A Complex Systems Approach to Describing Flow and Transport in Fractured-Porous Media

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1.1. INTRODUCTION

The study of complex systems has become recognized in recent years as a new scientific discipline. The primary goal of this chapter is to introduce an approach for the study of flow and transport in fractured-porous media through the use of complex systems theory. This approach will be based on (1) a review of complex systems theory, and (2) an analysis of the papers presented in this monograph, along with presentations given at the Fall 2012 AGU meeting session "Dynamics of Fluids and Transport in Fractured-porous Media," as well as other publications. Specifically, we would like to show that a fractured rock system may exhibit an emerging behavior resulting from interactions of its components.

The structure of the chapter is as follows: We will begin with the description of the general idea of the field of complex systems (including terminology), the general approach to the study of complex systems, central properties of complex systems, and the idea of emergence. Then, we will present the concept of a fractured-porous medium as a complex system, using a review of chapters included in this book, as well as abstracts of the presentations given at Session H071, "Dynamics of Fluids and Transport in Fractured-porous Media," of the Fall 2012 AGU Meeting held in San Francisco in December 2012. Our conclusion to the chapter will summarize the concept of a complex fractured rock system as one of the emerging trends in the field of hydrological science and technology, and answer the question whether the complexity sciences approach can benefit the field of flow and transport in fractured-porous media.

1.2. THE FIELD OF COMPLEX SYSTEMS

Adjectives such as *complicated*, *intricate*, *interconnected*, interwoven, self-organizing, and others are often used to describe complex systems, frequently in a qualitative sense. Despite much research on complex systems within different scientific fields, many such systems are not fully understood; there is no concise definition of a complex system [Ladyman et al., 2013]. In a general sense, a complex system may be defined as a system consisting of a large number of interacting components, which are described by a set of dependent variables and parameters requiring measurement, whose total behavior in space and time is nonlinear and cannot be derived from the summation (i.e., linear superposition) of individual component activities. This definition applies to complex systems from a wide array of scientific disciplines, and interdisciplinary research is often necessary for the study of complex systems. Whitesides and Ismagilov [1999] defined a complex system as"one whose evolution is very sensitive to initial conditions or to small perturbations, one in which the number of independent interacting components is large (three or more), or one in which there are multiple pathways by which the system can evolve. Analytical descriptions of such systems typically require nonlinear differential equations. A second characterization is more informal; that is, the system is 'complicated' by some subjective judgment and is not amenable to exact description, analytical or otherwise."

Werner [1999] explained that the complexity in natural landform patterns is "a manifestation of two key characteristics. Natural patterns form from processes that are nonlinear, those that modify the properties of the

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environment in which they operate or that are strongly coupled; and natural patterns form in systems that are open, driven from equilibrium by the exchange of energy, momentum, material, or information across their boundaries."

Complexity theory is generally used to characterize systems with many parts (variables) that interact with each other in multiple and complex ways. When such interactions are understood thoroughly, then the overall system may be represented by coupled sets of nonlinear ordinary or partial differential equations. Because complete understanding of these complex linkages is often lacking, experimental and theoretical studies with complex systems theory in mind are often the main goal of research in different fundamental and applied scientific fields, such as computer science, mathematics, sociology, physics, philosophy, chemistry, psychology, economics, and biology. However, despite great interest in studies of complex systems, universal laws governing all such systems have not been developed.

The main characteristics and common principles of complex systems are illustrated in Figure 1.1 (developed at

the New England Complex Systems Institute, http://www. necsi.edu/about/). Figure 1.1 illustrates that a complex system is composed of many parts that interconnect in complicated ways, and that the complexity of the system is related to the number and nature of the interconnections. In this chapter, we will show how these concepts can be linked to real examples of flow and transport in fracturedporous media.

1.2.1. General Approach to the Study of Complex Systems

Complex systems can be studied using a unified framework of theories and methods from all scientific and engineering disciplines. Complex system studies, in the first place, include research on how parts of a system give rise to the collective behavior of the system and how the system interacts with its environment, with the focus on both direct and indirect relationships between parts and the whole system. In 1948, Warren Weaver suggested two forms of complexity: disorganized complexity and organized complexity [*Weaver*, 1948]. In Weaver's view,



Figure 1.1 Main characteristics of a complex system. (Source: The New England Complex Systems Institute (NECSI), http://www.necsi.edu/projects/mclemens/sysrep.gif)

phenomena of disorganized complexity are treated using probability theory and statistical mechanics, whereas organized complexity deals with phenomena that escape such approaches and confront "dealing simultaneously with a sizable number of factors which are interrelated into an organic whole." Weaver's paper has influenced subsequent thinking about complexity.

As with simple systems, the nature of a complex system is intrinsically related to the behavior of its parts [*Bar-Yam*, 1997], but the emergent behavior of the complex system cannot be inferred directly from the behavior of individual components alone (http://www.necsi.edu/visual/systems.html).

To understand the behavior of a complex system, we must understand the concept of *dynamic interaction*. In other words, we must recognize the dynamic behavior of not only the system's parts but also how they act together to form the collective behavior of the whole system. The collective behavior of complex systems depends on many dependent and independent types of information and processes. It is also apparent that we cannot describe the whole system without describing its parts, and each part must be described in relation to other parts, which is the reason why complex systems are coupled and difficult to understand.

Describing the relationships among complex system parts is difficult, because the relationships are typically nonlinear. Moreover, a complex system is composed of groups of parts whose relationships (their nature, their degree) are more often than not poorly known or understood. Therefore, the emergent behavior of the system is difficult, if not at all possible, to predict, even though the behavior of individual components may be known, readily predictable, and observable.

Based on the theory of systems analysis, the behavior of an entire complex system cannot be understood by close study of its individual parts by themselves. Thus, experiments that isolate one part of a system while holding the other parts constant [*Smolin*, 2014] do not produce any real knowledge. It is necessary to look at parts in the context of the whole system, including the interaction with their surrounding environment, and account for these patterns in predictions using mathematical models. The notion of dynamic complexity can be applied to studies of different categories of complex systems, such as hydrodynamics (fluid flow, weather), climate, soil, composite materials, and earthquakes.

1.2.1.1. Emergent complexity and emergent simplicity of complex systems

Another property of complex systems is the phenomenon of emergence. This refers to a unique property that "emerges" (or appears) when the system components interact to develop a higher-level aggregate object, with a novel (often useful in a practical sense) property. A simple and well-understood example would be the development of a hive from the interaction of many individual bees. Presumably, no particular insect has the complete hive architecture in mind, but somehow it emerges from their many interactions (see http://dictionary.reference.com/ browse/emergent+property).

In studies of complex systems, it is important to determine how the complexity of the entire system is related to the complexity of its parts, and vice versa. However, collective behavior of a complex system is not readily understood from the behavior of the parts. Individual components of a complex system are often complex systems themselves, so it seems reasonable to assume that a collective behavior of the complex parts would also be complex. Still, even if a system were composed of simple parts, the collective behavior of these simple parts may become complex, which is called *emergent complexity*.

Another type of emergent behavior is *emergent simplicity*. A system composed of complex parts may exhibit a simple collective behavior, which is called *emergent simplicity*. A simple example is a planet, such as Earth, orbiting around a star, while the Earth itself is a complex system. This example illustrates that the collective system and its parts may behave *differently* at different scales. In other words, the system (and the system's components) may behave in a complex way on a smaller scale, but on a larger scale multiple complex details may not be relevant.

The following hydrogeological examples may be used to illustrate the concept of emergent simplicity and the difference between local emergence (when collective behavior appears within a small part of the system) and global (i.e., systems) emergence (when collective behavior relates to the whole system). For example, in the study of gas transport in fractured-porous subsurface media, two emergent properties of a gas are its pressure and temperature. These properties are emergent because they do not naturally arise out of the description of individual particles. Pressure and temperature become relevant to thermodynamic studies only when many particles are combined together, so that pressure and temperature can become local emergent properties of media. The pressure and temperature are local properties of the gas phase in the subsurface, and hydraulic pressure is a local property of the water in the subsurface. In physics, these local emergent properties are called intensive.

Phase transitions (e.g., solid to liquid and liquid to vapor) represent collective dynamics that are visible on a macroscopic scale but that can be seen in a microscopic sample as well, using modern detection methods (such as advanced spectroscopic, microscopic, and tomographic characterization techniques) to study biogeochemical interfaces in porous media (e.g., *Rennert et al.*, 2012).

Another example of a local emergent property is the formation of water from atoms of hydrogen and oxygen.

The properties of water are not apparent in the properties of oxygen or hydrogen gases, nor does an isolated water molecule reveal most properties of water. However, a microscopic amount of water is sufficient. In the study of complex systems (such as fractured rock), we are mainly interested in global emergent properties, which also depend on the surrounding environment.

1.2.1.2. Self-organization and feedback loops

Self-organized criticality, the spontaneous development of systems to a critical state, is the first general theory of complex systems with a firm mathematical basis. This theory describes how many of the seemingly disparate events of the world, from stock market crashes to mass extinctions, avalanches to solar flares, all share a set of simple, easily described properties.

The collective behavior and the emergence of a real complex system can spontaneously lead to the system's *self-organization* [*Peak and Frame*, 1994] and self-organized criticality, a feature of a complex system, related to an emergency [*Bak et al.*, 1987]. Self-organization is a process in which some form of global order or coordination arises out of the local interactions between the components of an initially disordered system. This process is spontaneous: it is not directed or controlled by any agent or subsystem inside or outside of the system; however, the laws followed by the process and its initial conditions may have been chosen or caused by an agent. It is often triggered by random fluctuations that are amplified by positive feedback. The resulting organization is wholly decentralized or distributed over all the components of the system.

The original "principle of the self-organizing dynamic system" [*Ashby*, 1947] states that any deterministic dynamic system would evolve toward a state of dynamic equilibrium (or in the terms of nonlinear dynamics and chaos, an attractor), so that the further evolution of the system is constrained to remain within the attractor. The presence of the attractor implies a mutual dependency or coordination between system components, with each component adapting to a state affected (to different degrees) by all other components.

The component adaptation is developed through a process that occurs in a feedback loop, including both positive feedback and negative feedback. *Positive feedback* is an influence on the process that enhances or amplifies the response of the system, when a small disturbance on a system increases in magnitude. Positive feedback loops normally do not cause endlessly increasing growth but rather have limited effects over time and space, resulting, for example, in the system's explosion, erosion, or collapse.

The positive feedback loops are often followed by a negative loop [*Meadows*, 1999]. *Negative feedback* occurs when the output of a system, process, or mechanism is fed back as a system (or one of its components) input to

reduce the system's output growth or fluctuations, which may lead to instability. Negative feedback generally reduces the effects of perturbations, promotes system's stability, and stimulates a state of equilibrium and stability.

Feedback loops in the emergent system result in coevolution, which in turn lead to further iterations of the system [*Main et al.*, 1994].

The complexity of a system must be a decreasing function of scale, because the information needed to describe a system on a larger scale must be a subset of the information needed to describe the system on a smaller scale: any finerscale description contains the coarser-scale description. (The Earth orbiting the sun is a relatively simple example.) In general, the complexity of system parts is described by the complexity of the system evaluated on the scale of the parts. When the behavior of the system depends on the behavior of its parts, the complexity of the whole must involve a description of the parts, thus it is large. The complexity of the entire system increases when the complexity of the smaller parts of the system is included.

1.2.1.3. Mathematical models: General approach

In classical mathematical theory, a model of any system is formed from simple elements whose states are correlated to a certain degree. Without correlations, emergent behavior is impossible. A model must be sufficiently rich in order to capture the phenomenon of global emergent behavior. The quantitative study of both simple and complex systems is based on the use of modeling using differential equations. Differential equations, like the equations that describe the relation between pressure and water flow, assume that a system is essentially uniform. The equations include effective parameters because the local-scale details are not important for the behavior of the system at larger scales.

However, such assumptions may not be generally valid for complex systems and may lead to significant uncertainties or errors in predictions. Alternative models such as fractals, percolation models, and nonlinear dynamical models may reduce such predictive uncertainty or error.

1.3. FRACTURED ROCK AS A COMPLEX SYSTEM

The goal of this section is to present the principal properties and characteristics of complex systems, described in the preceding section of this chapter, as they are related to fractured rock.

1.3.1. Methods of Field Measurements and Experiments

A fractured rock system is a complex system containing many interdependent parts. These parts need to be studied using different types of field and laboratory tests and experiments, using various monitoring techniques. Over the past 20–30 years, multiple surface and subsurface geophysical methods have been developed to characterize fractured rock and sediments. The most commonly employed methods include the heat pulse flow meter, the electromagnetic flow meter, and hydrophysical (or FEC) logging [*Pedler*, 2012]. These methods have been successfully applied in all types of hydrogeologic systems, including fractured bedrock, fractured sandstones, alluvium, massive and fractured clays, karst, and volcanic, for various practical applications, including remediation, geotechnical, mining, and water supply.

Karasaki et al. [2015, this volume] report on conducting a series of pump tests in isolated sections of two inclined ~200 m long boreholes, which were separated by a distance of ~130 m from each other. The boreholes penetrated the Wildcat Fault, a semivertical strike slip fault and a member of the Hayward Fault System, situated in the Berkeley Hills. The geology encountered in the boreholes was predominantly that of the Claremont formation, with extensively fractured and alternating sequences of chert, shale, and sandstone. The authors analyzed the drawdowns in four isolated sections within a vertical borehole (WF-1) and drilled adjacent to the fault at distances of ~45 m and ~95 m from each of the inclined boreholes. The permeability of the fault plane was found to be two orders of magnitude higher than that of the protolith, and anisotropic, with a ~10-fold higher permeability in the near-horizontal direction, which is somewhat expected for a strike slip fault. Buildup analysis suggests that the fault is asymmetric with higher permeability along the east side of the fault plane and lower along the west side. The results of this paper indicate that the field pumping tests provide an evaluation of the effective hydrogeological parameters on the scale of tens of meters, which relates to the idea of an emergent simplicity on a larger scale.

Wang and Hudson [2015, this volume] raise the question of how to determine the geometrical and hydrogeological properties of fractures in a specific rock mass, how to establish the link between hydrogeological fracture properties and other variables (such as the *in situ* stress state), and how to validate the results of experimental investigations at the full scale. The authors describe their progress in developing underground research laboratories (URLs) in both hard and soft rock, in housing large halls for particle detections at great depths, and in testing the energy and resource recovery capacities and waste disposal potential through borehole complexes.

Hawkins et al. [2012] present the results of an experiment in which the effect of channelized flow on fluid/rock heat transfer is measured using fiber optic distributed temperature sensing (DTS) and ground-penetrating radar. They showed that between wells with good hydraulic connection, heat transfer followed a classic dipole sweep pattern. However, between wells with poor hydraulic connection, heat transfer was skewed toward apparent regions of higher transmissivity (or larger aperture). The saline tracer test between the same wells confirmed that flow channeling significantly impacts heat transfer efficiency, even in single bedding plane fractures. The flowchanneling concept is similar to the idea of preferential flow in fractured rock.

In their studies of preferential flow paths in waste rock piles, *Broda et al.* [2012] demonstrate the importance of studies of various forms of unsaturated localized preferential flow processes, such as flow in macropores and fractures, and flow at heterogeneity-driven and gravity-driven unstable high velocity (with local hydraulic conductivity of several dozen meters per day).

Chan et al. [2012] demonstrate the need to use a variety of field tests, including saltwater tracer tests, hydraulic tests, and heat-pulse flowmeter tests, to locate the permeable fractures and detect the hydraulic connections between boreholes. Tracer cross-borehole tests included injection of zero-valent iron tracer with a magnet array specifically to locate permeable fractures and determine connectivity. Howar and Wohnlich [2012] use a series of push-pull tests, also known as single-well injection-withdrawal (SWIW) tests, with an application of tracer-cocktails consisting of fluorescent tracers (Uranine, Amidorhodamine G and Tinopal CBS-X) with different diffusion and sorption properties to characterize the fractured-porous media. Le Borgne et al. [2012] report on conducting a series of thermal and solute tracer tests to characterize the fractured crystalline aquifer of Ploemeur, France. Thermal tracer tests were performed by injecting continuously 50° C water in a fracture located at a 50 m depth. The breakthrough curves measured in an adjacent borehole show a significant time lag between the thermal and solute breakthrough due to the large coefficient of heat diffusion compared to molecular diffusion. Combining heat and solute tracer tests allows measuring tracer dispersion with Peclet numbers varying over orders of magnitude, thus providing important constraints on effective transport behavior [Klepikova et al., 2011].

DePaolo [2012] describes an application of isotopic and trace element sensors for fluid flow, heat- and mass transport in fractured rocks, including examples of useful analytical models and applications to available data from fluid-rock systems for helium and helium isotopes, Sr-O-H isotopes, uranium isotopes, U decay series isotopes, and radiocarbon. The application of these methods will allow scientists to better understand the nature of heat and mass transport in hydrothermal systems in fractured rock. Isotopic methods are used as a supplement to directly measuring flow and transport properties in fractured rock, taking into account mineral-fluid chemical reactions and transport in the interfracture rock matrix. *Ellis et al.* [2012] report on studying the leakage of CO₂ acidified brine, resolving and accounting for spatial variations in mineralogy along these leakage pathways, which is needed to improve the predictive models used to estimate the permeability evolution through reactive caprock fractures. Menke et al. [2012] studied CO, and H₂O leakage rates from the injection zone to overlying units as a result of geologic sequestration, and found that the water-leakage rate through the fault increases with decreased CO₂ injection rate. This inverse relationship is attributed to the complex relationships between relative permeability, saturation, pressure, and capillarity. Both papers on CO₂ transport are an illustration of the need to study the properties of complex systems in relation to the surrounding environment, along with coupled processes affecting the systems' emergent behavior.

1.3.1.1. Collective behavior, emergent complexity, and emergent simplicity of complex fractured rock systems

Ellis et al. [2012], in their studies of mineral spatial heterogeneity of a limestone fracture, determine that a doubling in fracture volume may overestimate the calculated values of permeability by as much as 40%, when dissolution is assumed to occur uniformly along the fracture. The authors indicate the importance of studies of bands of less reactive minerals perpendicular to the direction of flow, which restrict flow along the fracture, serving to control fracture permeability. These bands are a demonstration of the need to study different parts of the complex fractured rock, which may influence the behavior of the whole system.

Mourzenko et al. [2012] investigate the percolation and permeability of fracture networks in excavated damaged zones (EDZ) at the Mont Terri underground rock laboratory (Switzerland). This work is performed to study the characteristics of Opalinus Clay to assess its capacity to serve as a low-permeability formation for hosting radioactive waste repository sites [Mourzenko et al., 2011]. The authors found that the fracture density is an exponentially decreasing function of the distance to the wall of the EDZ with a characteristic length of about 0.5 m. They also found that the fracture orientation is anisotropic, most fractures are subparallel to the tunnel walls, and this can be approximated by a Fisher law. They demonstrate that a heuristic power-law model can accurately describe the results for the percolation threshold over the whole investigated range of heterogeneity and anisotropy, and a simple parallel flow model can be used to describe fractured rock transmissivity. The latter demonstrates the idea of conversion of the emerging complexity regarding the individual parts of the system, into an emerging simplicity, when the flow can be described using a simple parallel flow model.

To study the overall thermo-hydro-mechanical properties of the rock, *Ezzedine et al.* [2012] focus on how within fractured-porous rock, micropores and microfractures and their interactions affect the cumulative behavior of effective mechanical, thermal, and hydrological rock properties. The results are then used to infer uncertainty associated with the physical and chemical aggregates of tight shale rock and their parameterization, using bruteforce Monte-Carlo method. *Sun and Carrigan* [2012] also demonstrate the results of modeling of uncertainty in predictions of gas transport in fractured rock. Both papers confirm that uncertainty is an inherent feature of complex systems.

Field tests at various scales (1 to 100 m) demonstrate that the dynamics of multiphase flow in fracture networks is highly complex because of the coupling of inertial and viscous forces, gravity, surface tension, and wettability of fracture walls, as well as fracture intersections. Moreover, fracture intersections act as flow integrators and switches of flow pathways [*Wood and Huang*, 2015, this volume].

In their studies of candidate sites for radioactive-waste disposal, Geier et al. [2012] find many similarities and differences, which can be attributed to regional and local conditions such as stress fields, rock types, fractured-rock hydrodynamics, and paleohydrogeology. For example, while having broadly similar redox and pH conditions, there is more dissolved methane and lower sulfate below 300 m depth at the Olkiluoto site in Finland than at the Forsmark site in Sweden, although both sites are in hard crystalline rock (migmatite gneiss and metagranite, respectively) with groundwater flow mainly via fractures. Water-rock reaction modeling does not explain these and other differences in groundwater compositions and secondary minerals at the two sites. The conclusion, from the standpoint of complex system theory, is that the studies of individual parts of the complex system are insufficient for understanding the behavior of the entire system, or for understanding the relationships among the specific components of the system.

Boomsma and Pyrak-Nolte [2015, this volume] present the results of studies regarding the collective behavior of transport in fractured media, which is a manifestation of the emergent properties of the fractured rock system. The authors create a synthetic fracture-network model, using an Objet Eden 350V 3D printer, to build a network of fractures and show that the ability to transport cohesive swarms through the fracture network is a function of the flow rate and swarm volume. These experiments demonstrate conditions under which colloidal-size contaminants can be driven through a fracture network. High-speed transport of cohesive swarms depends on the volume of the swarm and the ambient flow rates that provide a balance of forces, preventing significant loss of particles from the swarm or deposition of particles along the flow path. Swarms that are transported cohesively travel along a highly localized path through a fracture network. The result of this investigation is clear evidence of collective, emergent behavior in the fractured rock system, which may occur in fractures in the subsurface as a result of both natural and anthropogenic/industrial processes (such as synthetic nano- and micro-particles from consumer products, chemical and mechanical erosion of geologic material, and hydraulic fracturing proppants). The degree of localization and speed of transport of such particles depends on the transport mechanisms, the chemical and physical properties of the particles and surrounding rock, and the flow-path geometry through the fracture. This chapter is an excellent example of the need to study the collective behavior of parts of the system.

Another example of collective behavior is given by *Fakcharoenphol et al.* [2015 (this volume)], who reported the results of experimental and numerical modeling studies conducted to evaluate the potential of low-salinity waterflooding of oil reservoirs in shales. The authors find that osmotic pressure, caused by a salinity contrast, can cause countercurrent flow of water and oil, both in oil-wet and water-wet shale formations, and showed that in conventional oil reservoirs, low salinity oil-recovery improvements of carbonate formations might be partly attributable to osmotic pressure induced by salinity contrast. The mathematical/numerical model includes osmotic pressure, gravity, and capillary effects, thus illustrating the need for consideration of the collective behavior at the field scale.

1.3.1.2. Upscaling is manifestation of emergent simplicity

The idea of upscaling is relevant to the notion of emergent simplicity. Karimi-Fard et al. [2012] present an application of discrete fracture modeling (DFM) and upscaling techniques to complex fractured reservoirs, including DFM techniques developed by Karimi-Fard et al. [2004], in turn based on an unstructured finitevolume discretization. The mass flux between two adjacent control volumes is evaluated using an optimized twopoint flux approximation. The method is designed for general purpose simulators, and any connectivity-based simulator can be used for flow simulations. The DFM technique can be used as a stand-alone or as part of an upscaling technique. Such upscaling techniques are required for large reservoirs, wherein the explicit representation of all fractures and faults is not possible [Karimi-Fard et al., 2006]. Using an empirical finite-sized scaling approach to understand the hydromechanical relationship of single fractures, Petrovitch et al. [2012] find that fluid flow can be represented at all scales by a single universal scaling function.

Using the results of air permeability measurements in vertical and inclined boreholes spanning a $30 \times 20 \times 30$ m³ site in unsaturated fractured tuff near Superior, Arizona, *Neuman et al.* [2012] show that a hierarchical structure of

fractured rock renders their attributes scale-dependent. The authors show that this behavior is consistent with sub-Gaussian random fields subordinated to truncated (monofractal) fractional Brownian motion (tfBm). Using the scaling theory, the authors develop a consistent statistical relationship between fracture length, aperture, density, and log permeability.

1.3.1.3. Feedback loops, hysteresis, and variations of parameters

In their study of stress-dependent permeability in fractured-porous media, Huo and Benson [2015 (this volume)] provide compelling evidence that flow and transport in fractured-porous media meets the criteria of a complex system, specifically self-organized criticality and forward feedback. Using a series of core flood experiments, the authors show that hysteretic behavior in both permeability and fracture aperture is due to repeated cycles of compression and decompression. When fractured rock is compressed axially, the fracture aperture is compressed, resulting in effective pressure increases and an exponential decrease in permeability, as expected from stress-dependent permeability theory. However, when the fractured rock is decompressed, permeability increases but does not follow the compression path to the original value. In other words, the phenomenon of hysteresis indicates the irreversible deformation of fracture asperities and friction between asperities, and corroborates the idea of forward and negative feedbacks in complex fractured rock systems.

Lee et al. [2012] study the evolution of the dispersion coefficient in the single rough-walled fracture before and after circulated flow near the wall. They show that dispersion in the variable-aperture fractures occurs by the combined effects of molecular diffusion, macro-dispersion, and Taylor dispersion. In particular, Taylor dispersion is proportional to the square of the velocity, while macrodispersion is proportional to the velocity. The results of the experiments conducted using a rough-walled fracture model show distinct dispersion regimes in different parts of the fracture and for different Reynolds numbers. For example, in the range of Re < 2.78, the dispersion coefficient was proportional to the power of *n* from 1 to 2, which corresponds to previously published data. However, the calculated dispersion coefficient decreased for Re > 2.78, which the authors explain by the generation of circulated flow near the fracture wall. It is the opinion of the authors of this chapter that Lee et al.'s experimental results correspond to the idea of forward feedback in flow through fractures.

Tsenn [2015 (this volume)] studies the effect of contact area on fracture permeability, based on the notion that chemical processes could alter both the contact-area fraction and the pattern of the fracture surface and fracture aperture. The author conducts numerical Monte-Carlo

modeling, using the boundary-element method to assess the fracture pressure and flux, and shows that (1) contactarea fraction has a much greater effect on fracture permeability than the contact-area pattern, (2) a near-linear relationship exists between contact-area fraction and normalized fracture permeability when the contact-area fraction is less than 0.2, (3) as the contact-area fraction increases, normalized fracture permeability decreases, with the spread of values possibly up to one order of magnitude, and (4) flow through fractures could be blocked for the contact-area fraction greater than 0.7. Moreover, these results show that the calculated fracture permeability based on the parallel-plate model may overestimate the fracture-network permeability by over one order of magnitude. Another important conclusion is that dynamic data, such as pressure transient tests, are needed to assess the equivalent hydraulic aperture or hydraulic conductivity for fractures in the fracture network. Tsenn's chapter provides an example of when an emergent complexity of the system on a small scale can be presented using a set of effective parameters, i.e., by means of emergent simplicity.

Petrovitch et al. [2012] present the idea of universal scaling of fracture hydraulic properties, based on the results of nonintrusive geophysical techniques. While seismic techniques have been developed to probe the mechanical properties of fractures, e.g., fracture-specific stiffness, there are no techniques by which to remotely characterize their hydraulic properties. In this study, an empirical finite-sized scaling approach was used to understand the hydrome-chanical relationship of single fractures. This paper is an example of reducing the level of complexity in the measurements of fractured rock properties by measurements of seismic and hydraulic properties, or the consideration of a more simple level of emergency.

Liu [2015 (this volume)] develops a hydraulic conductivity relationship for unsaturated water flow based on minimized energy dissipation, using the optimality principle. The basic idea of the optimality principle is that natural processes organize themselves in such a way that their functioning is optimal under given external forcing and steady state conditions. The optimality principle has been widely used in many scientific fields, including constraining hydrological models [Kleidon and Schymanski, 2008; Westhoff and Zehe, 2013]. Based on the assumption that a flow field will tend toward a minimum energy dissipation rate, Liu [2015 (this volume)] derives an unsaturated hydraulic conductivity function and shows that the ratio of water flux to water head (energy) gradient is a power function of water flux. Empirical evidence supports the validity of this relationship under gravity-dominated conditions. The finding that the hydraulic conductivity depends not only on capillary pressure (or saturation) but also on the water flux confirms a long-standing hypothesis developed for structured soils (e.g., Rode, 1965).

Seok and Gale [2012] address the long-standing idea of representative volume elements (RVE), which plays a central role in the mechanics and physics of random heterogeneous materials when predicting their effective properties. The authors conduct an experiment using one cubic meter of granitic rock with a single natural fracture, which is characterized by strong spatial variability in permeability and porosity. The experimental results were compared with those from simulations of flow, using average and spatially variable permeability in a discrete fracture. The comparison also includes the results of water injection tests in seventeen boreholes, both individually and in groups, to assess the local permeability and hydraulic head distributions over the fracture plane as a function of normal stress.

In Seok and Gale [2015 (this volume)], the authors present fracture pore space data, from coupled stressflow experiments, that had been measured using a resin technique on the scale of the fracture apertures over the entire 200 mm \times 300 mm area of a fracture plane sample. Using these pore space data, which essentially constitute a fully characterized part of one piece of the complex system, the authors were able to determine how much data were required to obtain a reasonable match between the measured flow rates and the numerical-model-simulated flow rates, when the complexity of the spatial variability of the fracture pore space was embedded in the numerical fracture-flow models. In addition, the fully characterized fracture pore space allows us to evaluate how the inherent spatial variability in just one part of the complex fractureflow system affects the fluid velocities (and hence solute transport) in fracture planes with highly variable fracture-aperture or pore-space distributions. The results of these experimental and 3D numerical modeling studies demonstrate that the complex flow and transport phenomena in fractured media can be simulated based on the idea of statistically similar RVE, using effective properties of heterogeneous media. This chapter [Seok and Gale, 2015 (this volume)] is another manifestation of the concept of RVE and effective parameters corresponding to the concept of emergent simplicity used in the theory of complex systems.

1.3.1.4. Connection to the surrounding environment

A complex adaptive system, such as a soil or fracturedporous system, responds by varying its behavior depending on its surrounding environment. *Dragila et al.* [2015 (this volume)] addressed the phenomena of complexity in gas exchange between the Earth's upper crust and the atmosphere, which controls to a large extent many important processes, such as the Earth-atmosphere water cycle, agricultural activities, and greenhouse gas emissions. Although diffusion was conventionally considered the main mechanism of gas exchange between the atmosphere and vadose zone, driven by gas concentration gradients, laboratory and field-scale studies have shown that advective gas transport mechanisms are governing these fluxes in fractured rocks and cracked soils. Convection driven by thermal gradients (free convection) and wind induction (forced convection) were found to play a major role in Earth-atmosphere gas exchange.

Nimmo and Malek-Mohammadi [2015 (this volume)] attempt to quantify water flow and retention in a partially saturated fracture-facial domain, using a three-domain flow model. Two of the domains are assumed to characterize water flow and water storage in a fracture-facial region, and the third domain is assumed to characterize the matrix water. The flow domain is modeled with a source-responsive preferential flow model, the roughness-storage domain is modeled with capillary relationships applied to the fracture-facial area, and the matrix domain is modeled using traditional unsaturated flow theory. The authors test the proposed model to characterize the hydrology of the Chalk formation in southern England, linking hydrologic data including recharge estimates, streamflow, water table fluctuation, imaging by electron microscopy, and surface roughness. The authors indicate that the concept of unsaturated roughness storage is the collective effect of all microcavities in unsaturated media, which is one of the main features of complex systems.

The chapter by *Sharma et al.* [2015 (this volume)] is an illustration of long-term temporal changes in local flow rates in a brine formation composed of multiple layers with different transmissivities over a period of months or years, for instance, as a result of seasonal or climatic changes, owing to the connection to the atmosphere. The chapter also illustrates the effect of self-organization and a feedback loop (both forward and negative feedbacks), as a consequence of supercritical CO₂ storage in the deep subsurface. The results of investigations show how the local flow pattern of the storage formation will be disturbed and may change over time, as low-density and low-viscosity CO₂ enters into the transmissive layers and interacts with water and rock.

1.4. MODELS AND APPROACHES: MODEL SIMPLIFICATIONS

Zimmerman [2012] reviews the history and role of the cubic law for fluid flow in fractured rock, starting from the seminal paper "Validity of Cubic Law for Fluid Flow in a Deformable Rock Fracture" by Witherspoon et al [1980]. The idea of the cubic law was initially developed based on the model of hydraulic transmissivity of a channel bounded by two smooth parallel walls separated by an aperture h, for which transmissivity is exactly equal to $h^3/12$. However, the walls of actual rock fractures are rough and are in contact at discrete asperities that

correspond to local regions of zero aperture. The presence of spatially varying apertures led to the development of the theory of hydraulic aperture or the evaluation of effective mean aperture, to account for the effect of aperture variability and contact area by suitable multiplicative factors. Zimmerman also emphasizes that normal stress will reduce the aperture in a nonuniform manner, so that the three factors, mean aperture, aperture variability and contact area, will influence the manner in which the transmissivity changes due to normal stress. Although the cubic law holds for flow between parallel walls up to the laminarturbulent transition that occurs at Reynolds numbers of about 2000, deviations from a linear relationship between pressure drop and flow rate in a rough-walled fracture occur at much lower Reynolds numbers, on the order of about 10, during laminar flow. Zimmerman's paper provides an example of the case in which positive feedback in fractured rock is followed by a negative feedback, leading to stability of the system.

Broda et al. [2012] simulate such flow patterns using a numerical 3D fully integrated surface/subsurface flow model HydroGeoSphere, in which material heterogeneity is represented by means of (1) the dual continuum approach, (2) discrete fractures, and (3) a stochastic facies distribution framework using TPROGS. The results of this paper demonstrate the need for an application of multiple models and corresponding observations on different scales.

Leube et al. [2012] perform a model reduction and multiscale simulations for solute transport in fracturedporous media, based on the application of the multirate mass transfer model (MRMT) with model block upscaling. Modeling also includes the application of temporal moments for generating the MRMT equations, which were used to analyze the multiscale arrival time statistics in fractured media, taking into account fracture network properties, matrix properties, heterogeneity, and mass transfer that leads to non-Fickian transport behavior.

Willmann and Kinzelbach [2012] develop a new stochastic particle-tracking method to model transport explicitly in both fractures and matrix. Contrary to the existing flow simulations using a superposition of two separate domains, the fracture and matrix domains with exchange particles between them, the authors use a model in which a particle stays in a fracture before being released again to the matrix, depending on the fracture aperture, with the matrix flux perpendicular to the fracture, and a molecular diffusion component. This stochastic model also takes into account weighted random choice at fracture intersections as well as a random component of molecular diffusion. The model is applied to assess a fractured sedimentary formation in Northern Switzerland, which is currently under investigation as a host rock formation for nuclear waste disposal.

van Genuchten et al. [2012] show that complex flow and transport processes at a uranium mining site having granular and fissured aquifers underneath can be simulated using Richards equation with a dual-porosity numerical model for variably saturated water flow and contaminant transport. In this model simulation, the composite (effective) unsaturated hydraulic conductivity function is used to account for the separate effects of the fracture and matrix domains, while uranium transport is simulated using a full dual-porosity formulation.

1.4.1. Multidisciplinary Hydrological, Geochemical, and Microbiological Research for Different Applications

Kahler [2012] presents a technique to promote mixing in dead-end pores to improve a pump-and-treat remediation approach, which is among the most common methods to remediate contaminated groundwater. A series of numerical and laboratory experiments illustrate that a change in pressure is needed to promote the pore-cleaning mechanism. The physical mechanisms of mixing were previously discussed in a number of publications (e.g., Ottino, 1990; Weeks and Sposito, 1998). Faybishenko [2005] showed that in fractured rock, mixing and dispersion of fluids result from two types of complex interactions between flow processes (even for small Reynolds numbers) on different scales: (1) drop length-scales, such as breakup, coalescence, and hydrodynamic interactions; and (2) agglomerate length-scales, such as surface erosion, fragmentation, and aggregation [Ottino, 1990], which are also caused by chaotic regimes in fractured-porous media [Faybishenko, 2003].

Winterfeld and Wu [2015 (this volume)] study geomechanically coupled processes in unconventional oil and gas reservoirs, showing that fracture networks provide highly permeable flow paths that allow for access to tight matrix blocks. Using as an example the results of water injection in Bakken, the authors illustrate how stress changes during water injection could induce microfractures that further extend the fracture network into the matrix. The stress change is calculated using equivalent mechanical properties for fractured rock, assuming that the deformation of fractured rock is the sum of the deformation of intact rock and fractures. The authors also apply the Hoek-Brown failure criterion to calculate when matrix rock fails. Simulation results indicate that viscous displacement and spontaneous imbibition processes are negligible because they cannot penetrate into the tight matrix block. Once matrix blocks are cracked via thermally induced stresses on the matrix surface, these processes become more pronounced and can improve oil production from the cracked tight matrix. The results of this paper are indicative of the sequence of positive and negative feedback processes in fractured media.

Peng et al. [2012] address the problem of reduced gas recovery in fractured Barnett shale, finding that the average first-year decline reported was 64%, which is attributed

to the coupled physical (such as tortuous flow pathways) and chemical (such as desorption) processes in the low permeability shale nano-porous matrix. Similar results of the long-term decline of gas production in shale were reported by *Patzek et al.* [2013] and *Monteiro et al.* [2012].

Mullally and Lowell [2012] investigate boundary layer flow, heat, and chemical transfer near an internally heated vertical borehole or borehole array emplaced in a homogeneous water-saturated porous medium, as a means of developing a large-scale hydrothermal experiment at the DUSEL site in the Homestake Mine, South Dakota, or elsewhere. The authors use a scale analysis to determine the relationships between vertical fluid velocity, boundary layer thickness, and the Rayleigh number, for both a single borehole maintained at constant temperature and a linear array of boreholes maintained at a constant heat flux. Based on the scale analysis, it is determined that thermoelastic stresses generated by heating the rock near the boreholes do not significantly impact the permeability for a low initial porosity of $\sim 5\%$, or when the initial crack aspect ratio is less than or equal to 10^{-2} . The scale analysis is also used to assess mineral dissolution within the boundary layer adjacent to the boreholes.

Molz et al. [2015 (this volume)] describe a decade long multidisciplinary research project, including field, laboratory, and modeling of plutonium (Pu) transport, first in field lysimeter soil, then in field soil containing grass roots, and finally in the roots and stems of corn (a type of grass) grown in laboratory pots. The overall system studied was certainly complex, involving natural climatic conditions driving variably saturated flow, coupled to oxidation and reduction of Pu species, species interaction with chelating agents secreted by plants and microbes, then rapid uptake by plant roots followed by transport in the transpiration stream and into the surrounding plant tissues. Many of the sub-processes occurred at very different time scales, but emerged simplicity was evident in several of these sub-processes. Downward transport of Pu in soil was dominated by the highly adsorbed oxidized Pu species, with only a couple of cm movement during the 11 year field period. A tiny fraction of Pu that was reduced on particle surfaces and released, in a repetitive manner, moved downward more rapidly. Pu uptake and movement in plants was millions of times faster than oxidized Pu in the soil, about 58 cm in 10 to 20 min. based on laboratory experiments. This rapid transport was probably due to Pu uptake by the biochemical apparatus of plants that was evolved to facilitate iron (Fe) uptake, an essential nutrient that is often held tightly to soil surfaces. In the lysimeter experiments, upward movement in the transpiration stream resulted in Pu being deposited on the soil surface due to grass dieback in the winter. Thus, biologically based complexation appears essential to the accelerated Pu and Fe movement in the soil-plant system. In this sense, a plant root in soil demonstrates some of the rapid transport features associated with a fracture in rock. Throughout the study, experiments motivated model development and modeling results motivated the performance of additional experiments, what the authors call computer-aided thinking due to microbiological activities in soils.

1.5. CONCLUSION: CAN COMPLEXITY SCIENCES BENEFIT THE FIELD OF FLOW AND TRANSPORT IN FRACTURED-POROUS MEDIA?

We apply the concepts of complex systems theory to the analysis of papers published in this volume and the papers presented at the Fall 2012 AGU Meeting, at the session titled "Dynamics of Flow and Transport in Fractured-Porous Media." Our analysis shows that fractured-porous media can be defined as a complex system formed out of many components with an emergent behavior. Certain properties of complex systems appear to be inherent to fractured-porous media, such as collective behavior, emergence, coevolution with their environment, connectivity of the fractured-porous media parts, feedback mechanisms, and self-organization. Moreover, all of these properties are intrinsically related to one another through multiple dynamic processes. Complex behavior is due to nonlinear dynamical effects, which under certain conditions may lead to the physically based phenomenon of chaos in natural systems (not due to numerical effects).

The relationships between different parameters and variables measured in the field are very complicated because the subsurface is composed of a hierarchy of structures and processes that span a large range of spatial and temporal scales. We show examples of both emergent complexity and emergent simplicity in the behavior of fractured-porous media. Due to the collective behavior of the components of a fractured rock system, the whole-system behavior cannot be simply inferred from the behavior of its components. Because the causes and effects in fractured rock are not obviously related, the problems of flow and transport in fractured rock are difficult to solve and are often hard to understand. In this perspective, the study of fractured rock as complex systems, based on the results of experimental field or laboratory investigations and modeling, is a new endeavor that strives to improve our ability to understand the processes of flow and transport, when a system is highly complex. Examples of fractured rock as complex systems that undergo guided developmental processes as part of their formation include infiltration tests or pumping and injection tests/experiments. During these tests, system developmental processes are guided by the boundary conditions.

The flow of fluids through fractured rock is critically important in many practical applications, including remediation, nuclear waste disposal, hydrothermal systems associated with geothermal energy production, base metal ore deposits, gas and oil recovery, and global geochemical cycles. The nature of mass, heat, and chemical transport in fractured rock systems is determined by the physical (spacing and volume) properties of fractures, the nature of chemical transport between fractures and matrix blocks, and the dissolution and precipitation rates of minerals in matrix blocks and on fracture walls. Fractured-porous media meet all criteria of the complex systems.

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