## Invasion percolation through minimum-weight spanning trees

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Invasion percolation is often used to simulate capillary-dominated drainage and imbibition in pore networks. More than a decade ago it was observed that the part of a pore network that is involved in an invasion bond percolation is a minimum-weight spanning tree of the network, where the weights indicate resistances associated with the bonds. Thus, one can determine a minimum-weight spanning tree first and then run the invasion bond percolation on the minimum-weight spanning tree. The time complexities of the two steps are  $O(m\alpha(m,n))$  and O(n), respectively, where m is the number of edges, n is the number of vertices, and  $\alpha(\cdot,\cdot)$  denotes the inverse Ackermann function. In this paper we (1) formulate the property of minimum-weight spanning trees that justifies the two-step approach to invasion bond percolation, (2) extend the two-step approach to invasion site percolation, and (3) further extend it to simulations of drainage (imbibition) that include trapping of the wetting (nonwetting) phase. In case of imbibition we also take snap-off into account. As a consequence, all these simulations can now be done in  $O(m\alpha(m,n))$ .

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### I. INTRODUCTION

Multiphase flow is a process that may occur in both natural and manufactured porous media, e.g., when (1) water flows in the partially saturated subsurface (the vadose zone), (2) oil is recovered from its natural reservoirs via water flooding, or (3) water flows in polymer-electrolytemembrane (PEM) fuel cells. Pore network models have been used extensively to study pore-scale characteristics of such flows and to then draw conclusions about macroscale flow behavior [1,2]. Pore networks represent real porous media by sites (the pore bodies) which are connected via bonds (passing through the pore throats). Simple rules, which account for local pore size, mass conservation, Poiseuille's equation for the viscous pressure drop (and extensions to noncircular pore throats or bonds), and capillary physics, are then used to model multiphase flow in a network. As a result, network models generally allow simulation of larger spatial domains than approaches that solve the Navier-Stokes equation or a lattice-Boltzmann equation.

Wilkinson and Willemsen [3] coined the term *invasion* percolation (IP) for network (lattice) models of two-phase flow, assuming that the flows are dominated by capillary forces and hence neglecting viscous forces. Two flavors of IP exist. Invasion bond percolation (IBP) describes the displacement of a wetting by a nonwetting fluid (drainage), while invasion site percolation (ISP) describes the displacement of a nonwetting by a wetting fluid (imbibition) [4]. In both IBP and ISP, the invading fluid advances at the location on the front between the two fluids where the resistance is minimal.

To specify what "minimal resistance" means during drainage, we denote by  $p_d(t)$  the critical capillary pressure (CP) between the two fluids at which nonwetting fluid invades a

pore throat t (and promptly the next pore body), provided that exactly one of the two pore bodies separated by t is filled with nonwetting fluid. In IBP, the critical CP  $p_d$  is inversely proportional to the size of t, proportional to the interfacial tension between the two fluids, and a function of contact angle.

To specify what minimal resistance means during imbibition, we denote by  $p_i(b)$  the critical CP between the nonwetting and the wetting fluids at which the wetting fluid invades a pore body b, provided that at least one of the pore throats incident on b is filled with wetting fluid. In ISP, the critical CP  $p_i(b)$  is inversely proportional to the size of b, proportional to the interfacial tension between the two fluids, and a function of contact angle, but it also depends on from how many and which throats the wetting phase seeks to invade the pore body b [5]. Generally, "cooperative pore filling" tends to increase the  $p_i$  values. There remains an issue about how one should exactly calculate  $p_i$  because of the complex shape of pores and the multiple fluid-fluid interfaces that merge in a complicated fashion during cooperative pore filling by wetting phase. Hence, network models exist that either do [6-8], in a typically heuristic manner, or do not [9,10] account for the effects of cooperative pore filling. As in [11], we call the pressure difference between the nonwetting phase and the wetting phase reservoir the external CP.

Minimal resistance during drainage (imbibition) now means that  $p_d$  ( $p_i$ ) is minimal (maximal) as compared to all pore throats (pore bodies) that are filled with the displaced fluid and that are incident on (adjacent to) the front. The external CP at which a given pore throat (pore body) in a pore network is invaded by the nonwetting (wetting) phase is determined by a path of minimal resistance from the nonwetting (wetting) phase reservoir to the pore throat (pore body).

More than a decade ago, Barabási [12] observed that running an IBP simulation (i.e., a primary drainage simulation) on a lattice amounts to constructing a minimum-weight spanning tree (MWST) [13,14] of the lattice with respect to the resistance values associated with the bonds of the lattice. This fact is very important, as it allows simulating drainage

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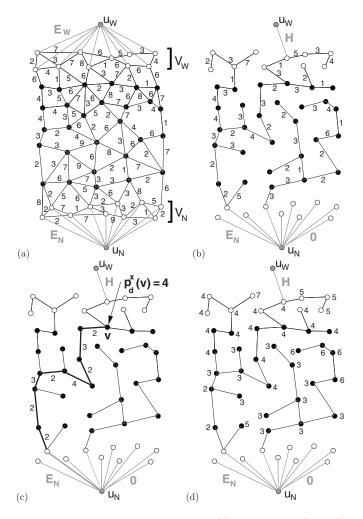


FIG. 1. Drainage without trapping. (a) A graph  $G^+=(V^+,E^+)$ . The numbers indicate values of  $p_d(\cdot)$ . (b) MWST of  $G^+$  with respect to  $\omega_d(\cdot)$ . The numbers at the edges indicate their  $\omega_d(\cdot)$  values, and H is a number higher than all  $p_d$  values. (c) The  $p_d^x$  value of a vertex v is the maximum of the  $\omega_d$  values along the unique path from  $u_N$  to v on a MWST of  $G^+$  with respect to  $\omega_d(\cdot)$ . (d) The  $p_d^x$  values for all  $v \in V \setminus V_N$ . They indicate the external CP at which drainage actually occurs.

much more effectively than algorithms that iteratively search the moving front between the invading and displaced fluids for the bond with the minimal resistance. Computational efficiency is crucial when networks are sought to span representative elementary volumes [15] or when they are used to determine fractal dimensions of sample spanning clusters, backbones, and minimal paths [4,16,17], because these properties only very slowly approach their asymptotic limits as the network size increases.

The objectives of this paper are (1) to rigorously show that primary drainage can indeed be simulated in pore networks by using a MWST; and (2) to develop a MWST method to simulate primary imbibition. In each case we demonstrate how one can take trapping into account. In the case of imbibition we also include snap-off [18,5], i.e., the imbibition of narrow ducts by the wetting phase due to the thickening of the wetting phase films.

Our method for simulating drainage (imbibition) works

only if the  $p_d$  ( $p_i$ ) values are known *a priori* (before the flow simulation). In particular, we do not take cooperative pore filling into account when simulating imbibition.

In the next section, we will introduce the formalism necessary to describe our method and prove its correctness. Then, we work out the graph-theoretical basics needed to relate the MWSTs to the flow simulations. After that, we show how drainage and imbibition can be modeled using MWSTs.

### II. SPANNING TREES OF PORE NETWORKS

In this paper, a pore network takes the form of an undirected connected graph G=(V,E) with vertex set V and edge set E [19]. We think of the vertices (edges) in V (E) as pore bodies (connections of pore bodies via their interfaces = pore throats). The vertices and edges are equipped with attributes given by the following functions.

- (a)  $p_d: E \mapsto \mathbb{R}$ , where  $p_d(e)$  indicates the CP that is critical for drainage through the pore throat represented by an edge e, provided that exactly one of the pore bodies represented by the end vertices of e is filled with nonwetting phase.
- (b)  $p_i: V \mapsto \mathbb{R}$ , where  $p_i(v)$  indicates the CP that is critical for imbibition of the pore body  $b_v$  represented by a vertex v, provided that at least one neighbor of  $b_v$  is filled with wetting phase.

We adhere to the general idea that a pore body  $b_v$  represented by a vertex v of G is wider than the pore throats between  $b_v$  and neighboring pore bodies, i.e.,  $p_i(v) < p_d(e_v)$  for all  $e_v$  incident on v. We specify the reservoir of the nonwetting (wetting) phase by means of a subset  $V_N(V_W)$  of V [see Fig. 1(a)].

In order to get a handle on the reservoirs we represent them by new vertices  $u_N$  and  $u_W$ , respectively. We then link  $u_N$  ( $u_W$ ) to all vertices in the nonwetting (wetting) phase reservoir, the new edges forming the set  $E_N$  ( $E_W$ ) [see Fig. 1(a)]. The extended graph thus obtained is the graph  $G^+$  with vertex set  $V^+$  and edge set  $E^+$  formally defined through

$$V^{+}:=V\cup\{u_{N},u_{W}\},\tag{1}$$

$$E_N := \{\{u_N, v\} \text{ with } v \in V_N\},$$
 (2)

$$E_W := \{\{u_W, v\} \text{ with } v \in V_W\},$$
 (3)

$$E^+:=E\cup E_N\cup E_W,\tag{4}$$

$$G^+:=(V^+,E^+).$$
 (5)

A spanning tree of  $G^+$ =( $V^+$ , $E^+$ ) is a subgraph T=( $V_T$ , $E_T$ ) of  $G^+$  that (1) is a tree, i.e., is connected and contains no circuits, and (2) contains all vertices of  $G^+$ , i.e.,  $V_T$ = $V^+$ . For an example, look at  $G^+$  depicted in Fig. 1(a) and the spanning tree of  $G^+$  depicted in Fig. 1(b).

In this paper, we express the resistances of the pore throats (pore bodies) to the invasion of the nonwetting (wetting) phase through weight functions  $\omega: E^+ \mapsto \mathbb{R}$ . There are no weights assigned to the vertices. The (total) weight of a spanning tree  $T=(V^+, E_T)$  with respect to  $\omega(\cdot)$ , also referred

to as the  $\omega$  weight of T, is defined as  $\Sigma_{e \in E_T} \omega(e)$ , and a MWST of  $G^+$  with respect to  $\omega(\cdot)$  is a spanning tree of  $G^+$  whose  $\omega$  weight is smaller than or equal to the  $\omega$  weight of any other spanning tree of  $G^+$ . The spanning tree in Fig. 1(b) is minimal with respect to a weight function  $\omega_d(\cdot)$  that coincides with  $p_d(\cdot)$  outside the reservoirs (the  $\omega_d$  values of the other edges are specified in Sec. IV).

Barabási's observation that running an IBP simulation amounts to constructing a MWST now takes the following form: IBP on  $G^+$  can be done by constructing a MWST of  $G^+$  with respect to  $\omega_d(\cdot)$  and running IBP only on the MWST.

Let us recast our objectives in graph-theoretical terms. We will derive a weight function  $\omega_d\colon E^+\mapsto \mathbb{R}$  ( $\omega_i\colon E^+\mapsto \mathbb{R}$ ) from the  $p_d$  ( $p_i$ ) values such that drainage without trapping (imbibition with neither trapping nor snap-off) can be done by (1) calculating a MWST of  $G^+$  with respect to  $\omega_d(\cdot)$  [ $\omega_i(\cdot)$ ], and (2) traversing the MWST. We then devise a weight function  $\omega_d^t(\cdot)$  [ $\omega_i^t(\cdot)$ ] such that a traversal of a MWST with respect to  $\omega_d^t(\cdot)$  [ $\omega_i^t(\cdot)$ ] allows us to take trapping (trapping and snapoff) into account during drainage (imbibition). Specifically,  $\omega_d^t(\cdot)$  allows us to locate trapped wetting phase after drainage, and  $\omega_i^t(\cdot)$  allows us to locate trapped nonwetting phase after imbibition.

### III. WHY MWSTs ARE USEFUL FOR IP

As laid out in the Introduction, the external CP at which a given pore throat (pore body) in a pore network is invaded by nonwetting (wetting) phase is determined by a path of minimal resistance from the nonwetting (wetting) phase reservoir to the pore throat (pore body). Often, the very large number of such paths prohibits the testing of them all. If, however, the paths of minimal resistance are contained in a certain MWST of the pore network, the paths are unique and no longer need to be tested. To build such MWSTs we will exploit a well-known theorem about MWSTs (see Theorem 1) and derive a proposition (see Proposition 1) that relates minimal resistance on a pore network to resistance on a MWST of the pore network. We will use the representation of the pore network by a graph  $G^+$ , as explained in Sec. II.

Let  $\Pi$  be a path on  $G^+$  given by a nonempty sequence of edges  $e_1, \ldots, e_k \in E^+$ , let  $\omega \colon E^+ \mapsto \mathbb{R}$  be a weight function, and let  $u \neq v \in V^+$ . We then set

$$\operatorname{Max}_{\omega}(\Pi) := \max\{\omega(e_i) : 1 \le j \le k\},\tag{6}$$

 $\operatorname{MinMax}_{\omega}(u,v) := \min \{ \operatorname{Max}_{\omega}(\Pi) :$ 

$$\Pi$$
 is a path from  $u$  to  $v$ }. (7)

Let the graph  $T=(V^+,E_T)$  be a spanning tree of  $G^+=(V^+,E^+)$ , and let  $e_T\in E_T$ . Removing  $e_T$  from T splits T into two trees  $T_1$  and  $T_2$ . Thus, the vertex set  $V^+$  of  $G^+$  is decomposed into vertex sets  $V_1^+$  and  $V_2^+$ . The set of all edges in  $E^+$  with one end vertex in  $V_1^+$  and the other end vertex in  $V_2^+$ , a so-called cocycle [13], is denoted by  $E^+(T,e_T)$ . We are now able to write down an important theorem about MWSTs (see Theorem 4.3.3 including a proof in [13]).

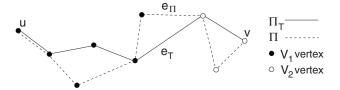


FIG. 2. Illustration to proof of Proposition 1.

Theorem 1 (cocycles of MWSTs). Let  $G^+ = (V^+, E^+)$ , and let the edge weights of  $G^+$  be given by a function  $\omega: E^+ \mapsto \mathbb{R}$ . Then, a spanning tree  $T = (V^+, E_T)$  of  $G^+$  has minimal weight with respect to  $\omega(\cdot)$ , if and only if the following holds for each  $e_T \in E_T$ :

$$\omega(e_T) \le \omega(f)$$
 for all  $f \in E^+(T, e_T)$ .

Proposition 1 [MinMax $_{\omega}(\cdot,\cdot)$  on  $G^+$  in terms of  $\mathrm{Max}_{\omega}(\cdot)$  on a MWST]. Let T be a MWST of  $G^+$  with respect to some  $\omega: E^+ \mapsto \mathbb{R}$ . Furthermore, let  $u \neq v \in V^+$ , and let  $\Pi_T$  denote the unique path between u and v on T. Then,  $\mathrm{MinMax}_{\omega}(u,v) = \mathrm{Max}_{\omega}(\Pi_T)$ .

Proof. Let  $\Pi$  be a path between u and v on  $G^+$  such that  $\operatorname{MinMax}_{\omega}(u,v) = \operatorname{Max}_{\omega}(\Pi)$ . Furthermore, let  $e_T$  be an edge on  $\Pi_T$  with  $\omega(e_T) = \operatorname{Max}_{\omega}(\Pi_T)$  (see Fig. 2). Removing  $e_T$  from T splits T into two trees  $T_1$  and  $T_2$ . Thus, the vertex set  $V^+$  of  $G^+$  is decomposed into vertex sets  $V_1^+$  and  $V_2^+$ , where u is contained in  $V_1^+$  and v is contained in  $V_2^+$ . Hence, when walking on  $\Pi$  from u to v, one traverses an edge  $e_\Pi$  with one end vertex in  $V_1^+$  and the other end vertex in  $V_2^+$ . According to Theorem 1 we have  $\omega(e_T) \leq \omega(e_\Pi)$ , and thus  $\operatorname{MinMax}_{\omega}(u,v) \geq \omega(e_\Pi) \geq \omega(e_T) = \operatorname{Max}_{\omega}(\Pi_T) \geq \operatorname{MinMax}_{\omega}(u,v)$ .

# IV. SIMULATION OF DRAINAGE WITHOUT TRAPPING

In a real experiment on quasistatic primary drainage, one starts with a wetting phase saturated porous medium at a low external CP (often 0) and then gradually and slowly increases the external CP. Simulating quasistatic primary drainage through IBP amounts to assuming that, if the external CP has risen to an intermediate value  $p^x$ , a pore body  $b_v$  represented by a vertex  $v \in V \setminus V_W$  has been drained at some point during the pressure increase to  $p^x$ , if and only if there exists a path between a vertex in  $V_N$  and v such that the maximal  $p_d$  value of the edges along the path is  $\leq p^x$ . This, in turn, is equivalent to saying that the external CP at which  $b_v$  is actually drained equals MinMax $_{\omega_d}(u_N, v)$ , where

$$\omega_d(e) := \begin{cases} 0 & \text{if } e \in E_N, \\ H & \text{if } e \in E_W \text{ or } e = \{u, v\} \text{ with } u, v \in V_N, \\ p_d(e) & \text{otherwise,} \end{cases}$$
(8)

and H is a number higher than all  $p_d$  values. We denote the external CP at which  $b_v$  is actually drained by  $p_d^x(v)$ . Due to Proposition 1,  $p_d^x(v)$  equals the maximum of all  $\omega_d$  values on the unique path between  $u_N$  and v on the MWST of  $G^+$  with

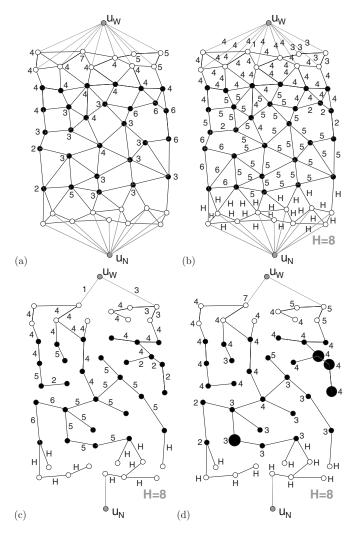


FIG. 3. Drainage with trapping. (a) The graph  $G^+=(V^+,E^+)$  from Fig. 1(a). The numbers indicate the  $p_d^x(\cdot)$  values. (b) The numbers indicate the  $\omega_d^l$  values of the edges. (c) MWST of  $G^+$  with respect to  $\omega_d^l(\cdot)$  (escape tree). (d) Critical escape pressures. The vertices with trapped wetting phase are emphasized. These are the vertices at which the critical escape pressure is lower than the  $p_d^x$  value.

respect to  $\omega_d$  [for an example see Figs. 1(b) and 1(c)]. Hence, the value  $p_d^x(v)$  can be determined by simply going from  $u_N$  to v along the unique path and updating the maximum of  $\omega_d$  encountered so far. Note that this gives us the  $p_d^x(v)$  values of all vertices on the unique path. More generally, any (recursive) traversal of the MWST of  $G^+$  with respect to  $\omega_d$  that starts at  $u_N$  allows us to determine the  $p_d^x(v)$  values of all vertices in  $V \setminus V_N$ . Since in such a traversal each vertex of  $G^+$  is visited exactly once, the computational complexity for determining the  $p_d^x(v)$  values of all vertices in  $V \setminus V_N$  is O(n), where n is the number of vertices in  $G^+$ .

## V. SIMULATION OF DRAINAGE WITH TRAPPING

To simplify our description, we call a vertex  $v \in V$  dry (wet), if the pore body represented by v is filled with non-wetting (wetting) phase. We first focus on a single wet vertex

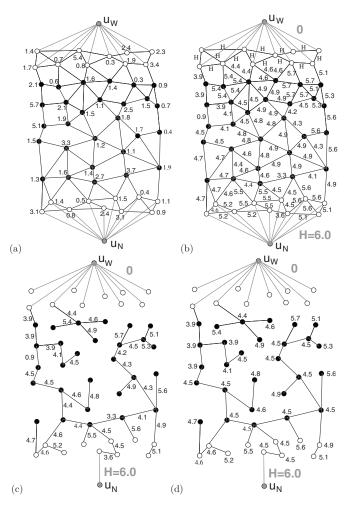


FIG. 4. Imbibition without trapping. (a) The graph  $G^+$  =  $(V^+, E^+)$  from Fig. 1(a). The numbers indicate  $p_i(\cdot)$  values of the vertices. (b) The weights  $\omega_i(\cdot)$  when H=6.0. (c) MWST of  $G^+$  with respect to  $\omega_i(\cdot)$ . (d) The  $H-p_i^x(\cdot)$  values of all  $v \in V \setminus V_W$ . The value  $p_i^x(v)$  indicates the external CP at which the pore body represented by v is actually imbibed.

v at the interface between the two fluid phases at some time during drainage. Then, v gets dry, if and only if (1)  $p_d(v) \le p^x$ , where  $p^x$  is the external CP, and (2) there exists a path from v to the wetting phase reservoir along which wetting phase can escape, i.e., all vertices along the path are wet.

If applied iteratively while the external CP is rising, the above criterion for a vertex getting dry amounts to a simulation of drainage with trapping of the wetting phase. The following definition of  $\omega_d^t(\cdot)$  ensures that the MWST of  $G^+$  with respect to  $\omega_d^t(\cdot)$  (see Fig. 3) captures the escape of the wetting phase:

$$\omega_d^t(e) := \begin{cases} H - p_d^x(v) & \text{if } e = \{u_W, v\}, \\ H - \min\{p_d^x(u), p_d^x(v)\} & \text{if } e = \{u, v\} \\ & \text{with } u, v \in V \setminus V_N, \\ H & \text{otherwise.} \end{cases}$$

(9)

Again, H is a number higher than all  $p_d$  values. To substantiate the definition of  $\omega_d^t(\cdot)$  we will first make sure that, if some  $v \in V \setminus V_N$  gets dry at all, it gets dry at the external CP  $p_d^x(v)$  defined in the last section. Indeed, as will be shown in the remainder of this paragraph, trapped wetting phase blobs do not cut crucial connections of nonwetting phase between v and the nonwetting phase reservoir. Until the first blob  $b_1$ of wetting phase is trapped, drainage proceeds exactly as described before in Sec. IV. When  $b_1$  is cut off, the  $p_d^x$  values of all vertices in  $b_1$  are higher than the  $p_d^x$  values of all vertices around  $b_1$ . Here, the vertices around  $b_1$  are the ones not in  $b_1$  but adjacent to a vertex in  $b_1$ . As the external CP continues to increase, and as long as  $b_1$  remains the only trapped blob, a vertex  $w_1$  not in  $b_1$  still gets dry at  $p_d^x(w_1)$ . Otherwise, the unique path  $\Pi$  from  $u_N$  to  $w_1$  on the MWST of  $G^+$  with respect to  $\omega_d$  would go through  $b_1$ . This is impossible, however, since the  $p_d^x$  values increase monotonically, as one walks from  $u_N$  to  $w_1$  along  $\Pi$ ; a contradiction to the  $p_d^x$  values in  $b_1$  being higher than those around  $b_1$ . Along the same lines one can show that, when a second blob  $b_2$  is formed, a vertex  $w_2$  neither in  $b_1$  nor in  $b_2$  still gets dry at  $p_d^x(w_2)$ , and so on.

From the description of drainage at the beginning of this section, the fact that the external CP is monotonically increasing during drainage, and the note above, it follows that a vertex  $v \in V \setminus V_N$  gets dry if and only if at the external CP  $p_d^x(v)$  there exists a path from v to the wetting phase reservoir such that all vertices along the path are wet, i.e., have a  $p_d^x$  value  $\geq p_d^x(v)$ . In other words, v gets dry if and only if  $H - \operatorname{MinMax}_{\omega_d^t}(v_W, v) \ge p_d^x(v)$ . The value H $-\operatorname{MinMax}_{\omega_d^t}(v_W,v)$  thus is the critical external CP for the wetting phase to escape from the pore body  $b_v$  represented by v. Nonwetting phase is trapped in  $b_v$ , if and only if H  $-\operatorname{MinMax}_{\omega_d^t}(v_W, v) < p_d^x(v)$  [see Fig. 3(d)]. As in the previous section, we can determine all wetting phase blobs by computing the H-MinMax $_{\omega_{J}^{t}}(v_{W},v)$  values for all  $v \in V \setminus V_{N}$ in a single recursive traversal of the MWST of  $G^+$  with respect to  $\omega_d^t$  starting at  $u_W$ .

# VI. SIMULATION OF IMBIBITION WITH NEITHER TRAPPING NOR SNAP-OFF

For the time being we take neither trapping nor snap-off into account. In a real experiment on quasistatic primary imbibition one starts with a nonwetting phase saturated porous medium at a high external CP and then gradually and slowly decreases the external CP. Simulating quasistatic primary imbibition through ISP amounts to assuming that, if the external CP has decreased to an intermediate value  $p^x$ , a pore body  $b_v$  represented by a vertex  $v \in V \setminus V_W$  has been imbibed at some point during the pressure drop to  $p^x$ , if and only if there exists a path between a vertex in  $V_W$  and v such that the minimal  $p_i$  value of the vertices along the path and not in  $V_W$  is  $\geq p^x$ . Note that the  $p_i$  values are assumed at the *vertices* of  $G^+$ . By extending the function  $p_i(\cdot)$  to edges via

$$p_{i}(e) := \begin{cases} \min\{p_{i}(u), p_{i}(v)\} & \text{for all } e = \{u, v\} \\ \text{with } u, v \in V \setminus V_{W}, \\ p_{i}(v) & \text{for all } e = \{u, v\} \\ \text{with } u \in V_{W}, v \in V \setminus V_{W}, \end{cases}$$

$$(10)$$

we get that  $b_v$  has been imbibed, if and only if there exists a path between a vertex in  $V_W$  and v such that the minimal  $p_i$  value of the edges along the path is  $\geq p^x$ . In other words,  $b_v$  has been imbibed if and only if there exists a path between a vertex in  $V_W$  and v such that the  $maximal\ H-p_i$  value of the edges along the path is  $\leq H-p^x$ . This, in turn, is equivalent to saying that the external CP at which  $b_v$  is actually imbibed—we denote it by  $p_i^x(v)$ —is given by  $H-p_i^x(v)=MinMax_{\omega_i}(u_W,v)$ , where

$$\omega_{i}(e) := \begin{cases} 0 & \text{if } e \in E_{W}, \\ H & \text{if } e \in E_{N} \text{ or } e = \{u, v\} \\ & \text{with } u, v \in V_{W}, \\ H - p_{i}(e) & \text{for all other edges } e \end{cases}$$
(11)

(for an example see Fig. 4). As for  $p_d^x$  in Sec. IV, all  $H-p_i^x$  values, and thus all  $p_i^x$  values [see Fig. 5(a)], can be obtained through a recursive traversal of the MWST of  $G^+$  with respect to  $\omega_i$ , this time starting at  $u_W$ .

## VII. SIMULATION OF IMBIBITION WITH TRAPPING AND SNAP-OFF

As in Sec. V, we call a vertex  $v \in V$  dry (wet), if the pore body represented by v is filled with nonwetting (wetting) phase. We first focus on a single edge e at the interface of the two fluid phases at some time during imbibition. Let e  $=\{u,v\}\in E$ , let u(v) be wet (dry), and let  $p^x$  be the external CP. Then, v gets wet if and only if (1)  $p_i(v) \ge p^x$ , and (2) there exists a path from v to the nonwetting phase reservoir along which nonwetting phase can escape, i.e., all vertices along the path are dry, and none of the pore throats represented by an edge on the path has been closed due to snapoff. Here, we assume that snap-off in the pore throat represented by the edge  $e = \{u, v\} \in E$ , with u, v both being dry, occurs if  $p_d(e)/2 > p^x$  [5,20]—a simpler approach than, for example, the one in [8]. We will take into account that snapoff contributes to the trapping of nonwetting phase blobs, but we require that imbibing wetting phase needs to be connected to the wetting phase reservoir (no imbibition originating from wetting phase blobs occupying single pore throats due to snap-off).

If applied iteratively while the external CP is decreasing, the above criterion for a vertex getting wet amounts to a simulation of imbibition that includes trapping and snap-off. The following definition of the weight function  $\omega_i^t(\cdot)$  ensures that the MWST of  $G^+$  with respect to  $\omega_i^t(\cdot)$  (see Fig. 5) captures the escape of the nonwetting phase:

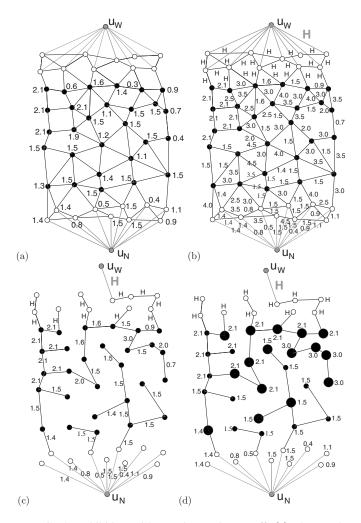


FIG. 5. Imbibition with trapping and snap-off. (a) The graph  $G^+ = (V^+, E^+)$  from Fig. 1(a). The numbers indicate the  $p_i^x(\cdot)$  values. (b) The numbers indicate the  $\omega_i^t$  values of the edges. (c) MWST of  $G^+$  with respect to  $\omega_i^t(\cdot)$  (escape tree). (d) Critical escape pressures. The vertices with trapped nonwetting phase are emphasized. These are the vertices at which the critical escape pressure is higher than the  $p_i^x$  value.

$$\omega_{i}^{t}(e) := \begin{cases} p_{i}^{x}(v) & \text{if } e = \{u_{N}, v\}, \\ \max\{p_{i}^{x}(u), p_{i}^{x}(v), p_{d}(e)/2\} & \text{if } e = \{u, v\} \\ & \text{with } u, v \in V \setminus V_{W}, \\ H & \text{otherwise.} \end{cases}$$

$$(12)$$

To see how the MWST of  $G^+$  with respect to  $\omega_i^t(\cdot)$  captures the escape of the nonwetting phase, note that, if some  $v \in V \setminus V_W$  gets wet at all (i.e., no nonwetting phase is trapped in the pore body represented by v), it gets wet at the external CP  $p_i^x(v)$  defined in the last section. This follows as in Sec. V.

From the description of imbibition at the beginning of this section, the fact that the external CP is monotonically decreasing during imbibition, and the note above, it follows

that a vertex  $v \in V \setminus V_W$  gets wet if and only if at the external CP  $p_i^x(v)$  there exists a path from v to the nonwetting phase reservoir such that (1) all vertices along the path are dry, i.e., have a  $p_i^x$  value  $\leq p_i^x(v)$  and (2) none of the edges along the path have been closed due to snap-off, i.e., all edges along the path have a  $p_d(e)/2$  value  $\leq p_i^x(v)$ . In other words, v gets wet if and only if  $\min \max_{\omega_i^t}(v_N,v) \leq p_i^x(v)$ . The value  $\min \max_{\omega_i^t}(v_N,v)$  thus is the critical external CP for the nonwetting phase to escape from the pore body  $b_v$  represented by v. Nonwetting phase is trapped in  $b_v$ , if and only if  $\min \max_{\omega_i^t}(v_N,v) > p_i^x(v)$  [see Fig. 5(d)]. As in the previous sections, we can compute the  $\min \max_{\omega_i^t}(v_N,v)$  values for all  $v \in V \setminus V_W$  in a single recursive traversal of the MWST of  $G^+$  with respect to  $\omega_i^t$  starting at  $u_N$ .

## VIII. SUMMARY AND CONCLUSIONS

In this paper, we have shown that not only IBP, but also ISP, can be done through constructing MWSTs of the pore network and traversing them. When simulating drainage through IBP we took trapping into account, and when simulating imbibition through ISP we took trapping and snap-off into account.

This was possible through (1) mapping ISP onto IBP using Eq. (10) and (2) calculating two MWSTs for drainage and two MWSTs for imbibition. In both cases, the second MWST was one with respect to new weights derived from the weights computed during a traversal of the first MWST, which does not account for trapping and snap-off.

Our method for modeling IBP and ISP (with and without trapping and snap-off) can be applied to any kind of pore network in any spatial dimension. Simulations can be performed in lattice networks, with randomly assigned resistance values for the bonds and sites, as in the seminal papers by Chandler *et al.* [21] and Wilkinson and Willemsen [3]. Simulations on network lattices are, for example, important for studying universality principles [22,23,4,16] in the general percolation-theoretical sense [24,25]. Our method, however, also works for irregular pore networks that represent real porous media [26–32].

Our method also implies that the time complexity of IBP and ISP, even when trapping and snap-off are included, is  $O(m\alpha(m,n))$ , where m is the number of network edges, n is the number of network vertices, and  $\alpha(\cdot,\cdot)$  denotes the inverse Ackermann function [33]—a bound considerably lower than  $O(m \log m)$  reported in [4,32]. Indeed, according to [34],  $O(m\alpha(m,n))$  is the time complexity to compute a MWST, and a traversal of a MWST takes only O(n). Since  $\alpha(\cdot,\cdot)$  is practically constant, one may say that IBP and ISP, even when trapping and snap-off are included, can now be done in linear time with respect to the number of network edges. This is optimal since, in any case, one needs to go through all edges.

Due to the improved computational complexity,  $O(m\alpha(m,n))$  instead of  $O(m \log m)$  [16], one can now run IP on larger networks than before. This ability could lead to improved estimates of the fractal dimensions of sample spanning clusters, backbones, and minimal paths [4,16,17]. Fi-

nally, the reduction of IP to MWST might provide new insights into the universality classes of IP along the lines of Dobrin and Duxbury [35].

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