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Connectivity metrics based on the path of smallest resistance

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ABSTRACT

Connectivity is an intrinsic feature of heterogeneous hydraulic conductivity fields which governs the paths of smallest resistance, along which water and solute fluxes concentrate. It is often organized as a network of channels which shows the fastest Darcy velocities and provides pathways for particles contributing to early time solute breakthrough. In subsurface hydrology the topological or static connectivity metrics are poorly defined, thus connectivity is usually characterized by dynamic connectivity indicators, derived from effective flow and transport behavior. We obtain a connected channel network using information about hydraulic conductivity only and define static connectivity metrics based on resistance of the individual channels as well as the channel width. Then we compare the static connectivity metrics with connectivity indicators derived from flow and transport simulations to check whether these connectivity metrics are able to predict effective flow and transport. We find a good agreement for flow and an acceptable one for transport for a large range of 2-D hydraulic conductivity fields with different connectivity structures. We conclude that our method provides a good estimate of effective hydraulic conductivity and early time solute breakthrough using our connectivity metrics based on information of the resistance and geometry of the connected channel network.

1. Introduction

Small scale heterogeneity cannot be resolved in most applications and has to be upscaled by using effective properties describing flow and transport. In weakly and intermediately heterogeneous hydraulic conductivity fields flow is upscaled by introducing an effective hydraulic conductivity which can be derived using two-point statistics [2–4,24,27]. In highly heterogeneous fields the flow structure is more complex and causes channeling [8,16]. Effective flow cannot be predicted from an ensemble alone [29]. Early solute arrival time is advanced, while late-time behavior shows delays which leads to tailing of solute breakthrough curves [20,28,29]. The reason of this complex behavior is topological connectivity: the position of more conductive areas relative to each other and in relation to low conductivity barriers.

In subsurface hydrology connectivity is not clearly defined [22]. Precise definition of topological connectivity exists in graph theory [5] and in percolation theory [11], in both cases it implies the existence of a connected cluster between opposite boundaries. Subsurface hydrology deals with continuous porous media and the above definitions are not easily applicable. Nevertheless the topological structure of the hydraulic conductivity field affects dynamic processes and its effect can be quantified in terms of flow and transport (extremely high or low values of effective flux, channeling, or early arrival of solutes) [1,7,13,14,22]. As they are not direct measures for connectivity but reflect a response due to connectivity on a hydrodynamic process like flow or transport they are named dynamic connectivity indicators. An example of a dynamic connectivity indicator is the effective flux through a domain divided by the flux through a homogeneous domain with hydraulic conductivity equal to the geometric mean [14].

A direct definition of connectivity in terms of the hydraulic conductivity field is called a topological or static connectivity metric [22]. Over the last years some attempts have been made to develop such static connectivity metrics and to relate them to effective flow and transport behavior. Knudby and Carrera [14] related two-point statistics (correlation length) to flow and transport connectivity indicators. Knudby et al. [15] studied a low conductive matrix with highly conductive regularly shaped inclusions. They found that effective hydraulic conductivity can be predicted by the size of inclusions and the low conductivity gaps between them. Ronayne and Gorelick [23] provided a flow upscaling law for binary media based on percolation theory. Oriani and Renard [19] studied the fields with complex topology and derived an upscaling rule for flow in binary fields using the solidity number. Most of these studies were conducted in 2-D but also the difference to 3-D was investigated [8,12].

Until now no static connectivity metric exists which is applicable to arbitrarily heterogeneous hydraulic conductivity fields. To obtain

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such metrics the connected channel network has to be obtained for a given hydraulic conductivity field. There are different methods to define connected channels: percolation theory is a powerful framework, but it requires an a-priori knowledge of the critical value [11,25]. Another way to describe such a structure would be a simple cut-off of hydraulic conductivity; but Edery et al. [6] showed that low conductive zones might provide large fluxes while the cut-off methodology recognizes them as not connected. Tyukhova et al. [26] presented a simple numerical method to delineate a connected network by finding iteratively the path of smallest resistance. The resulting connected channels represent a series connection of segments with different resistivities, thus, the overall resistance depends on the entire path. Depending on the type of connectedness the connected channels may contain sections of high resistance – bottle-necks – that plug channels and dramatically affect the dynamic processes. While it was shown that such connected networks are strongly linked to connectivity, no specific connectivity metrics based on them have yet been developed.

Our objective is to derive topological or static connectivity metrics from the network of connected channels. We then compare them with dynamic connectivity indicators derived from numerical simulations to test their capability to predict effective flow and early-time transport in a given aquifer.

2. Delineation of the connected channel network

To obtain the connected channels we use the method by Tyukhova et al. [26], which we briefly summarize here. The method is based on mathematical morphology corrected for continuity of hydraulic conductivity. The process is iterative and starts with a straight line at the inlet boundary. The line iteratively moves to the opposite boundary.

The points $\vec{x_j}$ of polygon i move normal to the line and the individual space steps are proportional to the hydraulic conductivity of the accommodating cell: $|\Delta\vec{x_j}| = \epsilon \frac{K(\vec{x_j})}{K_{max,i}}$, where ϵ is a fixed distance bounding the space step inside the most conductive cell (which should be less than the cell size to avoid crossing the entire cell), $K_{max,\,i}$ is the maximum value of hydraulic conductivity along the polygon-line, $K(\vec{x_j})$ is the hydraulic conductivity value at point $\vec{x_j}$. The points of two consequent polygons i and $i+1$ are separated by the resistance (Fig. 1a):

$$r_i = \frac{\epsilon}{K_{max,i}} \tag{1}$$

Due to the variability of hydraulic conductivity the line becomes irregular. We call this iterative line progression *"front movement"*. The front develops into the connectivity structure of the field. Reaching the opposite boundary at iteration n indicates the preferential path with cumulative resistance (Fig. 1):

$$R_{field} = \sum_{k=1}^{n} r_k \tag{2}$$

The field may contain several flow channels with various resistances, organized as a network. If the polygon front reaches the right boundary at another point we assume that the next channel has broked through and calculate its resistance R_i. The maximum number of iterations is not strictly defined and depends on the structure of the polygon. The number of channels also influences flow and transport. To quantify its influence we introduce the channel density Θ as the number of channels of comparable resistance per unit width of the field, L_y, summarizing all discernible channels [9]:

$$\Theta = \frac{R_1}{L_y}\left(\frac{1}{R_1} + \sum_{i=2}\frac{1}{R_i}\right) \tag{3}$$

3. Static connectivity metrics and dynamic indicators

Each individual channel is characterized by its resistance. It can be defined as a property of a the 1-D trajectory along the center line of the channel γ:

$$R(\gamma) = \int_{\gamma} \frac{1}{K(x,y)} ds \tag{4}$$

where $K(x, y)$ — is the point value of the hydraulic conductivity and s is the coordinate along γ. We are interested in paths γ that connect the opposite boundaries of the domain and have minimum values of resistance $R(\gamma)$. This concept is very close to the concept of the shortest path in Graph theory [10]. the path of the smallest hydraulic resistance is a center line of preferential flow channel.

The overall resistance is mainly controlled by low conductive bottle-necks along this path. A "bottle-neck" of thickness 10 and hydraulic conductivity of 0.1 has the same influence as one with a thickness of 1 and a hydraulic conductivity of 0.01.

To demonstrate how that our new connectivity metrics work, we define them in terms of measurable quantities: the effective flux and the first solute arrival. To quantify the amount of water passing through a channel, not only in the 1D-resistance, but also the thickness of the channel d and the channel density Θ have to be taken into account. The thickness may vary along the path. At bottle-necks the shape of the channel becomes wider than along relatively conductive parts [14,16]. As a width estimator we use the correlation length of the hydraulic conductivity field in the direction normal to the main flow, because it reflects the geometrical sizes of the more conductive parts.

A common dynamic connectivity indicator for flow is comparing the real flow through the heterogeneous domain with flow through a homogeneous domain with the geometric mean hydraulic conductivity, K_G [14]:

$$DCI_f = \frac{K_{eff}}{K_G} \tag{5}$$

where K_{eff} is effective hydraulic conductivity derived from true flux through the heterogeneous field $K_{eff} = \frac{QL_x}{L_y \Delta H}$, Q is the measured flux per unit depth, L_X and L_Y are domain sizes and ΔH is the hydraulic head difference.

We estimate a new effective hydraulic conductivity K_R based on resistance per length L_X, channel density, and thickness:

$$K_R = \frac{\Theta d L_x}{R} \tag{6}$$

and obtain a static connectivity metric describing flow:

$$SCM_f = \frac{\Theta d L_x}{R K_G} \tag{7}$$

To quantify early solute arrival we use a dynamic connectivity indicator relating the arrival time of particles driven by advection within an effective homogenized domain with observed arrival times of the first 5% of particles $t_{5\%}$ [14]:

$$DCI_t = \frac{t_{adv}}{t_{5\%}} \tag{8}$$

where

$$t_{adv} = \frac{L_x^2 n}{K_{eff}\Delta H} \tag{9}$$

Estimating $t_{5\%}$ by the smallest resistance:

$$t_{5\%R} = \frac{R}{\Delta H} \tag{10}$$

and including (6) into (9) instead of K_{eff} to estimate t_{adv}:

$$t_{adv\,R} = \frac{L_x^2 n}{K_R \Delta H} \tag{11}$$