Reply to comment by R. D. Braddock and J. Norbury on "On the continuum-scale modeling of gravity-driven fingers in unsaturated porous media: The inadequacy of the Richards equation with standard monotonic constitutive relations and hysteretic equations of state"

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1. Introduction

[1] Experimentally, one finds that as a gravity-driven finger (GDF) grows downward in an initially dry, water wettable, homogenous sand at low supply rates and where the air phase can escape freely, its tip oversaturates and then drains a distance behind, giving rise to a nonmonotonic signature in both time (at a given location) and space (up along the finger's profile) [*Glass et al.*, 1989]. In a hysteretic medium, such a nonmonotonic response induces heterogeneity in hydraulic properties and produces a finger core and fringe region structure that persists in time and over subsequent drainage and infiltration cycles. While a hysteresis-based theory [*Glass et al.*, 1989] allows the understanding of the persistence mechanism once a finger has formed, it says nothing about why an oversaturation of the tip should occur in the first place. In fact, it seemed obvious at the time when the nonmonotonic response was discovered that the traditional unsaturated flow theory, founded on the inherently diffusive Richards equation (RE) and monotonic properties, would not yield this initial oversaturation and thus could not be used to model GDF.

[2] Regardless, there has been interest on the part of many to explain GDF with traditional concepts of unsaturated flow. Since the RE is very nonlinear and we know that the media behaves hysteretically as well, emphasis in this quest was placed on numerical solution. *Nieber* [1996] was the first to publish what he believed to be a numerical solution of the RE that yielded GDF and its nonmonotonic response. This method was subsequently used in a series of papers concerning various aspects of GDF and its influence on solute transport as well as hydrophobic sands [e.g., *Ritsema et al.*, 1998a, 1998b; *Nguyen et al.*, 1999a, 1999b; *Nieber et al.*, 2000; *Ritsema and Dekker*, 2000]. However, after careful investigation, one finds that in *Nieber*'s [1996] method, numerical errors (more specifically spatial truncation error arising from his use of a downwind averaging method) cause numerical oscillations that, when combined with hysteresis, generate a GDF-like response. In fact, for the parameter values that yield a GDF-like response the errors are so large that one can show that the governing equation actually being solved numerically is not the RE at all.

[3] Our purposes and conclusions were stated in a previous paper [*Eliassi and Glass*, 2001a, sections 1 and 5]. We reiterate them here so that they are clear in context of both *Braddock and Norbury* [2003] (hereinafter referred to as BN03) and this reply. Our purposes were twofold: (1) To illustrate through artifact-free numerical simulations that the RE in conjunction with standard constitutive relations and hysteretic equations of state [*Mualem*, 1976; *van Genuchten*, 1980], which we refer to as standard monotonic properties (SMP), will not yield GDF and its nonmonotonic signature within parameter space where GDF has been found experimentally and (2) to demonstrate through detailed analysis that the numerical method used by *Nieber* [1996] and colleagues [e.g., *Ritsema et al.*, 1998a, 1998b; *Nguyen et al.*, 1999a, 1998b; *Nieber et al.*, 2000] relies on truncation error induced numerical oscillation associated with a downwind averaging, which in combination with hysteresis produces an "organized oscillation" that is GDF-like.

[4] Our conclusion, as stated in the last sentence of the abstract, was "Thus the RE along with standard monotonic hydraulic properties does not contain the critical physics required to model gravity-driven fingers and must be considered inadequate for unsaturated flow in initially dry, highly nonlinear, and hysteretic media where these fingers occur" [*Eliassi and Glass*, 2001a]. So let us be perfectly clear: Any simulation that looks like GDF in our paper [i.e., *Eliassi and Glass*, 2001a], those by J. L. Nieber and colleagues (i.e., those listed above), as well as the ones shown here, are not due to the physics explicitly represented in the model and instead arise purely from truncation error induced numerical oscillation.

[5] While we are happy that BN03 have given us the chance in this Reply to further emphasize the results of *Eliassi and Glass* [2001a], they are mistaken in what they perceive as oversights in our paper. They put forth three

such oversights: (1) that the basis of our assumptions on monotonicity are not fully met, (2) that the temporal truncation errors are leading to oscillation in the solutions, and (3) that these oscillations pose difficulties in the choice of switch value in the hysteresis relations. To each of these, we give our detailed reply in sections 2–4.

2. RE + SMP Yields a Monotonic Solution Where GDF Should Form

[6] BN03 state that published unsaturated flow theory only treats monotonicity as a one-dimensional (1-D) concept (both we and they reference the literature; note that we reference *Youngs* [1995] because of his simple description of the water content profile when the surface is subject to a constant flux, not that Youngs uses the word "monotonic"). BN03 point out that for 2-D situations, theory has yet to prove that RE + SMP can only yield a monotonic solution. While it may be true that no paper, published to date, explicitly proves the maximum principle for the general nonlinear 2-D case, there are literally hundreds of published papers that give analytic and numerical solutions to the RE + SMP in 2-D cases, all of which display monotonic results (of course, this is only true for a homogeneous medium with constant initial and boundary conditions as we study). Indeed, we show in our paper that when we solve the RE numerically and are careful to keep numerical errors in check, a monotonic solution is found for parameters representative of experiments where GDF occurs (e.g., refer to *Eliassi and Glass* [2001a], Figures 1d and 3b, for the second-order centered difference (CD2) result). That is why we conclude in our paper [*Eliassi and Glass*, 2001a] that the RE + SMP will not yield a nonmonotonic solution where it has been found experimentally, and thus the RE + SMP does not contain all the relevant physics to model GDF. We encourage BN03 in their quest for a more general proof of monotonicity; yet this is not necessary to support our thesis.

[7] However, if one is not convinced by the literature, experience, or numerical methods, we present the following example as suggested by BN03. Figure 1 presents the results for a 2-D simulation of RE + SMP where the flux at the surface is applied to the entire top region (i.e., a pseudo-1-D case, as BN03 refer to). Physical and numerical parameters (see caption for Figure 1) are those used in the baseline cases of *Eliassi and Glass* [2001a]. We see that for nonhysteric cases, first-order downwind (DW1, as used by *Nieber* [1996]), CD2 (simple arithmetic averaging) and first-order upwind (UW1, an inherently monotone averaging method) a horizontally uniform, 1-D wetting front (WF) advances into the domain. However, note that while for UW1 (Figure 1c) there are no oscillations present (that is, the saturation ranges from the initial value at the WF to its maximum asymptotic value imposed by the boundary condition), for DW1 (Figure 1a) and CD2 (Figure 1b) an oscillation is present at the WF. This is not at all surprising, because for coarse enough grids both DW1 and CD2 will yield oscillations. However, as we further refine the grid for CD2 (Figure 1d), the oscillation disappears, and the front becomes quite sharp and monotonic. Thus as BN03 would have it, the results in Figures 1c and 1d give an illustrative or pragmatic "proof" of the maximum principle for the nonlinear RE + SMP. As an aside, we also show a hysteretic simulation for the DW1 case (Figure 1e). Now we see that hysteresis allows the capture of the numerical oscillation at the WF in an organized oscillation that yields GDF-like fingers having saturated tip lengths representative of the physics and not the numerics.

[8] Finally, we note in passing that there is a vast literature dedicated to numerical techniques designed to ensure monotonicity in numerical solutions. These techniques include the total variation diminishing technique [e.g., *Harten*, 1983], flux-corrected transport [e.g., *Boris and Book*, 1973], *van Leer*'s [1977] second-order monotone scheme, *Leonard*'s [1979] quadratic upstream interpolation technique, and many others. All of these techniques have been developed and successfully applied to a variety of multidimensional problems in conjunction with advection-diffusion (and/or) dispersion equations with one common goal in mind: to ensure monotonicity whereby numerical oscillations do not mask the underlying physical processes being modeled. Indeed, implementing such techniques in the context of RE + SMP forces a monotonic solution in the parameter range where GDF occurs and thus suppresses spurious numerically based GDF-like behavior [*Eliassi and Glass*, 1997].

3. Spatial Truncation Errors in Nieber's Method Lead to GDF-Like Solutions

[9] One of the main purposes of our paper [*Eliassi and Glass*, 2001a] was to identify the numerical oscillations in *Nieber*'s [1996] method with the creation of near-physical, GDF-like solutions. To accomplish this, we analyzed the temporal and spatial leading truncation errors (LTEs) at the WF via direct calculation as a simulation progressed. We found the temporal LTE to be always much smaller and, indeed, negligible relative to that of the concurrent spatial terms' LTE. This resulted from the restrictions placed on the time step, which included a global maximum of 10^{-3} (not reported by *Eliassi and Glass* [2001a]). Thus we did not present or discuss the temporal LTE further in our paper (see our statement on this point [*Eliassi and Glass*, 2001a, last paragraph of section 3]). The negligibility of the temporal LTE is especially true near the WF where we are particularly concerned for the GDF problem. There, the temporal LTE for GDF-like solutions [e.g., *Eliassi and Glass*, 2001a, Figures 6a and 6b] can be many orders of magnitude smaller than the combined spatial LTE. Thus for the cases we have considered it is not the temporal term's LTE that drives and/or controls the artificial response that yields a GDF-like solution in *Nieber*'s [1996] method; rather it is the LTE of his downwind averaging method (and for that matter any averaging method that can cause oscillations at the WF).

[10] Beyond the fact that the temporal LTE can be shown to be negligible and therefore irrelevant in our simulations, let us turn our attention to BN03's linear analysis of the temporal LTE. For our problem, i.e., GDF in initially dry highly nonlinear porous media, analysis should be focused on the WF where state variables are changing rapidly. Because BN03's linear analysis applies only away from the WF, one must ask how it can shed light on the causes of the GDF-like behavior. For example, let us consider the error in the horizontal direction (i.e., η in our notation) across the artificial GDF-like solution [see *Eliassi and*

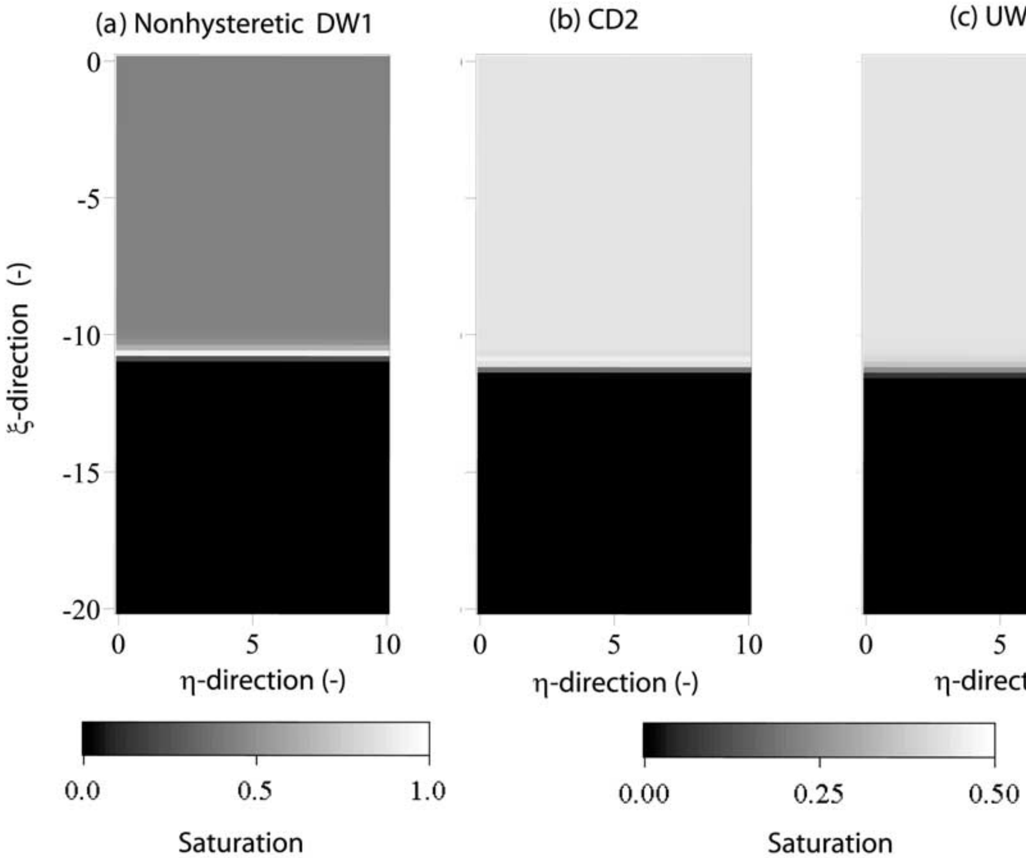

Figure 1. Saturation fields for two-dimensional numerical simulations, based on the Richards equation (RE) and standard monotonic properties (SMP), for constant flux infiltration, into an initially dry, highly nonlinear porous media, 10 dimensionless units wide and 20 dimensionless units tall, at a dimensionless time of $\tau = 50$. We illustrate in nonhysteretic simulations that while (a) the first-order downwind (DW1) and (b) the second-order centered (CD2) methods yield oscillatory solutions at the wetting front (WF) for coarse grids, using (c) the inherently monotone first-order upwind (UW1) or (d) CD2 methods with a more refined grid, the solution is monotonic (i.e., oscillation free). We do not recommend the use of the DW1 method (initially suggested by *Nieber* [1996]) and only present it here for the sake of consistency with our previous simulations [*Eliassi and Glass*, 2001a]. The solutions in Figures 1c and 1d clearly depict that monotonicity can be achieved for numerical solution of nonlinear RE + SMP. When hysteresis is included and the solution is oscillatory, GDF-like solutions result as we show in Figure 1e for DW1. The parameters for these examples are the same as for the baseline cases discussed by *Eliassi and Glass* [2001a]. For all cases here the initial saturation is uniform, having a value of $\Theta_i = 10^{-10}$; the dimensionless applied surface flux ratio is $R_s = q_s/K_s = 0.1$, with all other boundaries being of no flow condition, where q_s and K_s are the dimensional applied flux and saturated conductivity of the media, respectively. The SMP are determined using *van Genuchten*'s [1980] pressure saturation and *Mualem*'s [1976] relative permeability functions, where $n = 15$ and $\alpha^* = 1$ for nonhysteretic and $\alpha^* = 0.5$ for hysteretic properties (for details, see *Eliassi and Glass* [2001a]). Note that when the solution is monotonic, the maximum saturation yields an asymptotic value of $\Theta_A = 0.4355$, which can be found using the relationship $R_s = \kappa(\Theta_A)$, where κ is the relative permeability function at an asymptotic saturation of Θ_A. In fact, for all cases, $\Theta_A = 0.4355$ immediately behind the WF all the way back to the surface. The saturation in the color bar ranges from 0 to 0.5 for Figures 1b, 1c, and 1d to better show the solution near the WF across the various averaging methods. Other parameters used include uniform square grid spacing $\Delta\eta = \Delta\xi = 0.2$ in Figures 1a, 1b, and 1c and $\Delta\eta = \Delta\xi = 0.1$ in Figure 1d. See also *Eliassi and Glass* [2001a] for additional explanation on the choice of the parameter.

Glass, 2001a, Figure 9a]. From BN03's linear analysis (that results in the linear form of the telegraph equation), they explain the behavior of such a horizontal transect as a standing or traveling wave solution for the temporal LTE. On the contrary, one can show through direct calculation of the various LTE components that the horizontal behavior of the total LTE is due nearly entirely to the behavior of the spatial terms' LTE. In fact, the ratio of the temporal LTE to the total LTE (i.e., the sum of spatial and temporal LTE) throughout the entire domain, and in both the hysteretic and

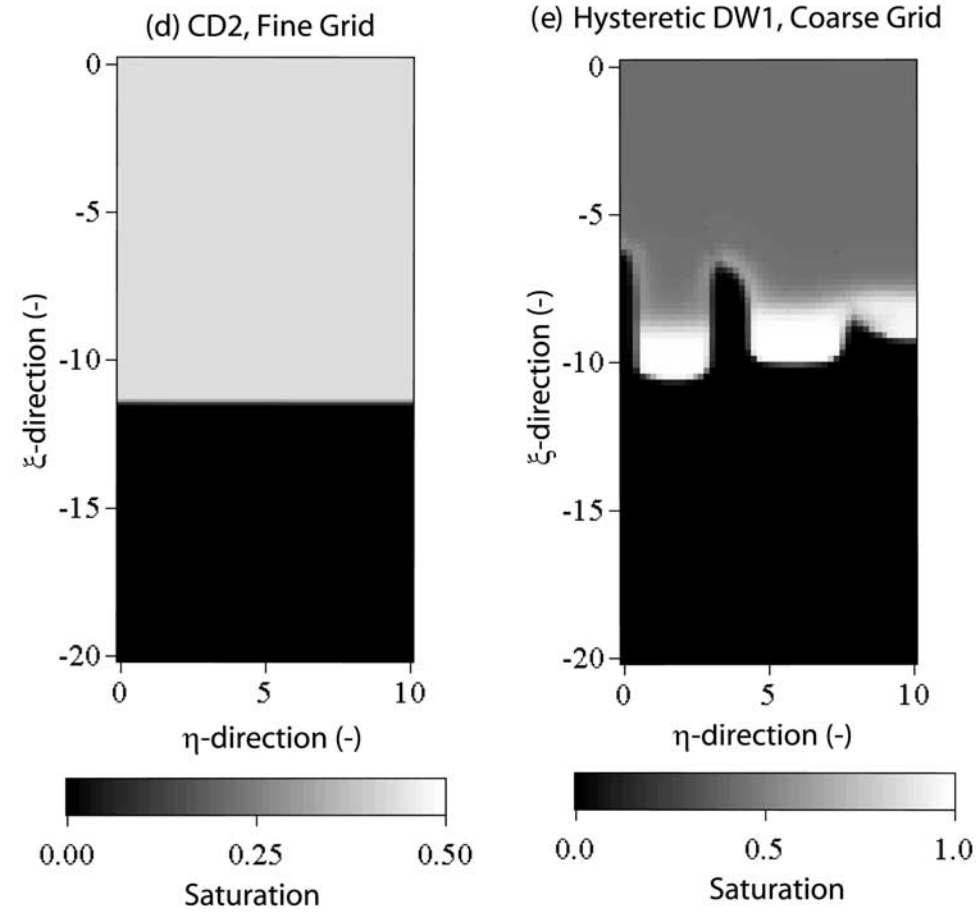

Figure 1. (continued)

nonhysteretic simulations [*Eliassi and Glass*, 2001a, Figure 9], never rises above a maximum of 1.7×10^{-5}.

[11] However, for the moment, let us put aside the fact that temporal LTE was negligible in our simulations. Let us consider whether the temporal LTE could indeed induce an artificial GDF-like response. With a spatial discretization given by CD2, which has reasonably low error, we can write the lowest-order, modified governing equation for constant grid spacing as follows:

$$\Gamma(\Psi)\frac{\partial\Psi}{\partial\tau} - \left\{\frac{\partial}{\partial\eta}\left[\kappa(\Psi)\frac{\partial\Psi}{\partial\eta}\right] + \frac{\partial}{\partial\xi}\left[\kappa(\Psi)\frac{\partial\Psi}{\partial\xi}\right]\right\} - \frac{\partial\kappa(\Psi)}{\partial\xi} = -\Gamma(\Psi)\left(\frac{\Delta\tau}{2}\right)\frac{\partial^2\Psi}{\partial\tau^2} - E_{\mathrm{cap}}(\eta,\xi) - \left(\frac{\Delta\xi^2}{6}\right)\frac{\partial^3\kappa(\Psi)}{\partial\xi^3} \quad (1a)$$

with

$$E_{\mathrm{cap}}(\eta,\xi) = \frac{\Delta\eta^2}{6}\left\{\frac{1}{2}\frac{\partial^2}{\partial\eta^2}\left[\kappa(\Psi)\frac{\partial^2\Psi}{\partial\eta^2}\right] + \frac{\partial}{\partial\eta}\left[\frac{\partial\Psi}{\partial\eta}\frac{\partial^2\kappa(\Psi)}{\partial\eta^2}\right]\right\} + \frac{\Delta\xi^2}{6}\left\{\frac{1}{2}\frac{\partial^2}{\partial\xi^2}\left[\kappa(\Psi)\frac{\partial^2\Psi}{\partial\xi^2}\right] + \frac{\partial}{\partial\xi}\left[\frac{\partial\Psi}{\partial\xi}\frac{\partial^2\kappa(\Psi)}{\partial\xi^2}\right]\right\}. \quad (1b)$$

The left-hand side of equation (1a) represents the standard form of the RE, and the three terms on the right-hand side (RHS) refer to the LTE terms for the temporal, capillary, and gravity components, respectively, where all variables are defined in *Eliassi and Glass* [2001a]. There, we refer to equation (1a) as the modified governing equation, since, depending upon the size of the various terms on the RHS of equation (1a), it is the actual equation that is being solved numerically.

[12] If we assume the spatial grid spacings, $\Delta\eta$ and $\Delta\xi$, are small enough (i.e., the spatial LTE are fairly small), while increasing the time step size, $\Delta\tau$, it is easy to demonstrate that the temporal LTE could indeed begin to dominate the RHS of equation (1a). In fact, the functional form of the temporal LTE is such that it could cause an oversaturation at the WF (i.e., yield the appropriate form of oscillation), which in combination with hysteresis might generate an artificial GDF-like response. However, one must be a bit careful here, since as $\Delta\tau$ increases, the numerical stability criterion may be violated, and the solution may not converge even if time implicit numerical solution methods are used.

[13] As a final point on this matter, BN03 believe that we should have used a higher-order temporal discretization. Given that we found temporal LTE to be negligible compared to spatial LTE, a further reduction in temporal LTE will not eliminate the driving spatial LTE that causes the oscillations at the WF. Instead, in combination with hysteresis, these spatial LTE-induced numerical oscillations create an organized oscillation that is GDF-like with a length scale that is associated with the physics and not the numerics.

This indeed was the reason why solutions of RE + SMP that yielded artificial fingers have been able to masquerade for physically based fingers for so long. Indeed, when the errors become this large, one must recognize that the numerical solution is no longer that of the RE + SMP.

4. The Choice of Reversal Threshold Value in the Hysteresis Relations for Our Problem Is Quite Clear

[14] If under conditions where the governing equation must yield a monotonic solution and if the truncation error that could induce nonmonotonicity is small enough, nowhere in the field will hysteresis be invoked. Since this is what we wish to demonstrate in our paper, we took the smallest possible value for the reversal threshold (just above machine error) so that any numerical artifact would be caught. In this way, if none are found the solution is indeed demonstrated to be monotonic (Figures 1c and 1d) (see also CD2 result of *Eliassi and Glass*, 2001a, Figures 1d and 3b). However, as we point out [*Eliassi and Glass*, 2001a, in the last paragraph of section 2.3 and in section 3.3], when such TE-induced oscillations are present, hysteresis will create an organized oscillation that yields a GDF-like solution. As an aside, we have shown in other work [*Eliassi*, 2001] that the organized oscillation is found over the range $10^{-15} \leq \epsilon_H \leq 10^{-3}$, where ϵ_H is the dimensionless hysteretic threshold. For $\epsilon_H \geq 10^{-2}$, one no longer obtains an organized GDF-like oscillation but rather a peaky oscillation as can be seen in our nonhysteretic simulations for large spatial LTE [see *Eliassi and Glass*, 2001a, Figures 5 and 6].

[15] As a final point on this matter, BN03 make their own suggestion for a way to calculate the reversal threshold based on their linear analysis of the temporal LTE that applies only away from the WF. Their arguments lead to the result that "the essential length scales of the finger need to be considered" [*Braddock and Norbury*, 2003]. Of course, as we have argued above, choice of the reversal criterion is problem-specific, and we are uncertain as to the exact problem that they are really addressing. However, we encourage BN03 to continue in this direction but hope that they implement their scheme within the context of a governing equation that incorporates physics beyond that embodied within RE + SMP.

5. Summary

[16] We concluded [*Eliassi and Glass*, 2001a] that the RE + SMP cannot support a nonmonotonic flow response for conditions where GDF has been experimentally observed. Since such physical nonmonotonicity is an essential characteristic of GDF, standard unsaturated flow theory (i.e., either the flux law and/or SMP) is insufficient to describe all aspects of unsaturated flow physics at least for infiltration in initially dry, highly nonlinear, and hysteretic media where GDF occurs. Recently, we have considered the extension of the RE to include the experimentally observed holdback-pileup (HBPU) effect [*Eliassi and Glass*, 2001b, 2002]. By postulating the HBPU effect as physically tied to WF sharpness the HBPU can be mathematically formulated in a variety of ways to include hypodiffusive, hyperbolic, and mixed spatial-temporal forms. For each an extended flux relation comprised of the Darcy-Buckingham flux plus an additional component due to the HBPU effect can be inferred. While parallels for each extended flux relation can also be found in the multiphase literature, it remains to be seen whether such porous continuum-scale models can be applied such as to increase our basic understanding of the GDF process. We do know, however, that GDF can be easily simulated using noncontinuum approaches based on modified invasion percolation (MIP) [*Glass and Yarrington*, 1989, 1996] including the underlying nonmonotonicity [*Glass and Yarrington*, 2001, 2003]. Because MIP approaches represent the physics of phase displacement at the pore scale with a set of fundamental, mechanistic, physical rules, they may provide a better context in which to increase our understanding of GDF.

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