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Controlling 2D Porous Media Characteristics Through Topology Manipulation

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Keywords

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Grain

Abstract

A systematic approach for controlling different 2D porous media (PM) characteristics is presented. Through the manipulation of the topology of the PM grain size, shape and distribution, different PM characteristics can be controlled/tailored as required. The presented approach is tested using a test 2D porous media to achieve a specific target porosity value and offers the possibility of tuning other fluid/solid dependent characteristics like the pressure gradient and maximum velocity. The demonstrated approach can be further extended to include other target characteristics through the inclusion of more topological parameters. It can also be extended to any generic PM structure. This approach opens many possibilities for the use of model 2D porous media in different applications and as a surrogate model for naturally occurring PM.

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1. INTRODUCTION

Porous media are encountered in many natural and industrial situations. Examples include oil reservoirs, heat exchangers, energy recovery systems, waste management, soil mechanics, composites for different machine components etc (Liu et al., 2017; Kumar & Muniamuthu, 2024). Due to this, different approaches have been proposed and used to study different phenomena in porous media. The most basic of these approaches is the fully experimental one. In which a sample of the physical system under consideration is brought to the lab where it gets tested under controlled experimental conditions then different conclusions can be drawn from the measured variables (Anguy et al., 1996; Mosser et al., 2017; Kharrat et al., 2022). On the other side of the spectrum lays the fully computational methods which can be divided into models that replicate the exact PM geometry (through a CT scan or a similar approach) and lumped models that only use the main PM properties like porosity without considering the exact geometry of the grains and their distribution (Miah et al., 2018; Di Palma et al., 2019; Yan et al., 2022).

Several studies have argued that computational models that do not consider the exact PM geometry may fail in predicting some features which are sensitive to the grain geometry such as the displacement interface geometry in the case of two-phase flow (Akhlaghi Amiri & Hamouda, 2014; Yong et al., 2014; Lu et al.,

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2018). The price paid to reflect the effect of the PM exact geometry is a detailed representation of the actual system through a CT scan or a similar approach (Di Palma et al., 2019). This approach, despite being more accurate, has two downsides. First, it is expensive since it is not fully computational as it needs a measurement part to get the full PM grain/bore geometry. Second, the obtained results cannot be generalized, or a sensitivity analysis cannot be done since the obtained results are specific to the tested PM sample.

A hybrid approach between these two extremes is the use of a model porous media that replicate some of the real PM under consideration without the need for a detailed description of the actual grain/bore geometry (Akhlaghi Amiri & Hamouda, 2014; Meinicke et al., 2020). Many studies adopted this approach while replicating the important parameters of the PM like porosity, grain size and shape (Rokhforouz & Akhlaghi Amiri, 2019). Based on this approach, a recent emphasis has been placed on 2D porous media which, in addition to being used as model for real porous media, are gaining popularity in many applications due to its unique properties and simplicity (Akhlaghi Amiri & Hamouda, 2014; Yan et al., 2022; Sun et al., 2023).

Synthetic porous media is another terminology widely used in scientific literature to reflect the use of different chemical and physical processes to produce porous media with desired target properties like specific surface area (Pfeiffer et al., 2016; Abdelrahman, 2018; Di Palma et al., 2019). Many studies have used model 2D and synthetic porous media to investigate its use for a specific application (Akhlaghi Amiri & Hamouda, 2014; Abdelrahman, 2018; Jahanshahi Javaran et al., 2010; Muniamuthu et al., 2016; Sun et al., 2023; Kumar & Muniamuthu, 2024) like waste management (Abdelrahman, 2018; Kumar & Muniamuthu, 2024), noise and vibration reduction (Kumar et al., 2016; Letaieff et al., 2017; Yuan et al., 2020; Sunil Kumar et al., 2024), control of thermal stresses in machine components (Kumar et al., 2023) and hydrogen storage (Pfeiffer et al., 2016). However, there is still no general approach/methodology that is generic enough to allow the determination of the 2D PM geometric parameters to fulfill a specific set of design targets.

The aim of this study is to show the possibility of designing/tailoring the 2D PM geometric parameters to achieve target properties (whether these properties are specified by the intended use of the 2D PM or they are used to replicate a physical PM) like a specific porosity value or other solid/fluid specific characteristics like the maximum velocity and the pressure gradient. The used approach relies on manipulating different topological parameters of the 2D porous media to achieve the required design targets. This approach can be made more sophisticated by controlling more topological parameters in order to achieve more PM characteristics. The approach is demonstrated through the study of the flow in a sample 2D porous media and how different target goals can be achieved through the change of the PM grain size, shape and size distribution.

2. PARAMETERS OF A 2D POROUS MEDIA

A model 2D porous media is normally used for one of two goals. To replicate a physical porous media which allows an easier way of analyzing its characteristics or to be used in a specific application. In both cases, a set of properties/characteristics needs to be replicated/achieved in the designed 2D PM. Some of these properties can be geometry related like porosity while others can be related to the used fluid/solid interaction like the required pressure gradient to pump the fluid through the PM with a certain flow rate/velocity or the maximum velocity in the bores between the PM grains.

Assume a simplified 2D PM model as shown in Figure 1. The model porosity depends on the number of grains and their size. In this case, for a target porosity value, many options can be tuned to achieve the required porosity, which include some or all of the following topological parameters:

1- Grain shape (e.g. circular, square, ... etc)

2- Grain size and distribution (e.g. equal size, two or more sizes with specific size ratio, distribution ... etc)

2- Grain relative arrangement to each other (e.g. inline, staggered, random ... etc).

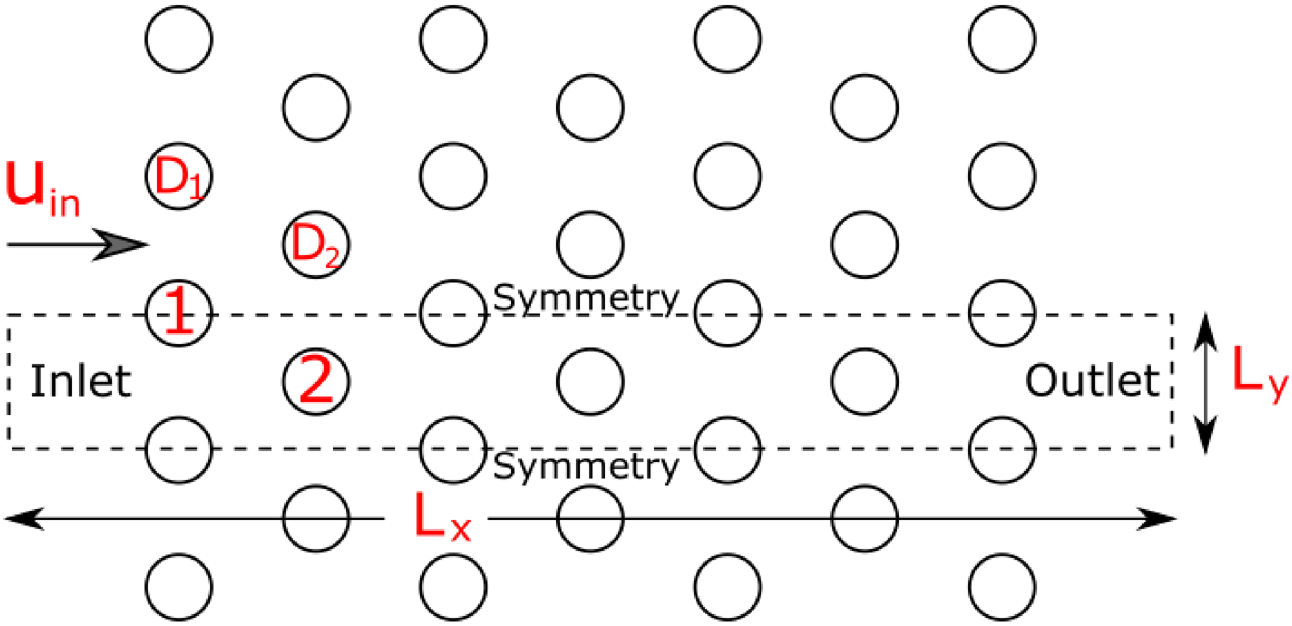


Figure 1. *Sample 2D porous media geometry*

Since the target porosity value can be achieved using any of these combinations, this adds more degrees of freedom to achieve other target design goals as well. If these goals are geometry-dependent (e.g. min. or max. throat diameter), the tuning of these topological parameters is enough. For other PM hydrodynamic characteristics that are solid/fluid dependent like the pressure gradient or the maximum velocity, a detailed numerical solution is needed to map the topological parameters space to the hydrodynamic parameters space. Once this mapping is done, the specific geometric configuration can be easily determined.

3. DESIGN OF A MODEL 2D POROUS MEDIA

Now let us consider a test 2D porous media for a certain application. The first parameter that needs to be replicated is the porosity. A generic representation for one of the many options that can be used to achieve this goal is the one depicted in Figure 1. In this model we only consider a staggered arrangement of grains (other arrangements can be considered as well). Another parameter that can be used is the grain shape. In the current study, we consider two shapes only cylinder and square. In addition to this we also add another geometric parameter that allows the use of different sizes of the grains in consecutive rows. Based on this we can have many combinations as shown in Table 1

where:

D_1: is the characteristic length of grains in row 1 (Diameter for a cylinder or side length for a square).

D_2: is the characteristic length of grains in row 2 (Diameter for a cylinder or side length for a square).

CC: denotes a configuration where both rows 1 and 2 contain cylindrical grains.

CS: denotes a configuration where row 1 has cylindrical grains while row 2 has square ones.

L_x: is the model 2D PM length parallel to the flow.

L_y: is the model 2D PM length in the normal to the flow direction.

Table 1.*Tuning of 2D porous media geometric parameters*

$[D_1^2/(L_xL_y)]x1000$	D_2/D_1	Porosity % (CC)	Porosity % (CS)
1.2	**1.0**	15	17
0.9	**1.7**	14	17
0.8	**2.1**	14	17
1.3	**1.0**	17	19
1.0	**1.5**	17	20
0.8	**2.4**	17	22
1.9	**1.0**	32	37
1.6	**1.3**	32	37
1.4	**1.6**	31	37
2.0	**1.0**	37	42
1.9	**1.2**	37	42
1.7	**1.3**	37	43

It is clear from Table 1 that a specific porosity value (like 17% or 37%) can be obtained with many combinations of the three main geometric parameters. Namely, the size of the grain with respect to the characteristic PM size, the ratio of the grain size between the two rows 1 and 2 and the shape of the grain. If the main objective is to design a PM with a target porosity then we have six options for each of these two porosity values.

Now, since we have six options, we can choose one of them according to other design targets. We can move to hydrodynamic design targets but before doing so we need to model the flow field of all the cases presented in the table above.

4. THE NUMERICAL MODEL

Due to the symmetry of the considered PM geometry, we only need to consider the part of the domain in the dashed box shown in Figure 1. The left boundary is set as velocity inlet while the right boundary is an outlet. The top and bottom boundaries are symmetry BCs and the solid grains are dealt with using the no slip BC.

Due to its computational efficiency especially for parallel processing, the Lattice Boltzmann Method (LBM) is used for the simulation of the flow field in the considered 2D PM for the cases considered above (He & Luo, 1997; Jahanshahi Javaran et al., 2010; Yan et al., 2022). The details of the used LBM model are given in Appendix A.

For all the test cases, the flow is assumed to be a steady-state laminar flow of a Newtonian fluid. The inlet velocity u_{in} is fixed for all cases to give a flow Reynolds number of 10 based on L_y.

$$Re = \frac{\rho\, u_{in}\, L_y}{\mu} \tag{1}$$

where: ρ is the fluid density and μ is the dynamic viscosity.

The normalized pressure gradient is calculated as follows:

$$\frac{dp}{dx} = \frac{\Delta p}{L_x}\frac{L_y}{p_0} \tag{2}$$

where: p_0 is the initial pressure in the domain.

Δp is the pressure drop along the porous media length L_x.

The normalized maximum velocity is the maximum velocity in the domain normalized by the inlet velocity.

$$V_{max} = \frac{u_{max}}{u_{in}} \tag{3}$$

where: u_{max} is the maximum velocity magnitude in the simulation domain.

For all cases, the simulation was run until a steady-state solution is reached. For the used Reynolds number, no oscillatory solution was observed for any of the tested cases.

5. RESULTS AND DISCUSSION

This section shows and discusses the results obtained following the proposed approach and simulation discussed in the previous section. The reported velocity fields are normalized by the inlet velocity u_{in} and the density fields are normalized by the initial density ρ_o.

Figure 2 shows the normalized velocity field for some of the test cases. The magnitude of the maximum velocity and its location seem to depend on both the grain shape configuration and the grain size ratio.

Figure 3 shows the density contours for the same cases. On average, the variation of the density on the cross stream-wise direction is limited to the neighbor of the grains and in some cases (case a) is almost constant across the PM cross section. It is also clear that the CS configuration in general results in higher pressure gradient due to the larger difference in the density between the front and rear stagnation points of the square grains compared to the smother variation in case of the cylindrical grains. For cases where the shape, size and configuration of the PM grains are more random/generic, the velocity and density fields will be less uniform.

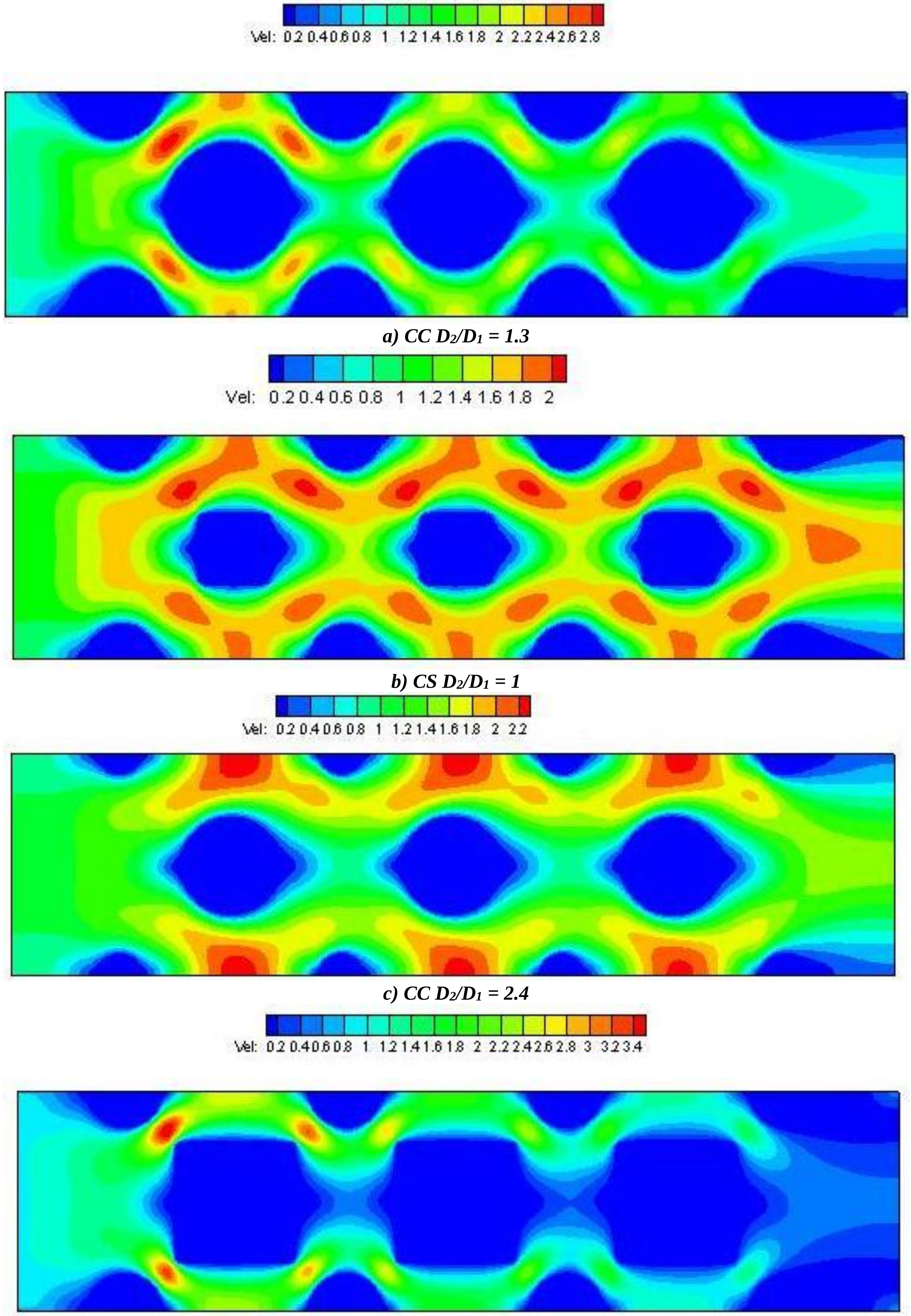
The previous two figures show that the change of the topological parameters of the 2D PM, for the same porosity value, has a profound effect on the resulting flow field (i.e. velocity and density fields). As will be shown, this will subsequently affect the 2D PM hydrodynamic characteristics which allows more freedom in selecting the appropriate set of geometric parameters that fulfills other hydrodynamic design targets.

Table 2 shows the calculated normalized pressure gradient and the normalized maximum velocity in all tested 2D PM configurations presented in Table 1. The highlighted cells show the normalized pressure gradient and normalized maximum velocity for PM configurations with the same porosity value.

The normalized pressure gradient and normalized maximum velocity for the configurations with a porosity value of 17% show almost no sensitivity to the grain shape configuration (CC vs. CS) with weak dependence on the grain size ratio (D_1/D_2). For other PM grain configurations/shapes, these parameters can be more sensitive to different size parameters.

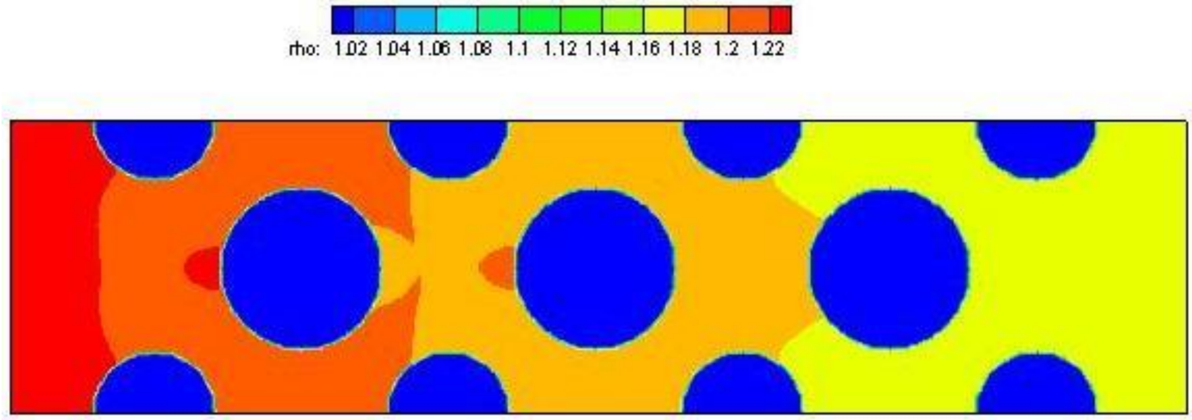
On the other side, cases with a porosity value of 37% show strong dependence of both the normalized pressure gradient and normalized maximum velocity on the grain configuration and grain size ratio. Based on this a specific configuration can be chosen or tailored to meet a specific pressure gradient and maximum velocity for the given porosity value.

GU J Sci, Part A 12(1) 319-331 (2025) 10.54287/gujsa.1611750

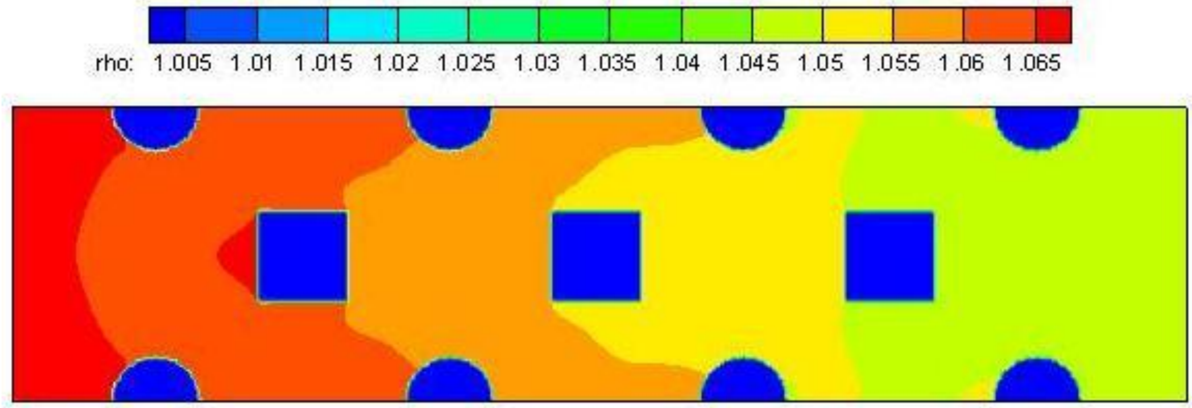


d) CS D_2/D_1 = 1.6

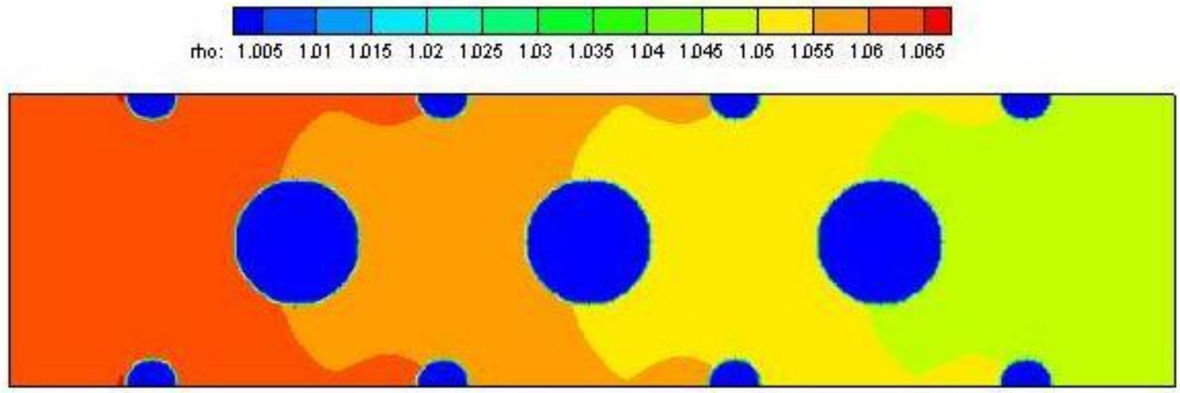
Figure 2. *The normalized velocity field for some of the test cases*



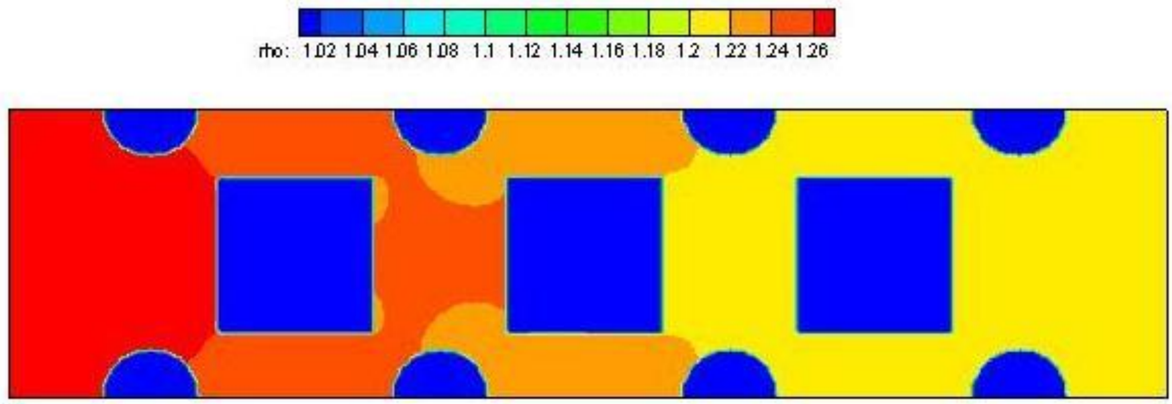
a) CC D₂/D₁ = 1.3



b) CS D_2/D_1 = 1



c) CC D_2/D_1 = 2.4



d) CS D_2/D_1 = 1.6

Figure 3. *The normalized density field for some of the test cases*

This sample set of test cases shows that by controlling only three topological parameters (grain shape, size ratio and grain configuration) three target parameters (porosity, pressure gradient and maximum velocity) can be fulfilled in the designed model 2D PM. Inclusion of other topological parameters like the type and parameters of the grains size distribution and a more generic grains arrangement will allow the control of more target design parameters like the max. and min. throat area in addition to other hydrodynamic parameters.

Table 2. *Hydrodynamic parameters of the tested cases*

Porosity % (CC)	Porosity % (CS)	dp/dx (CC)	dp/dx (CS)	V_{max} (CC)	V_{max} (CS)
15	17	0.47	0.58	2.04	2.08
14	17	0.44	0.58	2.03	2.24
14	17	0.41	0.56	2.11	2.34
17	19	0.51	0.66	2.06	2.18
17	20	0.50	0.70	2.05	2.28
17	22	0.48	0.70	2.35	2.55
32	37	1.23	2.03	2.65	3.62
32	37	1.21	2.17	2.63	3.75
31	37	1.10	2.06	2.67	3.62
37	42	1.57	2.78	2.95	4.42
37	42	1.57	2.97	2.93	4.59
37	43	1.59	3.15	2.91	4.79

6. CONCLUSION

In this work, a simple and systematic approach is proposed for the design of model 2D porous media. The approach relies on achieving the required design targets (whether geometric or hydrodynamic) through the manipulation of the PM topological parameters. The proposed approach is tested by a set of sample test cases to show how the topological parameters can be used in tuning the required 2D PM in order to achieve a predefined set of design targets. Geometric design targets can be fulfilled by just tuning the topological parameters of the PM while the hydrodynamic targets need the extra step of numerically modeling the flow field in the model PM to properly select the best configuration. The presented approach can be used to meet more design targets by including more topological parameters in the design of the model 2D PM. In addition to this, the proposed approach can be extended to more generic PM structures.

CONFLICT OF INTEREST

The author declares no conflict of interest

APPENDIX A:

The LBM solves the discrete Boltzmann equation on a lattice like the 2DQ9 which is used in the current work (Krüger et al., 2017).

$$g_i(x_i + c\Delta t, t + \Delta t) - g(x_i, t) = \Omega(g) \tag{1A}$$

where: g_i is a probability distribution function in lattice direction i, c is the lattice speed $c = {}^{\Delta x}/_{\Delta t}$ and $\Omega(g)$ is a collision operator. The lattice velocities c_i for the used D2Q9 lattice (Figure 1A) configurations are:

$$c_i = \begin{cases} (0,0) & i = 0 \\ (\pm 1,0)c, (0, \pm 1)c & i = 1:4 \\ (\pm 1, \pm 1)c & i = 5:8 \end{cases} \tag{2A}$$

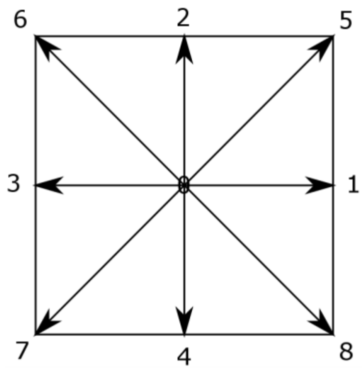


Figure 1A. *the D2Q9 lattice velocity set*

The single relaxation time (SRT) LBM uses the BGK collision operator but in the current work, the multiple relaxation time MRT LBM (Krüger et al., 2017) is utilized due to it improved stability especially for complex geometries. For this model, the collision operator is expressed as:

$$\Omega(g) = -N^{-1}.S.[n - n^{eq}] \tag{3A}$$

Where N is a matrix to transform g from the velocity space to the moment space $n = N.g$. The equilibrium distribution function g^{eq} is also transformed to $n^{eq} = N.g^{eq}$.

$$N = \begin{bmatrix} 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\ -4 & -1 & -1 & -1 & -1 & 2 & 2 & 2 & 2 \\ 4 & -2 & -2 & -2 & -2 & 1 & 1 & 1 & 1 \\ 0 & 1 & 0 & -1 & 0 & 1 & -1 & -1 & 1 \\ 0 & -2 & 0 & 2 & 0 & 1 & -1 & -1 & 1 \\ 0 & 0 & 1 & 0 & -1 & 1 & 1 & -1 & 1 \\ 0 & 0 & -2 & 0 & 2 & 1 & 1 & -1 & -1 \\ 0 & 1 & -1 & 1 & -1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & -1 & 1 & -1 \end{bmatrix} \tag{4A}$$

S is a diagonal matrix with diagonal elements representing the relaxation rate for each moment.

$$S = diag(0, s_1, s_2, 0, s_4, 0, s_6, s_\nu, s_\nu) \tag{5A}$$

The speed of sound for the D2Q9 is given by:

$$c_s = \frac{c}{\sqrt{3}} \tag{6A}$$

s_ν is related to the fluid kinematic viscosity as follows:

$$\nu = c_s^2 \left(\frac{1}{s_\nu} - \frac{1}{2}\right) \tag{7A}$$

The equilibrium probability distribution function g^{eq} is:

$$g_i^{eq} = w_i \frac{p}{c_s^2}\left[1 + \frac{c_i.v}{c_s^2} + \frac{(c_i.v)^2}{2c_s^4} - \frac{v.v}{2c_s^2}\right] \tag{8A}$$

Pressure p and velocity v are calculated from the moments of g :

$$p(x,t) = c_s^2 \sum_i g_i(x,t) \tag{9A}$$

$$v_j(x,t) = \frac{c_s^2}{p(x,t)} \sum_i c_{ij} g_i(x,t) \tag{10A}$$

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