

# A Comprehensive Review of the Simulation Methods for Analysis at the Pore-scale

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## Abstract

Fluid flow through porous material is relevant in different fields of engineering, such as in engine and vehicle development, and can be supported through CFD simulation. Numerical simulations at the pore-scale can be used to replace or reduce expensive laboratory measurements. These methods offer a valuable opportunity to connect the pore-scale properties of the porous material with displacement processes on the continuum-scale. Furthermore, they allow researchers to specify crucial flow properties, e.g., capillary pressure, which are crucial for REV-scale research. Three main methods, direct numerical, pore network modeling, and hybrid approaches, are widely used in order to analyze the pore-scale mechanics of fluid flow behavior through porous materials with CFD simulations. The present comprehensive review demonstrates and highlights the significant advantages, disadvantages, and critical challenges in the pore-scale fluid flow simulations. The main challenges include the characterization of material properties, and up-scaling process from pore to continuum or field-scale.

## Keywords

fluid flow, porous media, pore-scale, CFD-simulation, direct numerical methods, pore network methods

## 1 Introduction

Fluid dynamics and its various associated phenomena can be seen in everyday life. Individuals can observe surface force-driven 'bubbly' turbulent flow, wave propagation, or water channeling in common situations (Fu et al., 2021a). Fluid dynamics includes the understanding and utilization of flow problems and their scientific analysis. Moreover, in fluid dynamics, the study and explanation of complex phenomena requires in-depth scientific knowledge. For instance, a painting by Van Gogh, entitled "La Nuit Etoilee", demonstrates a unique and exciting phenomenon of cloud instability, known scientifically as a Kelvin-Helmholtz instability (Foullon et al., 2011). Every day's fluid dynamics is sponge's water absorption or sound phenomena of airflow over a solid object (Fattahi Evati, 2017).

The discipline of transport in porous media, also called microstructure, has been transformed by our ability to imagine – in 3D – the pore-space of materials at numerous length scales, from nanometer to millimeter-scales and at different resolution levels (Fu et al., 2021a; Shams, 2018; Xu et al., 2020). Recent advances of different imaging

techniques, which are able to represent the porous geometry, can help in geometric representation with negligible loss in pore topology definition in millimeter-scale porous media, i.e., 1–10 mm (Ambekar et al., 2021). Geometry representation methods are critical because the 3-D image is an input parameter of the numerical simulations (Yin, 2018). Therefore, physical mechanisms and processes can be developed at this level by simulations. It supports the specification of the essential parameters of the macroscopical model. Furthermore, the calculated pore-scale parameters can be widely used in REV-scale (Representative Elementary Volume) models (Pawar, 2016) though experimental setups for some practical questions may be impossible to realize. Theoretical research in fluid dynamics supports the improvement of simulation approaches at different scales such as micro and continuum-scales (Ambekar et al., 2021). Furthermore, the practical application of theoretical methods (e.g., automotive industry) requires in-depth scientific knowledge of the behavior of the fluid, as well as knowledge of

multi-phase flows, multi-physics problems, and the interaction of fluid flow with other physical phenomena for instance (Fattahi Evati, 2017; Zöldy and Vass, 2019).

Different complex physical phenomena can occur on different scales in a porous medium (Fattahi Evati, 2017). For example, the length scale in a given porous media can vary from the pore-level (a few nano or micrometers) to the field-level (meter or kilometers). Proper handling of relevant scales still remains a challenge in mathematical and computational modeling. Generally, the variation of the modeling approaches is fully dependent on the applied scale of the porous material. The illustration of these different scales is shown in Fig. 1 (Oostrom et al., 2014).

## 2 Analysis at the pore-scale

Pore-level modeling is connected to the microscopic-scale of microstructures and it is based on the well-known physical laws (e.g., transport equations) through porous medium (Mahamudul et al., 2020). As its name suggests, this method studies the individual pores', ranging from  $10^{-6}$  to  $10^{-3}$  m (Mukherjee et al., 2011). Flows at the pore-scale are described by the solid's complex geometry, which limits the flow of the liquid as the boundary according to the Navier-Stokes (N-S) equations (concretely conservation of momentum, mass and energy). Solving the N-S equations is necessary for the appropriate boundary conditions (i.e., no-slip) and to determine the pressure, velocity distribution in the pore geometry. Modeling at the pore-scale allows a direct description of the fundamental physical processes that determine the behavior of fluids, making its application more favorable than rigorous physics-based approaches. With this approach, the flow behavior and different transport processes in microstructures can be better understood (Oostrom et al., 2014).

Furthermore, pore-scale CFD simulation offers various opportunities to up-scale the calculated parameters (pore-scale) to the macroscopic-scale, where experimental determination is complicated. Despite its advantages, the main challenge involved in micro-scale techniques is the representation of actual pore geometry. Detailed specifications of the porous material are crucial for simulations at pore-scale, which for complex, real pore networks are often challenging (Ficzere, 2018; Oostrom et al., 2014). Additionally, the analysis at the pore-scale ensures an extraordinary opportunity to understand and study processes in various complex porous materials including multi-phase flow (Sobieski and Lipinsky, 2017), or multi-physics problems (de Carvalho et al., 2017). These are still not known in detail due to the applicability of the experimental methods and the dependency of inherited structure-performance (Mukherjee et al., 2011).

Simulation at the pore-scale allows excellent flexibility in the design of numerical analysis tailored to the experimental operating conditions for evaluation of essential closure relations, e.g., multi-phase correlations (Sobieski et al., 2018) regarding the capillary pressure and the relative permeability. Although, these are challenging to obtain by expensive laboratory tests (Oostrom et al., 2014). Recent advantages of different modeling techniques (Fu et al., 2021a), allowing real modeling of the fundamental pore-morphology at a reasonable computational cost, are the main reasons for the increasing attraction in predictive micro-scale modeling (Zhu et al., 2016). In general, micro-scale techniques cater to the mesoscopic modeling system. This contains the impacts of mesoscale physics and pore morphology on the macroscopic transport attitude. Despite the increasing demand, there are still various limitations regarding pore-scale modeling which should be resolved (Gommes et al., 2009).

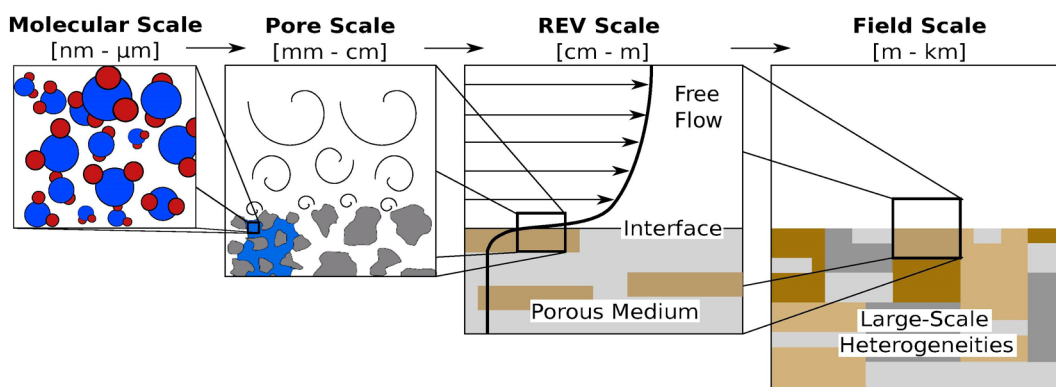


Fig. 1 Connection between various scales – namely the molecular/atomic-, pore-, REV/continuum-, and the field-scales adapted from Mosthaf (2014)

The pore-level modeling and simulation technique considers comprehensive natural processes. Thus, they are complicated and require significant computational power. Scanning electron microscopy (Borel et al., 2014), transmission electron microscopy (Alvarez et al., 2019), and micro-CT (Matrecano, 2011) are three of the widely used techniques to illustrate the pore geometry. Other techniques can also be applied to find the optimal method for CFD input (Mahmoodlu et al., 2020).

Nowadays, pore-scale modeling is at an advanced position in predicting the physical properties of a micro-structure due to recent developments in geometry representation methods. Fig. 2 shows two examples of porous media which are meshed by a pre-processing tool (Ramstad et al., 2019; Vuong, 2016).

### 3 Flow regimes in terms of Reynolds number

Until now, the Darcy's Law has already been widely used in research of numerous micro-structure analyses regarding the fluid flow behavior at the pore-scale. However, in real systems applicability of the classical Darcy equation is strongly narrowed, due to assumptions about fluid flows in the porous medium (Das et al., 2018). For this reason, use has been limited (pre-and post-Darcy flows) and often has to be modified, extended, or replaced entirely by considering the suitable theoretical foundations. Therefore, numerous scientists (Bloshanskaya et al., 2017; Das et al., 2018; Dukhan et al., 2014; Kovalchuk and Hadjistassou, 2019; Oostrom et al., 2014; Wu, 2016) have sought to work out alternative methods for the determination of porous media flows, along with the prediction of domain onset or an additional zone termination (Das et al., 2018).

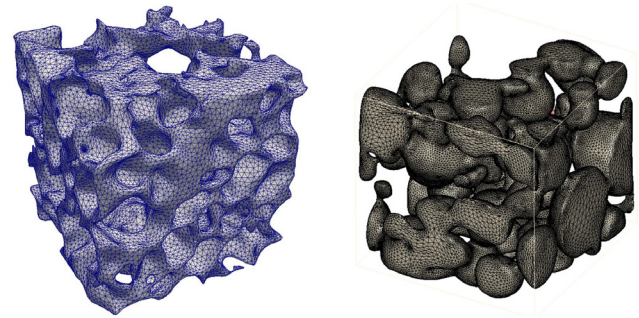


Fig. 2 Two numerical models of porous media in the field of engineering adapted from Ramstad et al. (2019) and Vuong (2016)

Commonly, the Reynolds number (Re) is used to differentiate between flow regimes. Flow transitions in porous material are treated as smooth if there are no specific limits. (Kovalchuk and Hadjistassou, 2019) The Reynolds number (Re) in porous materials can be determined by Eq. (1).

$$Re = \frac{u \times d}{\nu}, \tag{1}$$

in which  $\langle u \rangle$  denotes the volume-averaged fluid's velocity,  $d$  represents the average diameter of the grains, and  $\nu$  marks the fluid's kinematic viscosity. Considering the recommendation of (Kovalchuk and Hadjistassou, 2019), 4 different specific flow regimes and the 'no flow zone', illustrated by Fig. 3, can be detected based on the porous material's properties and the pressure gradient  $\nabla\langle p \rangle$ .

Every flow zones' boundary is based on the volume-averaged velocity  $\langle u \rangle$  – pressure gradient  $\nabla\langle p \rangle$  connection spectrum. These 5 different domains are related as (Kovalchuk and Hadjistassou, 2019):

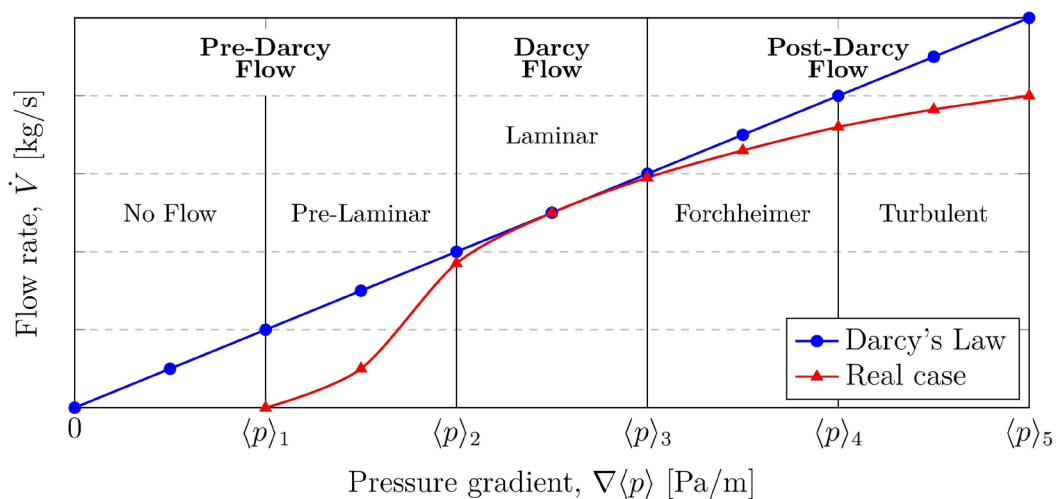


Fig. 3 Flow regimes according to the flow rate – pressure gradient relationship, based on Fattahi Evati (2017); Kovalchuk and Hadjistassou (2019)

1. *No-flow*: In this phase, the real flow rate is equal to zero.
2. *Pre-Darcy (pre-laminar flow)*: Reynolds number (Re) has less relevance in this case. In this domain, the flow is characterized by the strong interaction between surface and fluid. Therefore, it is conditioned by the material and fluid properties.
3. *Darcy (Laminar flow)*: The region's Reynolds number (Re) is smaller than one. The dominating force is the viscous force and the pressure gradient is approximately linear by the flow rate.
4. *Post-Darcy (Forchheimer flow)*: It can be characterized by intensive inertia influence. The function of pressure gradient ( $\nabla p$ ) produces a fluid velocity  $\langle u \rangle$  parabolic in shape.
5. *Post-Darcy (Turbulent flow)*: It can be characterized as a deeply unsteady, unstable, and chaotic flow with the corresponding Reynolds numbers greater than 300. There is also a slightly smaller pressure drop than calculated from the laminar flow equation, namely from the Darcy's law.

Transition between pre-Darcy and Darcy flows and between Darcy and post-Darcy flows are often related to the dimensionless Reynolds number, defined in Eq. (1), as it represents the ratio of inertial forces to the viscous forces (Bloshanskaya et al., 2017; Kovalchuk and Hadjistassou, 2019). Moreover, every transition zone between the different flow domains is smooth. For this reason, it is not possible to apply a correct Reynolds number (Re) limitation setting for porous materials. Therefore, between the defined regimes, so-called "transition zones" should be determined (Aminpour et al., 2018; Bloshanskaya et al., 2017; Kovalchuk and Hadjistassou, 2019). Instead of Reynolds number, the pressure gradient  $\nabla \langle p \rangle$  will be used as the specific characteristic value for the transition among the different flow domains (Zimmerman, 2018).

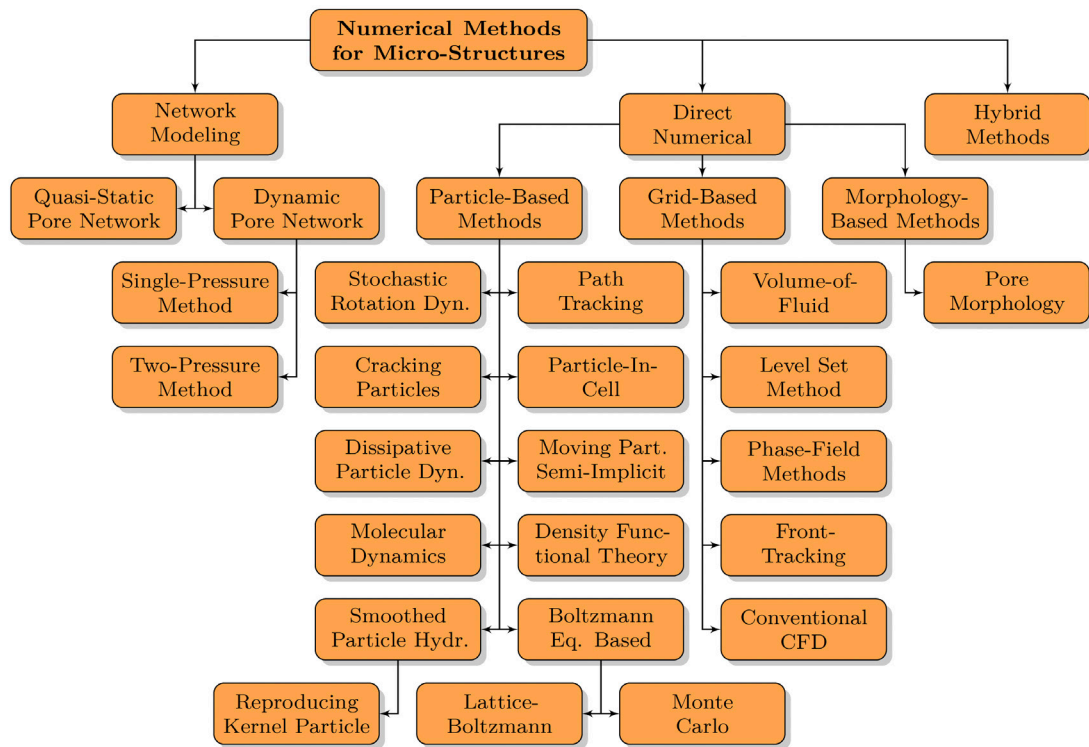
#### 4 Simulation methods of pore-scale

Numerical simulations have been widely demonstrated as one of the more powerful techniques to characterize the dynamics of fluids and for the characterization of several flow regimes in porous materials. For the determination of fluid flow characteristics, it is essential to understand the previously defined flow domains, the transition between them, and finally, the different processes of energy transfer, e.g., dissipation (Fattahi Evati, 2017). Numerous pore-scale approaches have been developed for the analysis of the flow behavior of fluids through porous materials and

for material properties determinations (Mahmoodlu et al., 2020). In general, three major numerical methods can be used at the pore-scale. The first class directly simulates flow and transport phenomena on the complex pore geometries. The second class simulates the accurate geometry of the material using a conceptualized pore network. A combination of these two specific methods can also be used constituting a third class (de Carvalho et al., 2017). Fig. 4. shows an overview of these three main classes.

The first class of the techniques is commonly known as direct numerical methods (DNM). Naturally, it contains conventional computational fluid dynamics (CFD) with the purpose of solving the partial differential equations (either the Navier-Stokes or other governing equations i.e., Boltzmann, Darcy equations) directly (Mahmoodlu et al., 2020). Additionally, a high-quality representation (3D) of the porous (solid) geometry is needed for these methods (de Carvalho et al., 2017). Fundamentally, the direct modeling techniques are able to recognize the fluid as the particles' mixture, as well as mimic the particles' collision and transfer (Mahmoodlu et al., 2020).

In the other class, the pore spaces are demonstrated as a connected pore-network with idealized pore throat and body geometries, and the applicable governing equations are calculated on top of this PN over time through the media. This technique attempts to maintain the exact pore space's topology but does not produce geometric structures of all pore bodies/throats to achieve reduced computational cost (Mahmoodlu et al., 2020). In the pore-network modeling (PNM) class, various approaches have been introduced in the last decade. Notably that the technique which will be chosen for realizing the pore-network strongly depends on the used modeling mechanisms (Yin, 2018). The techniques of this class (Ramstad et al., 2019) use a combination of flow step series for every individual pore body to simulate and calculate the fluid flow behavior in a 3D pore geometry. Mainly, two methods are utilized here to represent the micro-scale network, also called pore-network (PN). In some applications, a normal PN is established utilizing pore size, synchronization number and throat size (pore connection). After that, these parameters have to be adjusted and then validated against test data. On the other hand, in other applications, a similar network is built adopting pore connection (throat) size and the quantified pore body is obtained through imaging methods. However, the PN approach cannot be applied for fluids having gel, foam, or polymer; especially for domains in which fracture exists (Mahmoodlu et al., 2020).



**Fig. 4** Overview over the numerical approaches for pore-scale analysis based on Ambekar et al. (2021); Bear (1972); Blunt (2017); Brandon and Kaplan (2008); Clayton et al. (1995); Dai et al. (2017); de Carvalho et al. (2017); Fattahi Evati (2017); Friis et al. (2019); Golparvar et al. (2018); Griebel et al. (1998); Joekar-Niasar (2016); Kovalchuk and Hadjistassou (2019); Landers et al. (2013); Lieb and Schrader (2013); Montellá et al. (2020); Mosthaf (2014); Mukherjee et al. (2011); Ohwa and Sasaki (2020); Oostrom et al. (2014); Pawar (2016); Rabbani and Babaei (2019); Ramstad et al. (2019); Regaieg (2015); Shams (2018); Vuong (2016); Yang et al. (2019); Yang et al. (2021); Yin (2018); Zhang et al. (2011); Zhao et al. (2016); Zhu et al. (2016); Zhu (2017)

### 5 Direct numerical methods

Today, using direct numerical methods has not been widely adopted at the pore-scale yet. This method is not as attractive as others due to the complex algorithms needed to resolve the complex mesh and governing equations of the porous material on a pore-scale (Oostrom et al., 2014). Furthermore, the porous effect has to be studied on a larger-scale (up-scaling), such as continuum-scales, which denotes the most significant problem of numerical simulations at the microscopic-scale (Mukherjee et al., 2011).

Nowadays, with significant improvements in computational power (CPU, RAM) and numerical methods, different discretization schemes have been developed for direct numerical simulations at the pore-scale (Shams, 2018). Generation of conforming or boundary-fitted meshes can be an extremely complicated procedure, particularly if coarse meshes (in order to decrease computational cost and time), as well as high-quality solutions, are necessary in 3D. The quality of topology triangulation affects the solution's quality. Discretization schemes such as the finite difference (FDM), finite element (FEM), finite volume method (FVM), spectral/hp element (high order FEM),

or boundary element (BEM) that discretize the governing equations on the whole computational domain must be applied in each simulation (Oostrom et al., 2014).

Generally, CFD simulation methods use FVM discretization of governing equations (the Law of conservation of momentum, mass, and energy). Various applications of these methods concern macroscopic flows and include aerodynamics, free-surface flow, and turbulence (Oostrom et al., 2014). The application of these methods in fluid flows through porous media is also quite active (Anderson, 2009; Griebel et al., 1998). Numerous commercial CFD software that simulate at the pore-scale are generally described as direct numerical simulations. The main reason for this is that the governing equations (NS) for transport phenomena and fluid flows are solved on a generated grid that retains the whole microstructure's geometry in 3D. Much of the research using CFD techniques include flow simulations of various geochemical, chemical, biological components, or in the engineering process development, e.g., characterization of vortex development. Consequently, both laminar and turbulent flows can also be calculated in 3D at the pore-scale (Oostrom et al., 2014).

Depending on the treatment of the fluids within the implemented mathematical model, direct numerical methods can be classified into (Golparvar et al., 2018):

1. Particle-based methods
2. Grid-based methods
3. Morphology-based methods.

### 5.1 Particle-based methods

Normally, in particle-based approaches, the fluid domain is illustrated as corresponding sets of many particles whose motion is a result of interactions within the pore space as well as the solid particles. Generally, different numerical methods are considered to fall within the general class of particle-based methods (Dai et al., 2017; Friis et al., 2019; Zhu et al., 2016) such as:

- |                                    |      |
|------------------------------------|------|
| 1. Molecular Dynamics              | MD   |
| a. Lattice-Boltzmann               | LB   |
| b. Dissipative Particle Dynamics   | DPD  |
| c. Monte Carlo                     | MC   |
| d. Density Function Theory         | DFT  |
| 2. Path Tracking                   | PT   |
| 3. Smoothed Particle Hydrodynamics | SPH  |
| a. Reproducing Kernel Particle     | RKP  |
| 4. Stochastic Rotation Dynamics    | SRD  |
| 5. Moving Particle Semi-Implicit   | MPS  |
| 6. Particle-In-Cell                | PIC  |
| 7. Cracking Particles Method       | CPM. |

### 5.2 Grid-based methods

Each approach in this class is based on the well-known Navier-Stokes (or Stokes – convective term is neglected) equations. A computational algorithm based on iterative or direct solvers helps to couple and solve the resulting system of partial differential (PDE) equations. Grid-based methods, because of their greater ability and high computational efficiency to calculate the flow of fluid with high viscosity ratios and densities, are regularly preferred for practical applications. In these techniques, the major challenge is modeling and simulating moving interfaces; there arises a need for an additional algorithm for modeling the interface, containing its evolution, shape, and location with time (Golparvar et al., 2018; Shams, 2018). Therefore, grid-based approaches are often implemented to adapt various algorithms for modeling interfaces between fluids, and consequently, all of them are able to take multi-phase fluid into account. On the other hand, particle-based techniques are computationally cheaper, because the momentum equation (i.e., not the conservation of momentum, rather the Darcy equation) is simpler. The listed numerical approaches are

generally considered to fall within the general class of grid-based method (Golparvar et al., 2018; Shams, 2018):

- |                    |     |
|--------------------|-----|
| 1. Volume-of-Fluid | VoF |
| 2. Level-Set       | LS  |
| 3. Phase-Field     | PF  |
| 4. Front-Tracking  | FT. |

### 5.3 Morphology-based methods

Morphology-based methods use a fundamentally different technique for calculating fluid flow behavior in porous materials. Pore morphology approaches are based on the mathematical morphology study of the reconstructed 2D or 3D actual porous material. These models intend to connect the various macroscopic processes of the material, e.g., the relation of the capillary pressure and the saturation, to the porous media's real representation directly through the morphological data input (Golparvar et al., 2018). Maximal inscribed sphere (MIS), also called the ball (MIB) technique (Clayton et al., 1995), is a particularly powerful algorithm that is used in morphology-based approaches for modeling different fluid configurations (i.e., capillary interactions or equilibrium configurations) at the micro-scale (Widiatmoko et al., 2010). The so-called "MIS approach" can simulate the fluid configurations and the curves of the capillary pressure in different 3D pore-structure materials.

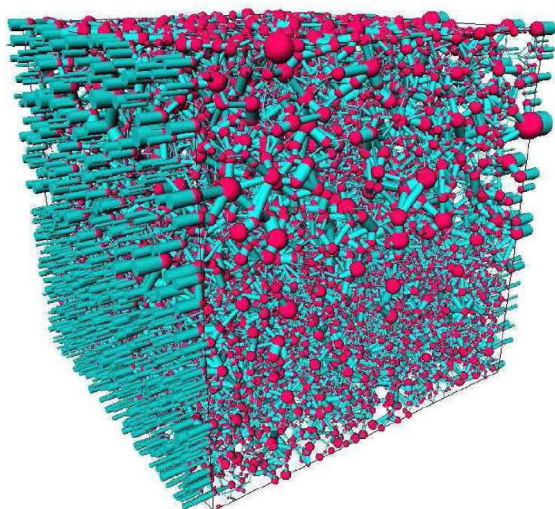
Independently of the MIB, a novel function of the capillary pressure (dimensionless) has been formulated by Silin and Patzek (Golparvar et al., 2018) that improves the conventional J function (Thakur and Penumadu, 2020).

## 6 Network modeling methods

As an alternative, the commonly named pore-network (PN) approach is widely applied to study fluid behavior in microstructures. Pore-network models require less computational power than the fully resolved grid-based techniques. On the top of that, PN is computationally also cheaper than the particle-based approaches (Montellá et al., 2020). Therefore, PN is commonly used in several fields of engineering (Ambekar, 2021). Pore network modeling is presently an effective, well-established method for the numerical investigation of numerous micro-scale phenomena, which are not reproducible by simple REV-scale numerical models. Pore-network approaches determine the flow of fluid or gas through an ideal network connected by various elements (throats). Consequently, the porous materials can be modeled as numerous interconnected pore elements, which represent the void space in the investigated material (Zhao et al., 2016).

Numerous investigators (Ambekar, 2021; Montellá et al., 2020; Mukherjee et al., 2011; Shams, 2018) considered the pore network as a large number of pores or compartments connected by a network of narrower channels or throats. Others use only one type of elements (bonds) to build their network models (Regaieg, 2015). This technique holds the entire structure of the real pore space but does not require the exact geometric structures of all pore bodies and connection elements (throats) to be introduced to the simulation as in other methods. The pore-network algorithms, which are effectively used to a wide range of computational problems, have notably lower computational costs than the direct numerical techniques. This is because the solution of the governing equations for the whole PN is reduced to the concurrent solution of a set of analytical flow concepts in every individual network component (Yang et al., 2021). Pioneers in this field have developed an algorithm which can extract the network of pores connected by throats from high quality micro-CT pore-space image (Wanek et al., 2011; Yeung et al., 2007). Then, flow equations are solved, usually semi-analytically, through the network elements. This methodology's essential step is extracting highly realistic networks from images of the pore-space. Naturally, there are various algorithms employed in order to partition the pore space into pore- and throat-bodies and for determining their connectivity (Shams, 2018). An illustration of the pore network representation showing pores and pore bodies is given in Fig. 5.

Generally, in the PN technique, the involved processes are calculated in specific pores and the microscopic-scale data is firstly summed and secondly averaged to REV-scale



**Fig. 5** Graphical demonstration of a PN model illustrating the complex structure of bodies and throats adapted from Oostrom et al. (2014)

(Regaieg and Moncorgé, 2017). Therefore, by using laws which govern transport and the flow of fluids in the throats and pores, macroscopic features are estimated across the structure. PN techniques are not typically computationally demanding compared to direct numerical methods. In spite of the low computational time, the porous material as an input parameter should be idealized as a network, which cannot hold generally (Golparvar et al., 2018). Furthermore, different processes at the surface cannot be correctly taken into consideration because it is not accurately represented (Oostrom et al., 2014).

The field of displacement mechanisms has extended recently (Ambekar, 2021) and includes several mathematical expressions derived applied for pore-network modeling (Golparvar et al., 2018; Oostrom et al., 2014). PN techniques (Lyras et al., 2020; Ovaysi and Piri, 2010; Shen and Chen, 2007) can be classified into 2 individual sets of fluid flow models in network modeling (Yin, 2018):

1. Quasi-static models have been used favorably to predict the connection between the capillary pressure-saturation and relative permeabilities, especially in the case of multi-phase flow.
2. Dynamic PN approaches are required when the capillary-dominance assumption is no longer valid, and the viscous force must be examined with capillary force. Dynamic PN algorithms essentially fall into two categories: single-, and two-pressure algorithms.

Quasi-static and dynamic models have a large computational demand; although, their applicability is restricted to flow domains in which capillary forces are dominated typically occurring at low capillary numbers (Zhang and Yang, 2014). The motivation in this category is to overcome and solve these shortcomings with the combination of the best dynamic and quasi-static pore network models. They are to employ powerful adaptive PN simulations, which are founded on a common single-pressure dynamic PN technique published by Regaieg and Moncorgé (2017). Their technique has been successfully applied in different analyses and in the validation against microstructure tests on a pore-by-pore basis. It has also found success in the comparison of some macroscopic parameters (for instance, relative permeability, saturation, and the profiles of saturation) (Regaieg and Moncorgé, 2017).

In pore network-based approaches, an instance of an original porous sample's equivalent pore network can be simplified into 2 specific, individual elements: the pore, which contains the bulk volume of fluids, as well as the

throat, which is treated as a fluid conduit between the individual pores (Oostrom et al., 2014). The major steps of any pore-scale network modeling (Regaieg, 2015; Shams, 2018; Zhao et al., 2019) can be classified into network construction and fluid flow simulation process. In the last decade, regular networks have been examined, which consisted of elements with only circular cross-sections. Hereafter, networks have been founded on statistics that are randomly generated and more sophisticated. Angular cross-sectional shapes (star or triangle) have been added into PN models in order to better represent more angular porous materials. Dynamic or quasi-static techniques can be used, depending on whether the capillary forces dominate the viscous forces or the converse situation (Golparvar et al., 2018; Yin, 2018). If the specific cross-sections and the aspect ratio range are known (i.e., first fluid phase's entry pressure), the semi-empirical correlations can be derived by solving the well-known N-S equations. Elementary methods are used to monitor the contact line between liquid and solid, and the interface between liquids at every time step. The angle of contact and the corner angle of the displaced and displacing fluids are also monitored (Montellá et al., 2020). Using search algorithms, the fluid configuration's actual state at every individual element can be captured as the fluid flows. The possibility of adding a new set of fluid configuration displacements is assessed for each element. This is also true for the validity of the previously added displacement mechanism (Ambekar, 2021). Equations and criteria have improved, which can be used for modeling normal percolation and invasion percolation phenomena (for instance, formation/collapse of layers; snap-off or film/layer flow) (Golparvar et al., 2018).

The pore-network model is a practicable tool for analyzing fluid flow behavior at the micro-scale, which has low computational demand (Liu et al., 2016). PN techniques are commonly found in the effort to idealize pore geometries against others that are hydraulically similar, though they are simplified elements (for instance, cylinder, sphere) in regular networks (Oostrom et al., 2014). All of the PNs are extracted from the simplified representations of real porous materials. Every PN demonstrates the porous geometry statistically without the consideration of the local structure of the material, which restricts their predictive capability and accuracy (Ambekar, 2021; Liu et al., 2016). PN algorithms use simplified fluid flow models (i.e., Poiseuille flows) in order to govern the flow dynamics in porous geometry, that is constructed of various tubes or geometrically similar shapes. Previously,

in these PN approaches, only spheres and cylindrical throats were used, but today real and complex geometries can also be used (Oostrom et al., 2014).

Generally, in the last decade, pore network techniques were used to characterize the relative permeability of micro-structure in the case of single-phase flows. Recently, PNs have shown the ability to calculate multi-phase flow properties at the continuum-scale such as the saturation-capillary pressure and the saturation-permeability relations (Carrillo et al., 2020; Golparvar et al., 2018). Although, the PNs are not able to fully capture the microscopic-scale flow mechanisms as a result of the idealization/simplification of the pore-space topologies, which leads to the loss of topological and geometrical data. What's more, the temporal changes in the single-pore are not comprehensive, as each pore (body and throat) is normally reconstructed as an individual node. Therefore, though the PNs have been shown to be acceptable to predict the continuum-scale parameters of the material, the use of the PN technique for the calculation of multi-phase (i.e., two phases) flow dynamics in a porous material has various limitations (Ambekar, 2021).

## 7 Hybrid approaches

Finally, the so-called "hybrid models", the last class of simulation techniques, try to overcome and solve the present limitations by coupling models across scales. These approaches are focusing on various challenges of the general problem and difficulties (Mahmoodlu et al., 2020). The hybrid models combine, typically, direct numerical (described in Section 5) and network modeling (see Section 6) approaches in order to perform accurately and with computational efficiency. Furthermore, these hybrid methods are capable to bridge the different scales. Three widely used techniques are introduced in the following (Montellá et al., 2020).

Montellá et al. (2020) published a novel multi-scale technique integrating the traditional PN methods' effectiveness along with the original LB methods' accuracy. Their introduced algorithm is founded on the granular assembly's decomposing into smaller subsets. The pore-level multi-scale approach provides an approximation sequence to direct numerical methods (DNM) with controllable accuracy. The approach recommends dividing the computation domain for reproducing the physics at the micro-scale applying the LB and continuum scale models too (Landers et al., 2013). The macroscopic impacts of dynamic conditions of flow (viscous) at the micro-scale



can be analyzed by using LB for the pore scale, combining the PN and LB results in less computational cost and higher computational speed (Montellá et al., 2020).

Researchers, namely Miller and Hilpert (Chan and Govindaraju, 2011) extended the general pore morphology method to take accurate and complex porous material morphology into account for quasi-static pore throat in a porous material, which is water-wet. They use approaches from morphology-based algorithms to get the distributions of the fluid. This model of quasi-static fluid phase distributions depends on the discretization of the pore-space by a set of voxels, inhere in a cubic lattice (the calculated parameters are also characterized by voxels). Moreover, the interfacial area is slightly over-estimated, and the pore-space voxelization renders the calculated capillary pressures to assume discrete values (Mukherjee et al., 2011). Other researchers, namely Adalsteinsson and Hilpert (Chan and Govindaraju, 2011; Mukherjee et al., 2011) extended and developed this model further. Their approach treats the pore spaces and solid phases not as voxels, but rather as a correct discretization of a fundamental, continuous representation for drainage simulations. The modified pore morphology-based model reduced the computational cost and shows reasonable agreement with the practical results from experiments. This approach can be considered as a compromise between the simplified pore morphology-based PN model and the computationally intensive LB model, particularly for quasi-static fluid flows in accurate and realistic microstructures (Mukherjee et al., 2011).

From the work of Rabbani and Babaei (2019), a novel approach is offered. This method is able to couple the mentioned Lattice Boltzmann (LB) technique and each general pore network modeling (PN) utilizing the advantages of the two techniques simultaneously. The extraction of the pore network is realized with representations of twelve specific 3D porous materials using the watershed-segmentation approach. Every individual throat's permeability can be calculated by using the Lattice-Boltzmann approach (Landers et al., 2013) and is replaced in the PN approach rather than applying the cylindrical formulation found in the Hagen–Poiseuille equation. The solution of Boltzmann equations for each individual throat results in an exact flow-representation, however, the algorithm suffers from a substantial computational cost. Lattice-Boltzmann methods can be implemented into modeling the steady-state incompressible flow of fluids to mitigate the increased computational cost. Moreover, an artificial neural network

(ANN) can also be used to imitate the permeabilities of connecting elements (throat) sections found on the cross-sectional images. Consequently, the throat's averaged distance is positively correlated with the throat's permeability calculated by a particle-based technique (i.e., LB). It has been shown that even an elementary empirical correlation could correctly specify the connection between the defined parameters. The results demonstrated that the recommended hybrid technique produces an equivalent estimation of permeability along with a significant decrease in computational cost (Rabbani and Babaei, 2019).

## 8 Summary

All of the numerical methods for pore-scale analysis (Fu et al., 2021b; Macini et al., 2011) have strengths and weaknesses in areas such as flexibility, accuracy, computational cost (e.g., computational speed), and scalability (i.e., up-scaling). Therefore, it is necessary to compare the presented models using different computational problems (Zhang and Yang, 2014). While each method of the three main types has been widely used to calculate fluid flow and further different processes at the pore-scale. Moreover, comparatively small number of systematic comparisons of these algorithms have been published for a complex system regarding actual microstructure. A series of nonreactive solute transport measures through porous materials were conducted and the data was offered to the micro-structure simulating community for investigations (Regaieg, 2015).

Comparisons between various numerical approaches showed that each pore-scale model can simulate the laboratory experiments satisfactorily, but revealed no unique solution for the idealization of microstructures (Joekar-Niasar, 2016; Pawar, 2016). It should be noted that these comparisons were limited to simplified microstructures with steady-state tracer simulations and regular pore arrangements. Furthermore, relatively few intercomparison analyses based on 3-D reconstructed porous materials have also been published in which real and complex microstructures were represented in extremely high resolution (Yu et al., 2020). Specifically, the complex porous material can be scanned using different techniques, such as -CT (Ficzere et al, 2021; Mel'gunov and Ayupov, 2017). Depending on the computational power, both simplified and real pore geometries can be tested (Lyras et al., 2020). Consequently, actual pore structures are useful both for pore networks and direct numerical methods, and also for hybrid approaches. Finally, these two categories and

the third hybrid approaches demonstrated their ability to predict fluid properties accurately and achieved excellent agreement with the results of the experiments (Yu et al., 2020).

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