Sinkholes and the Engineering and Environmental Impacts of Karst

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EDITED BY
Lynn B. Yuhr
Technos, Inc.

E. Calvin Alexander, Jr.
University of Minnesota

Barry F. Beck
P.E. LaMoreaux & Associates, Inc.

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LATTICE-BOLTZMANN SIMULATIONS OF CARBONATE SYSTEMS

Stuart D.C. Walsh, Scott C. Alexander, and Martin O. Saar

ABSTRACT

Carbonate bedrocks encompass a vast range of primary porosities and permeabilities, which are further modified by the addition of secondary porosities as a result of fissure, fracture, and conduit development. The wide variety of primary and initial secondary porosities found in carbonates further complicate the already difficult task of modeling speleogenic processes. Understanding carbonate dissolution requires consideration of the aqueous speciation of a host of chemical elements (e.g., H, O, C, Ca, Mg, and S). It also requires simultaneous solution for the complex, typically non-Darcian, flow field over a wide range of spatial and temporal scales as the flow field affects the degree of advection and diffusion of the chemical species to and from the host rock.

Lattice-Boltzmann methods are particularly suited to modeling the complex fluid dynamics involved in carbonate dissolution. Lattice-Boltzmann simulations are adept at reproducing complex and changing boundary geometries, as well as turbulent and laminar flows, multiphase-multicomponent flow, and buoyancy-induced convection due to solute and thermal gradients. Here, we present some preliminary numerical models, using lattice-Boltzmann simulations, to reproduce permeability development over a range of length and time scales for two different karst systems: continental Paleozoic systems and modern carbonate platforms.

INTRODUCTION

Carbonate rocks contain many of our most productive aquifers and petroleum reservoirs (Ford and Williams 2007). This high productivity is the direct result of dissolution processes that significantly increase the connected porosity and the permeability of the original formation (Figure 1). However, poorly constrained are the rates

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1Department of Geology & Geophysics, University of Minnesota - Twin Cities, MN 55455; saar@umn.edu
of carbonate dissolution and the complex feedback mechanisms between these dissolution rates and the flow field (Klimchouk 2005) – factors that ultimately determine the shapes, storage capacities, and permeabilities of carbonate aquifers and petroleum reservoirs. An improved understanding of how the various feedback mechanisms between fluid flow and host-rock dissolution result in productive aquifers and petroleum reservoirs, would improve our ability to detect and quantify such systems (Heward et al. 2000).

In particular, formation of larger fissures or conduits by carbonate dissolution increases permeability and thus fluid flow rates, which, in turn, increase rock dissolution rates (White and Longyear 1962). The latter further widens fissures, eventually forming conduits, thus closing the feedback loop. The increase in carbonate dissolution rate with an increase in flow rate is due to the flow maintaining the Ca-ion gradient near the host rock and providing a fresh source of the chemical species that facilitate dissolution, both of which are greatly enhanced with the onset of eddy diffusion in the transition from laminar to turbulent flow (White and Longyear 1962; Buhmann and Dreybrodt 1985a; Buhmann and Dreybrodt 1985b). Understanding carbonate dissolution requires consideration of the aqueous speciation of the elements H, O, C, Ca, Mg, and S (Plummer et al. 1979; Hill 1995). It also requires simultaneous solution for the complex, typically non-Darcian, flow field over a wide range of spatial and temporal scales as the flow field affects the degree of advection and diffusion of the chemical species to and from the host rock (Dreybrodt et al. 2005; Ford and Williams 2007).

![Carbonate Dissolution Processes](image)

**FIG. 1.** a) Schematic illustration of carbonate dissolution features due to carbonic acid from CO$_2$ and water at the water table, sulfuric acid formation above marine shales, and due to freshwater mixing corrosion. Also shown is corrosion due to freshwater-saltwater mixing of brines from deep sources both with less-salty ocean water or with freshwater. b) Illustration of the three spatial scales considered in the proposed study. The spatial scale affects fluid flow rates which, in turn, affect dissolution rates over multiple temporal scales, as discussed in the main text.
Lattice-Boltzmann simulations are capable of modeling a wide variety of fluid-mechanical processes encountered in speleogenesis. Lattice-Boltzmann simulations are adept at reproducing complex and changing boundary geometries (Aharonov and Rothman 1993; Bosl et al. 1998; Hersum et al. 2005), turbulent and laminar flows (Benzi and Succi 1990; Chen et al. 1992), multiphase-multicomponent flow of miscible and immiscible fluids (Succi et al. 1991; Pan et al. 2004), and buoyancy-induced convection due to solute and thermal gradients (Alexander et al. 1993). This paper discusses lattice-Boltzmann modeling methods for reproducing permeability development at the three different spatial and temporal scales illustrated in Figure 1b, for a range of different primary permeabilities and porosities: the first is an explicit method that simulates the slow growth of small fissures under diffusion-dominated conditions; the second model simulates the development of meso-scale permeability; and the third is an implicit method capable of simulating development of, and flow through, systems at the conduit scale.

MULTI-SCALE LATTICE-BOLTZMANN SIMULATIONS

Microscale Fissure Initiation

At the smallest scale, the simulation employs a diffusion-controlled dissolution model, based on that given in Verhaeghe et al. (2005), to simulate the formation of fluid-bearing fissures in carbonate rocks and subsequent solute transport. Figure 2b compares the model’s predictions to the analytical solution for the classical, one dimensional Stefan moving boundary problem (Stefan 1889). The model has been extended to account for dissolution in the presence of multiple chemical species (Figure 2c). Here for simplicity, we consider calcite dissolution in response to aqueous carbon dioxide. The same techniques can be employed to include the Sulfur system (S, H$_2$S, H$_2$SO$_4$, SO$_4$) when considering the effect of underlying marine shales (Figure 1a) that provide a Sulfur source. In this scenario, the order of chemical species release from the marine shales is conducive to productive reservoir formation as the Sulfur is released first from the marine shale, thus forming sulfuric acid that enhances dissolution of overlying carbonates, into which subsequently formed hydrocarbons can migrate (Ford and Williams 2007).

The lattice-Boltzmann simulation models calcite dissolution by tracking the behavior of three chemical species: 1) the fluid controlling the advective transport of the other dissolved phases; 2) aqueous CO$_2$; and 3) dissolved Ca$^{2+}$ ions. Our lattice-Boltzmann model simulates flow of the fluid phase employing an algorithm with a standard three-dimensional, nineteen-velocity lattice (Qian et al. 1992). As in all lattice-Boltzmann models, the fluid is represented by a set of discrete fluid packets, each with a given density and velocity (Figure 3). At each timestep, the fluid packets are first propagated between neighboring lattice nodes in a so-called “streaming step” and subsequently redistributed in a “collision step.” The collision step for the fluid
phase representing the solvent redistributes the fluid packet densities according to
\[ f_{\alpha}^{\text{out}} = (1 - \lambda) f_{\alpha}^{\text{in}} + \lambda f_{\alpha}^{\text{eq}}, \]

where \( f_{\alpha}^{\text{out}} \) is the outgoing fluid packet density along lattice direction “\( \alpha \)”, \( f_{\alpha}^{\text{in}} \) is the incoming fluid packet density after the streaming step, \( \lambda \) is a collision frequency, which determines the viscosity of the fluid, and \( f_{\alpha}^{\text{eq}} \) is the equilibrium fluid packet density. For the models discussed in this paper, the equilibrium fluid packet densities are given by
\[ f_{\alpha}^{\text{eq}} = \rho w_{\alpha} [1 + 3u \cdot c_{\alpha} (1 + 3u \cdot c_{\alpha}/2) - 3u \cdot u/2] , \]

where
\[ \rho = \sum_{\alpha} f_{\alpha}^{\text{in}} \]

is the net fluid density,
\[ u = \frac{1}{\rho} \sum_{\alpha} f_{\alpha}^{\text{in}} c_{\alpha} \]

is the net velocity of the incoming fluid packets, \( c_{\alpha} \) are the fluid packet velocities, and \( w_{\alpha} \) are weighting constants specific to the lattice. The latter two are given by
\[ c_0 = (0, 0, 0); \quad c_1 \ldots c_6 = (\pm c, 0, 0), (0, \pm c, 0), (0, 0, \pm c); \]
\[ c_7 \ldots c_{18} = (\pm c, \pm c, 0), (\pm c, 0, \pm c), (0, \pm c, \pm c), \]

and
\[ w_0 = 1/6; \quad w_1 \ldots w_6 = 1/18; \quad w_7 \ldots w_{18} = 1/36 \]

where \( c = \Delta x/\Delta t \) is the lattice velocity, i.e., lattice spacing divided by timestep duration.

Advection and diffusion of the two soluble phases are modeled with appropriate diffusion lattice-Boltzmann models as described in Dawson et al. (1993). These diffusion models are similar to standard lattice-Boltzmann methods, except the velocity
FIG. 3. Part of a two dimensional lattice-Boltzmann lattice (a). The fluid packets are propagated between nodes during the streaming step (b) and redirected during the collision step (c).

used to obtain the equilibrium packet density is calculated from the original fluid phase, rather than the dissolved phase. Dissolution and precipitation of calcite at the fluid boundaries is controlled through a mass-balance approach: First aqueous carbon dioxide and calcium ion concentrations are calculated at the boundary nodes and concentrations of the dissolved species at the boundary are adjusted to the equilibrium concentration; the location of the boundary is then adjusted according to the local gain or loss in calcium carbonate. Sub-grid scale adjustments are made to the location of the boundary using the interpolated boundary condition described in Verhaeghe et al. (2005).

**Mesoscale Fracture Features**

As the rate of fluid flow grows relative to the speed of host-rock dissolution, it becomes increasingly impractical to simulate the dissolution with an explicit, diffusion-controlled model. Fluid flow and dissolution rates in fracture systems of even moderate size often differ by several orders of magnitude (Dreybrodt et al. 2005). Therefore, development of meso-scale fracture features is instead modeled with a multi-speed simulation that employs a rate-controlled dissolution model (Figure 4). In this approach, the lattice-Boltzmann method is used to find the distribution of the dissolved solutes under steady-state conditions. The rate of host-rock dissolution at each node is then calculated based on an empirical model (Palmer 1991) for the water-CO$_2$-limestone system as a function of Ca-undersaturation in water. As with all of the models discussed in this paper, other components (oil, $S$, etc.) can be accommodated as well. With this information the boundary conditions and locations are updated to reflect host-rock dissolution and the process is repeated. This method allows the growth of mesoscale features (~1m) to be simulated (Figure 4).

The numerically modeled widening of a fracture shown in Figure 4 resembles similar features found in caves. For example, Figure 5b is a cross-sectioned Light Distance And Ranging (LIDAR) image through a cupola (Ford and Williams 2007) or similar dissolution pocket in Mystery Cave, south-eastern Minnesota. The field data is not symmetric due to natural variation of the cave surface, however, the typically ob-
FIG. 4. At the mesoscale, a multi-speed model is used to accommodate the different timescales associated with the fluid velocity (~m/s) and the rate of dissolution (~cm/year): 1) The model first calculates the steady-state solution for the fluid flow and dissolved solutes on the short timescale. 2) The rate of dissolution at the boundaries is found based on the short-time steady-state solution. 3) These dissolution rates are then used to increment the boundary positions on the long timescale, and the process is repeated for the new boundary conditions (shown are modeling results).

FIG. 5. LIDAR image of a fracture opening in Mystery Cave, southeastern Minnesota: a) rendered surface view and b) cross-sectional view, as indicated in panel a, for comparison with the widened fracture image in Figure 4.

served concave dissolution shapes can be seen on the right side of the cross-sectional LIDAR image.

Macrosopic Conduit Systems
On yet larger scales, we simulate the development of conduit features using an implicit method, modified from the partial-bounceback approach of Dardis and McCloskey (1998) and Thorne and Sukop (2004). This model, described in greater detail in Walsh et al. (2008), employs a probabilistic method to simulate host rocks of varying primary permeability and is particularly suited to systems with rapidly changing
heterogeneities (Figure 6) as is found in modern carbonate platforms.

In the partial-bounceback approach, a proportion of the incoming fluid packets are reflected in the opposite direction during the collision step, according to

$$f_{\alpha}^{\text{out}}(x, t) = (1 - n_s) f_{\alpha}^{c}(x, t) + n_s f_{\alpha}^{\text{in}}(x, t),$$

(7)

where the portion reflected at each node is controlled by a model parameter known as the solid fraction, $n_s$, such that $0 \leq n_s \leq 1$. The solid fraction should be regarded as an internal model parameter from which the permeability is derived, rather than a reflection of the actual proportion of solid material at each node. Under the standard partial-bounceback model the relationship between the intrinsic permeability, $k$, and the solid fraction, $n_s$, is given by

$$k = \frac{(1 - n_s)\nu}{2n_s},$$

(8)

where $\nu$ is the kinematic viscosity of the fluid (Walsh et al. 2008). The partial-bounceback method can simulate other solid-fraction/permeability relationships by introducing

$$k = k(n_s(n_s^*)),$$

(9)

where the function $n_s = n_s(n_s^*)$ converts the actual solid fraction to the model value corresponding to the desired permeability. The dissolved phases are simulated using a modified lattice-Boltzmann model that accounts for the effect of the local variations in pore fractions on the species transport (Walsh and Saar 2008).

The dissolution “fingers” of the macroscopic conduit system (Figure 6), generated by our implicit lattice-Boltzmann method for large-scale flow systems, resemble flank margin cave development as depicted by Mylroie (1988), although we stress that different mechanisms are involved in both cases. The present very simple model represents dissolution under a constant head gradient. To more accurately simulate the flank margin environment we will have to add fresh/salt water mixing, tidal forces, and density effects.

**CONCLUSION**

Lattice-Boltzmann methods provide a means for simulating the complex hydrodynamic processes encountered in karst development. Although we have concentrated on carbonate systems, each of the methods discussed in this paper can also be extended to examine systems involving the action of other chemical components.

This paper has presented three methods for simulating the development of permeability in carbonate systems over a range of length and timescales, with a variety of initial permeabilities and porosities. Standard lattice-Boltzmann methods allow the
FIG. 6. The macroscopic model employs a partial-bounceback lattice-Boltzmann method to simulate host rocks of varying permeability. The figure shows a) the final solid fraction (dark=zero, light=maximum) and b) the fluid speeds (light=zero, dark=maximum, overall flow is from left to right) in an initially random heterogeneous medium (see gray scale matrix in panel a), where focused dissolution and related permeability increase of the host rock has been simulated.

The simulation of carbonate dissolution on small scales. However, for larger scale simulations, the disparity in fluid flow rates and dissolution timescales requires alternative methods. At subcave scales, and in systems with low intrinsic permeability, carbonate dissolution can be simulated using a two-speed method. Over short timescales, the lattice-Boltzmann method is used to simulate fluid flow and solute transport, which is in turn used to calculate the dissolution of the rock matrix over larger times. On yet larger scales and in systems with an initial intrinsic permeability, an implicit partial-bounceback method is used to simulate the flow of fluid through porous media.

Comparisons of our numerical speleogenesis models and field observations are encouraging. Specifically, simulations of fracture widening as well as development of dissolution “fingers” closely resemble features found in natural systems. However, the presented numerical methods have to be developed and tested further, including coupling of the three scale-dependent modeling techniques, to better constrain the proposed causality of some observed karst features and to improve comparisons with field observations.

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