

# EVALUATION OF IMBIBITION PROCESS IN POROUS MEDIA BY INVADDED PERCOLATION PROBABILITY

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**ABSTRACT:** The water retention capacity of soil is determined by the texture and structure of the soil and the physical properties of the grain surface. Specifically, it is influenced by various factors such as size and shape of pore, connectivity to neighboring pores, and the contact angle of grains in a bottom-up manner. The water retention curve, a relationship between retained water in soil and matric potential, can exhibit different shapes depending on such factors. However, in our previous numerical experiments with a pore-network model, we suggested that the various water retention curves can be integrated into an almost identical curve regardless of different pore-size distributions when variously saturated porous media are evaluated by an evaluation index derived from the percolation theory. The evaluation method is called invaded percolation probability here, and it was extended from the percolation probability, which evaluates the degree of network connectivity. In this study, more detailed numerical experiments for imbibition process were conducted and the applicability of the invaded percolation probability was investigated. Our results indicated that a common curve of the invaded percolation probability was obtained if pores in the pore-network did not have any correlation with their neighboring pores. In a case where the pore-network had some spatial structure, we found that a different curve of the invaded percolation probability was obtained, and this evaluation method was applicable unless the structure was disturbed.

*Keywords: Water Retention Property, Pore-network, Percolation Theory, Invasion Percolation*

## 1. INTRODUCTION

The soil is essential not only for agriculture but also all terrestrial flora and fauna, including humans. Among various soil properties such as physical, dynamic, and chemical ones, hydraulic properties are quite important for crop production since water retention characteristics and permeability have a large influence on crop growth. Many models such as van Genuchten-Mualem model [1], [2], one of the representative functional models based on the bundle of capillary tubes model, have been utilized. In addition, to reproduce the hydraulic properties of soil in a bottom-up manner, an approach with a network of pores has been utilized, focusing on the importance of connectivity of pores [3], after Fatt et al. proposed a pore-network model [4]. This approach has also been employed to analyze pore structure [5], [6]. Recently, detailed shape of pores and frequency of pore size have studied directly due to the development of observation apparatus such as a high-resolution X-ray computed tomography (CT) scan [7].

On the other hand, invasion phenomena such as imbibition and drainage processes can be put together into a single curve based on the percolation probability from the analysis with the

percolation theory [8]. The curve, which is referred to as the invaded percolation probability in this study, shows a relationship between invadable and invaded pores. Moreover, the curve resembles the water retention curve showing a relationship between matric potential and saturation or water content in the soil. Although physical indices are used in both axes in the water retention curve, proportions of invadable and invaded pores to the total pores are used in the invaded percolation probability. The matric potential in the water retention property corresponds to the proportion of invadable pores in the invaded percolation probability, and saturation to the proportion of invaded pores. By introducing this evaluation method, there is a possibility that various water retention curves obtained from different soil type are treated in a unified way, and this deepens the understanding of invasion processes as a basic principle. In this study, the applicability of the evaluation method and factors that determine the shape of the invaded percolation probability were investigated through numerical experiments.

## 2. MODEL

### 2.1 Pore-network Model

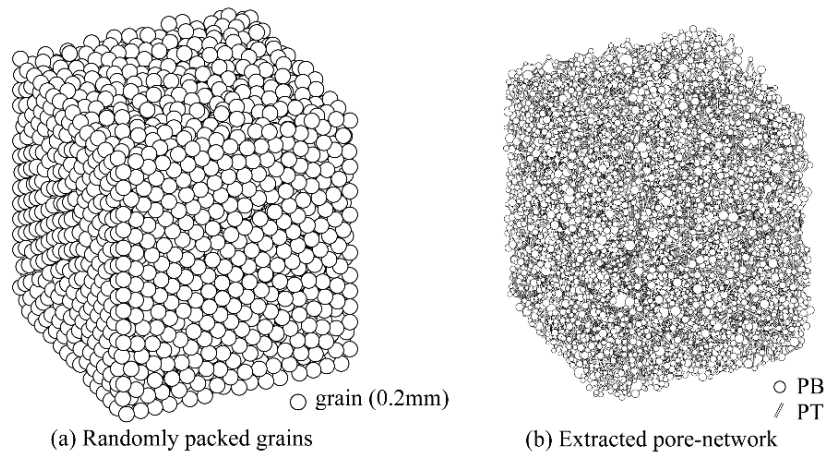


Fig. 1 Virtual porous medium (Network1)

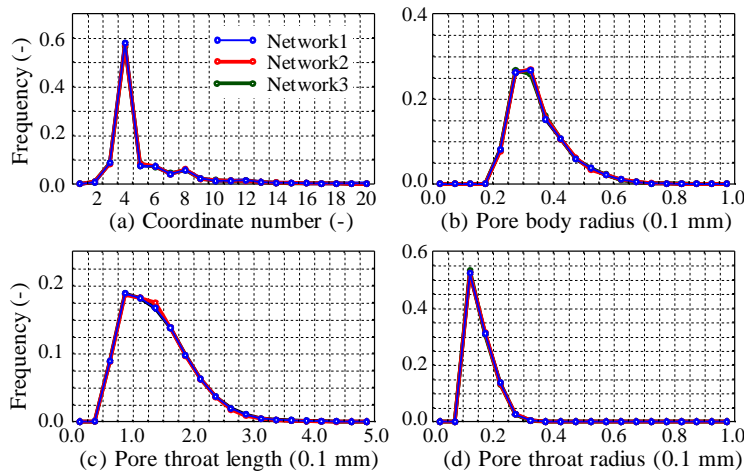


Fig. 2 Histograms of coordinate number and pore sizes

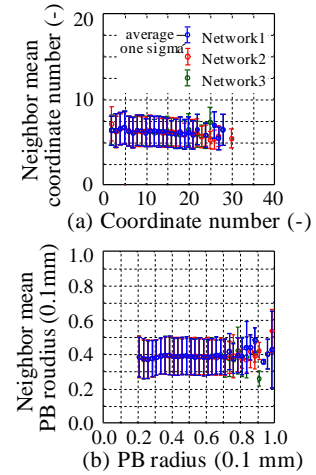


Fig. 3 Correlation of neighbor PBs

A pore-network model was utilized to conduct numerical experiments, described in the following section, and it was extracted from a virtual porous medium prepared by using the discrete element method. A virtual porous medium is composed of equal-sized spherical grains packed randomly in a cubic container. A pore-network was extracted from the porous media with the modified Delaunay tessellation method [9]. Fig. 1 shows a virtual porous medium formed by 5800 spherical grains of 0.2 mm in a 9 mm<sup>3</sup> cube container and a pore-network extracted from the porous medium.

A pore-network consists of pore bodies (PBs) and pore throats (PTs). PBs are relatively large and are represented by circles in Fig. 1. PTs are relatively small and connect two PBs; these are represented by tubes here. The extracted pore-network referred as Network1 here in Fig. 1 (b) includes 14,000 PBs and 35,500 PTs. Moreover, frequency distributions of pore sizes and coordinate number, the number of PTs that a single PB connects, are shown in Fig. 2. Figure 3 shows the correlations between coordinate numbers, and between the radii of PBs and other PBs

surrounding them. Except for the vicinity of the right ends of both graphs, where values disperse since the number of samples in each dot is small, the shape of the graphs was generally flat, which showed that neither coordinate number nor PB size had a strong spatial correlation with their neighbors. However, the level of low radii was slightly lower compared to others, meaning that small PBs tend to connect small PBs.

## 2.2 Percolation Probability

In the percolation theory, a network is represented by sites and bonds, which correspond to PBs and PTs, respectively, in a pore-network model. In an analysis using networks, two processes are considered on a network, namely, site and bond processes in which sites and bonds play the main roles, respectively. In a site process, each site takes one state out of two possible states: 'open' or 'close'. When a site is open, it can convey something, which depends on an objective system (e.g., information, electricity, and infectious disease) [10]. In this study, open sites

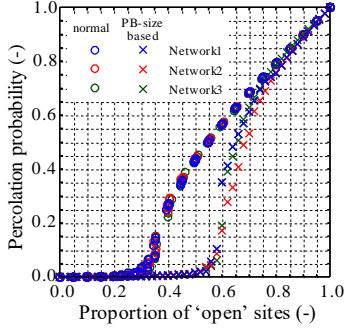


Fig. 4 Percolation probability

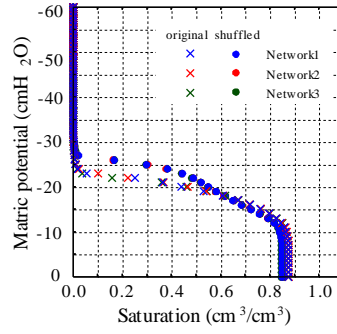


Fig. 5 Water retention curves

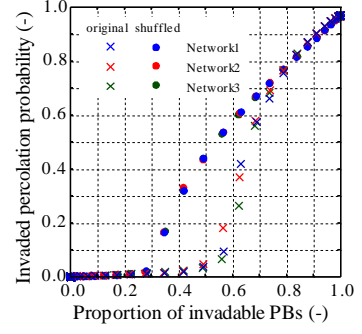


Fig. 6 Invaded percolation probability

represent invadable pores small enough, and close sites represent non-invadable pores large in imbibition process. Then, the conveyed matter is water. In drainage process, open (invadable) pores are large enough and the conveyed matter is air. Basically, the imbibition process into normal (hydrophilic) soil can be treated as a site process because PBs regulate the water invasion. This means that if water can invade into a certain PB, it can also inevitably invade into the PTs connected to the PB because the connected PTs are smaller than the PB. Moreover, the drainage is treated as the bond process for the same reason.

The percolation probability is an index of connectivity inside a network and represented by a relationship between the proportion of all open elements (sites or bonds) in a network and that of the largest open cluster, which is the maximum subnetwork formed by open elements, among all open clusters in the network. Normally, as the proportion of open elements increases, the number of open clusters decreases and eventually one large subnetwork is formed by connecting each other.

Fig. 4 shows two types of percolation probabilities of the site process. One type is a normal percolation probability as a network in which the percolation probability is computed based on random numbers given to sites. The other type is a percolation probability computed based on the PB size. These show a typical shape of the percolation probability. As the proportion of open sites increases, the percolation probability rises suddenly at a point and approaches a diagonal line asymptotically. The point of sudden rise is referred to as the percolation threshold, and it shows phase transition because the system changes from non-conveyable to conveyable at this point. In soil physics, the transition point has an important meaning because it corresponds to the point where water begins to invade into the soil at the water-entry pressure of the soil in imbibition process. In other words, when the pressure passes across the water-entry pressure, the proportion of invadable pores becomes large enough to form a large subnetwork spreading from one side to the opposite. In drainage process, transition point

corresponds to air-entry pressure.

### 2.3 Invasion Percolation

An invasion percolation [11] is utilized as the relevant model for a process of displacement by immiscible fluids (e.g., water and air). Invasion percolation is a temporally and spatially discretized progressive process model whereby invaded elements on interfaces change from one state to the other if certain conditions are met. The water-entry pressure for imbibition and air-entry pressure for drainage determine whether the fluid enters the element or not in fluid invasion in a pore-network. In an imbibition process, water can enter objective pores filled with air if the water-entry pressure  $p_{we}$  is greater than the capillary pressure  $p_c$  as follows:

$$p_{we} > p_c \quad (1)$$

with

$$p_c = p_{air} - p_{water} \quad (2)$$

$$p_{we} = P_{water} \sigma \cos \theta_{adv} / R_{imb} \quad (3)$$

$$R_{imb} = A_{water} / P_{water} \quad (4)$$

where  $p_{air}$  and  $p_{water}$  are the air and water pressures at the vicinity of the air-water interface,  $\sigma$  is the interfacial tension,  $R_{imb}$  is the hydraulic radius,  $A_{water}$  and  $P_{water}$  are the cross-sectional area and the wetted perimeter of the objective pore, respectively, and  $\theta_{adv}$  is the advance contact angle of the pore wall. Here it is assumed that the air pressure is constant, and the water pressure is hydrostatic. Therefore, when some pressure is applied to the bottom of the porous medium the water pressure at an objective pore is represented as follows:

$$p_{water} = p_{btm} - (z - z_{btm}) \quad (5)$$

where  $p_{btm}$  is the water pressure at the bottom of the medium,  $z$  and  $z_{btm}$  are the  $z$  coordinates of the objective pore and the bottom. To represent the degree of ease with which a fluid invades a pore filled with the other fluid, invadability is defined as follows:

$$I_{imb} = p_c - p_{ac} \quad (6)$$

where  $I_{imb}$  is the invadability for an imbibition process.

In addition to the conditions for water-entry, an accessibility rule is imposed for movement of the interfaces between the invading and invaded fluids. Specifically, each fluid needs to connect to its outside reservoir through pores filled with the same fluid type.

In this study, the invading fluid enters an arbitrary number of invadable pores, in the same way as in Takeuchi et al. (2016) [5]. In the original version of invasion percolation, the invading fluid enters the most easily invadable pore in each time step [11]. Takeuchi et al. (2016) show that the number of pores invaded in one-time step affects the residual amount of invaded fluid [5].

The procedure of invasion percolation for an imbibition process is described below:

1. As an initial state, all pores are filled with air, and a certain pressure is imposed on the bottom of the pore network.
2. Those pores filled with air and connected with water-filled pores satisfy the accessibility rule and they are sorted in descending order of invadability for an imbibition process.
3. The top  $N^{ip}$  pores are invaded by water (i.e., the air in these pores is discharged through other air-filled-pores), simultaneously, where  $N^{ip}$  is the number of pores that are invaded in one-time step.
4. Processes 2 and 3 are iterated until no pores change their state, which means that the pore-network has reached a steady state under the imposed pressure at the bottom, and the saturation of the pore-network is calculated.
5. The pressure imposed at the bottom is changed (increased in the case of an imbibition process), and the process returns to stage 2.

Regarding the state of the pore-network, there are two possible options: either the state obtained from the previous pressure condition is used as an initial state in the next pressure condition or a fully dried state is used as the initial state. The former option corresponds to the suction method in which one soil sample is used for various pressures and changed gradually and the latter option corresponds to the soil column method in which a separate pressure is imposed on each stacked soil sample in the column.

#### 2.4 Invaded Percolation Probability

As mentioned in the previous sub-section, percolation probability is a static property of a network, and the percolation threshold is very important to estimate the network behavior. If the proportion of 'open' pores exceeds the critical percolation threshold, the system begins to convey

the fluid. However, the percolation probability alone cannot be used to estimate fluid invasion into porous media because the invading order has a strong influence on whether one fluid invades a pore filled with the other fluid or not, due to the accessibility rule. In this study, the invasion percolation probability is proposed for a dynamic process such as imbibition and drainage. Although the normal percolation probability is obtained solely from a network, the invasion percolation probability changes depending on both of the number of pores invaded in one step and the number of pores connected to the invading fluid at the beginning of the process. Computation of the invasion percolation probability is conducted in the same way as the normal percolation probability for a finite network. In a graph representing the proportion of potentially invadable pores on the horizontal axis and the proportion of the maximum subnetwork filled by invaded fluid in the whole network on the vertical axis, the results of invasion percolation from various proportions of potentially invadable pores were plotted to create a scatter graph showing the invasion percolation probability.

### 3. NUMERICAL EXPERIMENTS

Based on the extracted pore-networks, various pore-networks with the different frequency distribution of pore sizes were generated, and two numerical experiments of the imbibition process were conducted in this study. The top and bottom are open to air and water, respectively, and the four sides are enclosed by walls. In this case, air and water cannot go in and out through the sides. Water is supplied from the bottom, and the air is discharged from the top freely in an imbibition process. The maximum number of pores invaded in one-time step is set as 10,000, which gives no substantial limit.

#### 3.1 Different Packings of Grains

Three pore-networks extracted from different porous media made from a randomly-perturbed initial position of grains were used to investigate the individual difference of the pore network. The frequency distributions of the coordinate number and pore sizes, the correlation with neighbor PBs, and the percolation probability were almost identical, although these three pore-networks have different topology (Figs. 2–4). Besides, the computed results of the water retention property and invaded percolation probability (Figs. 5 and 6, respectively) were also almost identical. These results assure that the volume of porous media employed in this study is sufficient, and this volume exceeds the representative elementary volume (REV).

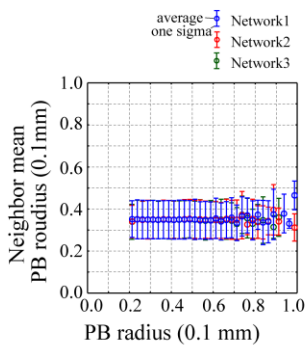
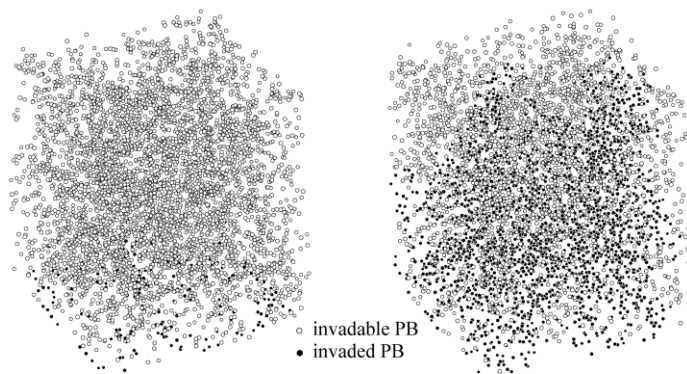


Fig. 7 Correlation of neighbor PBs (shuffled)

In addition to the verification of porous media volume, another experiment was conducted to investigate the effect of the arrangement of PBs. In the normal percolation probability, each site is treated equally. Hence, whether a site is open or close is given stochastically. However, the size of each PB is used as a value in the PB-size-based percolation probability. Thus, 0.3 in the horizontal axis in Fig. 4 means that 30% of sites (pores) from the smaller ones are open. The arrangement of PBs is responsible for the discrepancy between normal and PB-size-based percolation probabilities (Fig. 4). The percolation threshold of the normal and PB-size-based percolation probabilities were 0.35 and 0.55, respectively. This result indicates that the networks as a pure network have potential to form an open subnetwork which expands sufficiently if 35% of sites are open. However, the network as a pore-network needs 55% of open sites (invadable PBs). This result implies that small PBs do not exist uniformly in the pore network. This inference is supported by the fact that the small PBs whose radius is 0.03 mm or less tend to connect to small PBs (Fig. 3).

Another three virtual pore networks in which PB size is randomly shuffled in each network were created from the three pore networks. Here, the generated and original pore-networks are referred to as ‘shuffled’ and ‘original’, respectively. The computed water retention curves and invaded percolation probability are shown in Figs. 5 and 6. These figures show that the difference between each type of pore-network is small enough, and water entry pressure of the original pore-networks is larger than that of the shuffled pore-networks, reflecting the large percolation threshold of the original pore-networks.

Fig. 7 shows the correlation of neighbor PBs of the shuffled pore-networks. Unlike that of the original pore-networks in Fig. 3 (b), totally flat graphs are obtained except for the right end, which shows each size of PBs connect evenly to all size of PBs. Fig. 8 shows spatial distributions of



(a) Original network (34.9%, 1.4%) (b) Shuffled network (34.9%, 16.4%)  
Fig. 8 Invadable and invaded PBs in Network1 (percentages of invadable and invaded PBs to total PBs)

invadable and invaded PBs in the original and shuffled pore-networks of Network1 when the percentage of invadable PBs is 34.9%. At this time, the water pressure applied to the bottom of the pore-network is -26 cmH<sub>2</sub>O, and only a little amount of water invades from the bottom face in the original pore-network when water spreads in the shuffled pore-network (Figs. 5 and 8). Table 1 shows that invadable PBs forms separate small clusters in the original pore-network, and a big cluster is formed in the shuffled pore-network.

Table 1 Properties of invadable clusters

	original	shuffled
the number of pores	14060	
the number of invadable pores	4907	
the number of clusters	1860	1045
the minimum of NIP <sup>†</sup>	1	1
maximum of NIP	54	2364
mean of NIP	2.7	4.8
standard deviation of NIP	4.1	73.6

<sup>†</sup>NIP is the number of pores in an invadable cluster.

### 3.2 Various Distributions of Pores

In this subsection, three different types of pore-size distribution such as average-shift type, variance-change type, and bimodal type are given to PBs and PTs of Network1 to investigate the effect of pore size distributions on water retention property and invaded percolation probability (Fig. 9). In the average-shift type, the distributions are shifted upward or downward without changing their original distribution shape (A3), and in the variance-change type, the variance of distributions are larger or smaller from the original distribution (V3). A3 and V3 are equal to Network1. In the bimodal type, bimodal distributions were generated by mixing two different distributions of B1 (=A1) and B5 (=A5) at various rates. The cumulative distributions of invadable pores to the

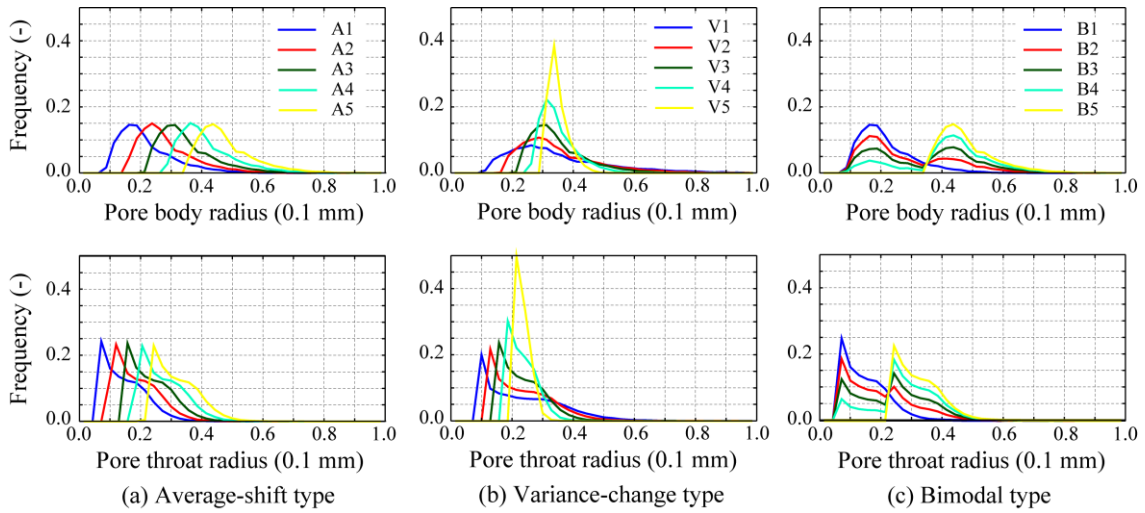


Fig. 9 Pore-size distributions

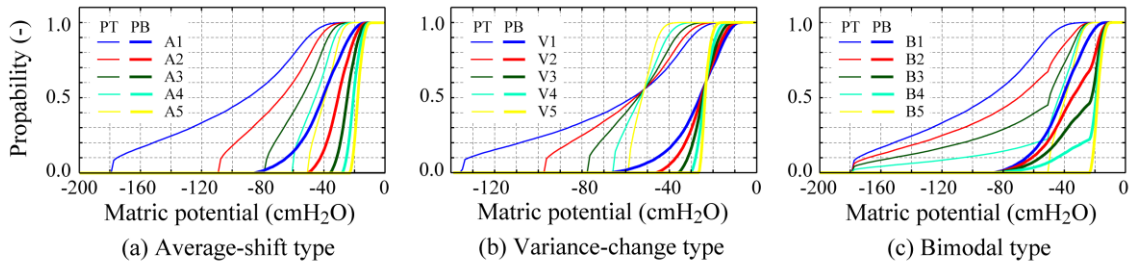


Fig. 10 Cumulative distributions of invadable pores

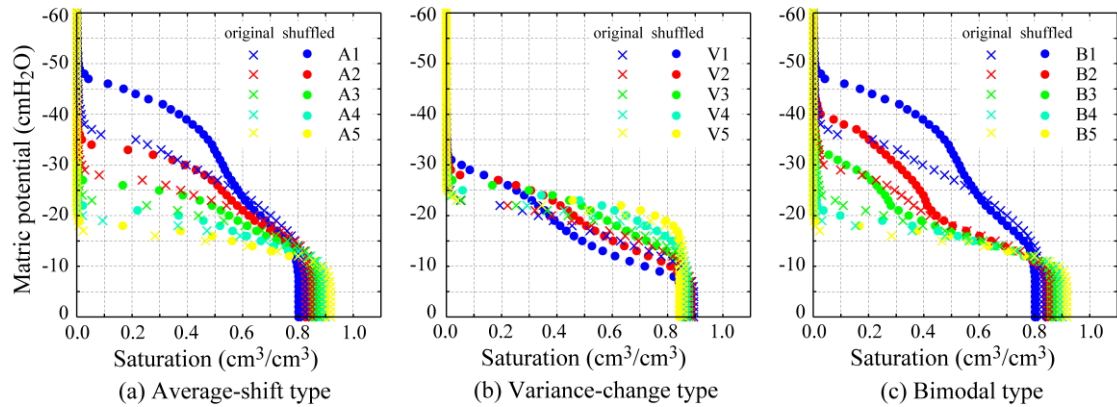


Fig. 11 Water retention curves of different pore-size distributions

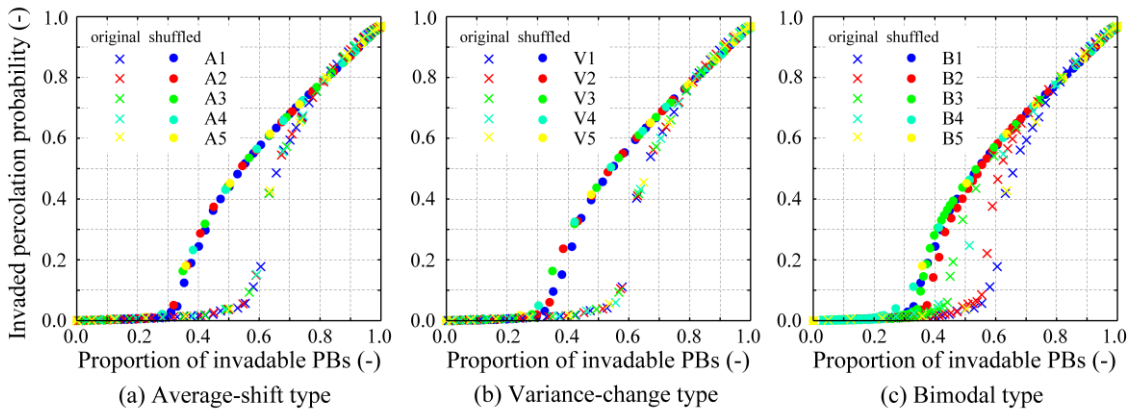


Fig. 12 Invaded percolation probability of different pore-size distributions

matric potential of each distributions type are shown in Fig. 10. In the same way with the previous subsection, pore-size-shuffled versions of each pore-network were also generated.

The computed water retention properties and the invaded percolation probabilities are shown in Figs. 11 and 12. We found that although the shape of water retention curves changed variously depending on the pore-size distributions, all the obtained invaded percolation probability were almost identical except for the bimodal distribution in the original pore-network, and shapes of the invaded percolation probability was the same with those in Fig. 6 and derives from the percolation probability of the site process shown in Fig. 4.

In the original pore-network with the bimodal distribution, the invaded percolation probability of B2, B3, and B4 deviated from others because the structure of small pores, which form many clusters of several pores in the pore-network, was destroyed by the mixing of pores of different sizes. However, even in a case of the shuffled pore-network, the obtained invaded percolation probability of the bimodal distributions was almost identical to those of other distributions since shuffled pore-network does not have such structure.

Furthermore, we found that the water-entry pressure of a pore-network can be estimated from the percolation probability of the site process (Fig. 4) and cumulative distribution of invadable pores (Fig. 10). As an example, a case of A1 is explained here. We found that the percolation thresholds of the original and shuffled pore-networks are about 0.55 and 0.35, respectively (Fig. 4), and the values of the matric potential of both were about -39 and -48 cmH<sub>2</sub>O when the cumulative probability of those were 0.55 and 0.35 (Fig 10 a). This value was identical to the water-entry pressure of A1, which were about -38 and -48 cmH<sub>2</sub>O (Fig. 12 a).

#### 4. CONCLUSIONS

In this study, two types of numerical experiment were conducted using extracted pore-networks from virtual porous media to investigate the applicability of the evaluation method called invaded percolation probability. In the first numerical experiment, we showed that porous media randomly packed with equal-size spherical grains had a spatial structure that small pores form separate clusters compared to the uniformly distributed pore-network, and the shape of the percolation probability and invaded percolation probability depended on the structure. In addition, we found that the structure obstructed water invasion and made the water-entry pressure higher as a result. In the second experiment with various pore size distributions, we showed that almost identical invaded percolation probability in each type of pore-network were obtained unless the pore structure was destroyed although various water retention curves were obtained depending on the different pore size distributions. This finding showed the feature of the evaluation method that the same type of network had the same shape of invaded percolation probability. Hence, we concluded that this evaluation method based on the percolation theory is applicable, but the shape of the percolation probability is valid only in the same soil type.

#### 5. ACKNOWLEDGEMENTS

This study was supported by JSPS KAKENHI Grant Number 16K07971.

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