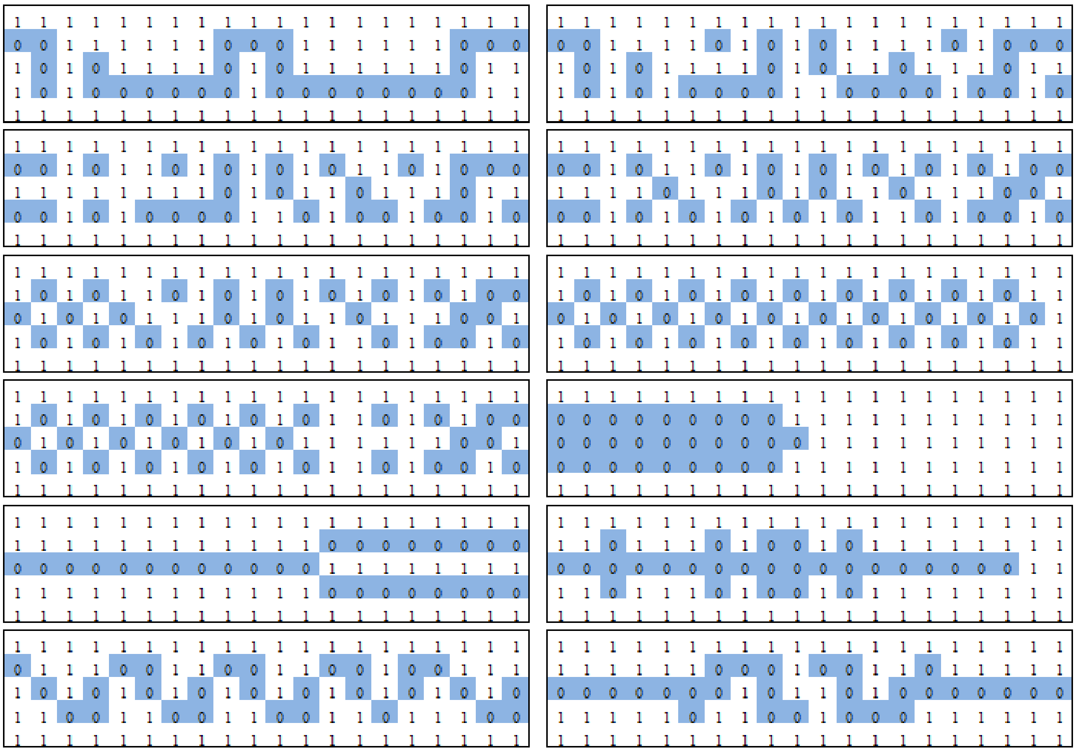

Figure 10. Some microstates (ϕ = 0.28) which do not have tortuosity.

For now it is assumed impossible to figure out how many configurations which can construct a single tortuosity value. It is the reason why equation (16) considers only one microstate. Figures 7-9 shows only some possibilities, while there are still a lot of others to be found.

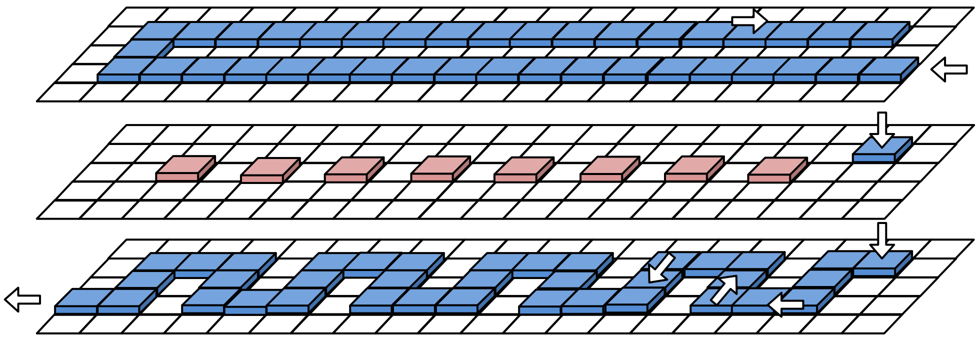

Figure 11. Maximum tortuosity $T_{\max}$ in system 5×20×3 for porosity ϕ = 0.28 with 8 unconnected voids.

Supposed that the system is increased in H direction from 1 to 3, which means that current 5×20 (2-d) system is changed into 5×20×3 (3-d) system as shown in figure 11. Number of additional materials grids will be

$$N_{\varphi} = \max(0, N - N\varphi - 6N_L) \tag{20}$$

from equation (14). Then N = 300 and similar porosity (ϕ = 0.28) will required N_{φ} = 96, number of random number to be generated or simply 84 voids inside the 5×20×3 grids. Figure 11 gives the maximum possible tortuosity $T_{\max}$ = 3.8 for the system. It can be understood that porosity between

0.253 and 0.280 will have the same value of T_{max}, since the unconnected voids do not give any contribution to T_{max}. In future work permeability must also be investigated related to tortuosity instead only related to porosity [12], since tortuosity determines permeability more than porosity. Current results are still not sufficient to show relation between tortuosity to porosity in the forms as shown in [5, 6], which are very handy for further use. More microstates are required in order to obtain such formulation.

4. Summary
System in two-dimension for modeling tortuosity of single channel fluid path has been developed. Based on statistical physics postulate, thermodynamics probability of a certain porosity value to produce a tortuous channel is very small, in order of 10^{-17}. This means that the postulate only is not sufficient to predict how such channel can be formed in nature.

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