

NONLINEAR SOLVER BASED ON FLUX-FUNCTION TRUST-REGIONS FOR ACCURATE MODELING OF CO2 PLUME MIGRATION IN AQUIFERS

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Summary. We describe a Newton-based nonlinear solver for immiscible two-phase transport in the presence of significant viscous, buoyancy, and capillary forces. The evolution of CO2 plumes in heterogeneous saline aquifers, especially during the post-injection period, is an important example of this class of problem. The flux (fractional flow) function, which is strongly nonlinear function of saturation, is divided into trust regions. The delineation of the regions is dictated by the unit-flux point and inflection points in the flux function. Within each trust region, the standard Newton iterative scheme is guaranteed to converge. For problems where the dynamics are dominated by buoyancy and capillary forces, the proposed scheme allows for taking much larger time steps than existing Newton based solvers. The nonlinear solver is demonstrated using challenging problems dominated by buoyancy and capillary forces in heterogeneous domains with emphasis on the CO2 post-injection period.

1 INTRODUCTION

The transport problem in porous media is usually described by nonlinear hyperbolic conservation laws. To solve the governing mass conservation equations, explicit time integration schemes often lead to severe restriction on the time step size. In theory, implicit time integration allows for taking arbitrarily large time steps. In the fully implicit method, a Newton-based strategy is used, whereby a sequence of iterations, each involving the construction of the Jacobian matrix and solution of the resulting linear system, is performed until the solution is obtained for the target time step. While the implicit scheme is unconditionally stable, there is no guarantee that the nonlinear solver will converge for the a-priori chosen timestep [1]. In reservoir simulation, this problem is usually overcome by time step cuts based on heuristics. The heuristics are usually guided by experience with a certain sub-class of problem. The use of such heuristics often leads to time step sizes that are either too conservative resulting in unacceptably large computational time or too large, such that timestep cuts occur too often during a simulation run. [2].

To improve the convergence behavior of the Newton method, solution chopping (or damping) techniques have been developed ([3]). Such strategies select a scaling factor on a cell-by-cell basis using physical arguments to limit the overshoot of local Newton updates. Recently, Jenny et al. [4] proposed a modified Newton method for hyperbolic conservation laws in the absence of gravity and capillarity. In [4], it is observed that the nonlinearity of the residual for the transport problem (saturation equation) is dictated by the structure of the flux function (fractional flow curve). For viscous dominated multiphase flow in porous media, the nonlinear flux function (normalized phase flux vs. saturation) is usually S-shaped. That is, it has an inflection point. Since the nonlinearity in the residual equation is dominated by the nonlinearity of the flux function, if the solution (saturation) resides on one side of the inflection point on the flux function, it is hard for the Newton method to converge if the initial guess is on the other side. So, if the Newton update would cross the inflection point, it is scaled back to the saturation value at the inflection point. Combined with phase-based potential ordering (Kwok and Tchelepi, 2007 [5]), Jenny et al.'s modification results in a convergent method for arbitrarily large time step sizes, and that allows one to choose the time step size based on accuracy considerations only.

Things get quite complicated when the buoyancy and/or capillary force are significant. Note that when buoyancy forces are significant, it is possible for each phase to have a different flow direction. This is known as countercurrent flow. Capillarity is treated as a nonlinear diffusion term that has a significant impact on the nonlinear character of the residual equation.

In this work, we propose a nonlinear solver based on flux-function trust-regions for accurate modeling of nonlinear immiscible two-phase transport in porous media. The mathematical model for two-phase flow in porous media is introduced in section 2. In section 3, an unconditionally convergent nonlinear solver for one-dimensional transport that is rigorous and efficient across the entire viscous-gravity-capillary parameter space is described. Numerical examples are presented in section 4. Finally, in section 5 we present our conclusions.

2 MATHEMATICAL MODEL

We consider the transport problem for immiscible, two-phase (wetting and non-wetting) in porous media. For a 1D domain, assuming that the total velocity, u_t , is constant, the transport equation can be written as

$$\phi \frac{\partial S_w}{\partial t} + u_t \frac{\partial F_w}{\partial x} = 0. \quad (1)$$

where S_w is the wetting-phase saturation and ϕ is the porosity. Here, $F_w = \frac{u_w}{u_t}$ is the flux (fractional flow) for the wetting phase. It is defined as

$$F_w = \frac{\lambda_w}{\lambda_t} - kg \frac{\lambda_w \lambda_n}{\lambda_t} (\rho_w - \rho_n) \frac{\nabla h}{u_t} + k \frac{\lambda_w \lambda_n}{\lambda_t} \frac{\nabla p_c}{u_t}, \quad (2)$$

where $\lambda_\alpha = \frac{k_{r\alpha}}{\mu_\alpha}$ is mobility of phase α , $p_c = p_c(S_w)$ is the capillary-pressure versus saturation relationship, and the total mobility $\lambda_t = \lambda_w + \lambda_n$. We introduce two dimensionless quantities:

$$N_g = \frac{k(\rho_w - \rho_n)g\nabla h}{\mu_n u_t}, \quad (3)$$

and

$$P_e = \frac{u_t \mu_n L}{k \bar{p}_c}, \quad (4)$$

where L is the characteristic length of the domain and \bar{p}_c is a characteristic capillary pressure. N_g is the gravity number, which is the ratio of buoyancy to viscous forces, and P_e is the Peclet number, which is the ratio of the viscous to capillary effects. With these definitions, the expression of F_w can be written as

$$F_w = \frac{\lambda_w}{\lambda_t} - \frac{k_{rn}\lambda_w}{\lambda_t} N_g + \frac{\lambda_w k_{rn}}{\lambda_t} \frac{\nabla p_c}{\bar{p}_c/L} \frac{1}{P_e}, \quad (5)$$

in which the three terms on the right-hand side account for the viscous, buoyancy, and capillary fluxes, respectively. We denote the flux that accounts for both the viscous and buoyancy forces as

$$f_w = \frac{\lambda_w}{\lambda_t} - \frac{k_{rn}\lambda_w}{\lambda_t} N_g. \quad (6)$$

Since the total velocity is assumed constant, we can make the transport equation dimensionless by defining $t_D = \frac{tu_t}{\phi L}$ and $x_D = \frac{x}{L}$. Then the 1D dimensionless transport equation is

$$\frac{\partial S_w}{\partial t_D} + \frac{\partial F_w}{\partial x_D} = 0. \quad (7)$$

From here on, we drop the subscripts, so we can write the equation in a more concise form:

$$\frac{\partial S}{\partial t} + \frac{\partial F}{\partial x} = 0. \quad (8)$$

3 NONLINEAR SOLVER FOR 1D TRANSPORT

In the absence of gravity and capillarity, $F = \frac{\lambda_w}{\lambda_t}$. For multiphase flow in porous media, the flux function, $F = F(S)$ in Eqn. 8, is usually S-shaped (not uniformly convex or concave). An S-shaped flux function is shown in Fig. 1(a). F is a monotonic function of saturation. The inflection point (represented by red dots in Fig. 1(a)) is where the convexity of the flux function changes. The presence of gravity or capillarity changes the shape as well as the monotonicity of the flux function. Fig. 1(b) shows a typical example of the flux function with strong buoyancy, i.e. $N_g = -5$. In this case, F is not a monotonic function of saturation. In fact, there are two inflection points (red dots in Fig. 1(b)), a sonic point (green dot) and a unit-flux point (yellow dot). The sonic point is where flux function is maximum; unit-flux point is where the flux function equals to

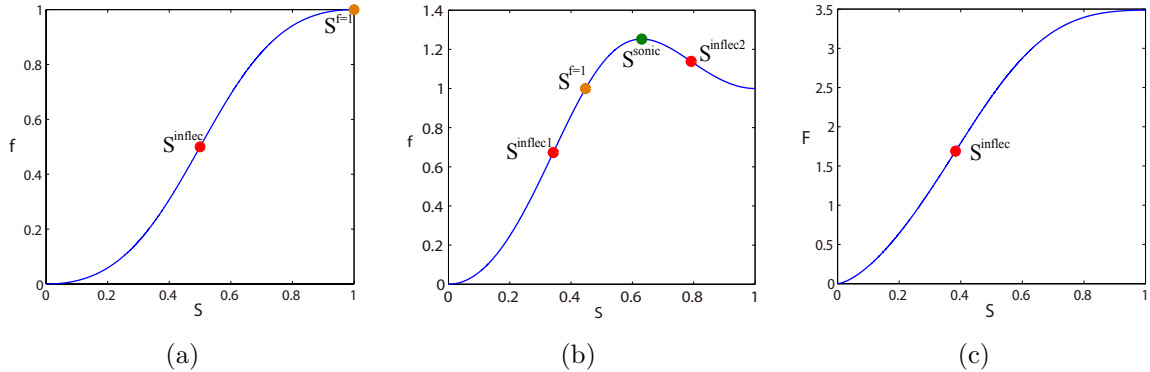


Figure 1: flux functions: (a) Viscous flux ($M^0 = 1$, $N_g = 0$, $P_e = \infty$); (b) Viscous and buoyancy flux ($M^0 = 1$, $N_g = -5$, $P_e = \infty$); (c) Viscous and capillary flux ($M^0 = 1$, $N_g = 0$, $P_e = 0.2$). Red dots represent inflection points; yellow dots are unit-flux points; and green dots are sonic points.

one at a point $S \leq 1$. On the other hand, Fig. 1(c) shows that the presence of strong capillary forces ($P_e = 0.2$) changes the shape, as well as, the inflection point of the flux function. We divide the flux function into trust regions. The delineation of the regions is dictated by the inflection and unit-flux points in the flux function. Within each trust region, the standard Newton iterative scheme is guaranteed to converge.

We now describe a nonlinear solution strategy based on saturation trust regions for problems with viscous, buoyancy and capillary forces. The proposed solver performs chopping based on trust regions in the flux function. Specifically, we apply chopping on iterative updates at the unit-flux point of flux function f (Eq. 6), where f includes the viscous and gravitational forces, and inflection points of flux function F (Eq. 5), where F includes viscous, gravitational, and capillary forces. The algorithm is summarized in Fig. 2.

4 NUMERICAL EXAMPLES

The modified Newton method is demonstrated using several examples. For all the test cases, we compare the results with the standard Newton method.

4.1 Single cell problems: convergence map

We start with a single-cell problem. Nonlinear analysis of a single-cell transport problem reveals some fundamental conclusions that are valid for multiple cells and even large-scale simulation. Consider the single-cell problem under strong buoyancy ($N_g = -5$) and strong capillarity ($P_e = 0.2$). The right boundary condition is fixed as $S_R = 1$. The target is to find the solution S^{n+1} of the nonlinear transport problem (Eqn. 8). We investigate the convergence behavior for arbitrary combinations of the left boundary condition (S_L) and the initial guess ($S^{n+1,0}$), if the root of the residual equation is found by Newton's method as the number of iterations, $\nu \rightarrow \infty$, for all possible starting points $S^{n+1,0} \in (0, 1)$.

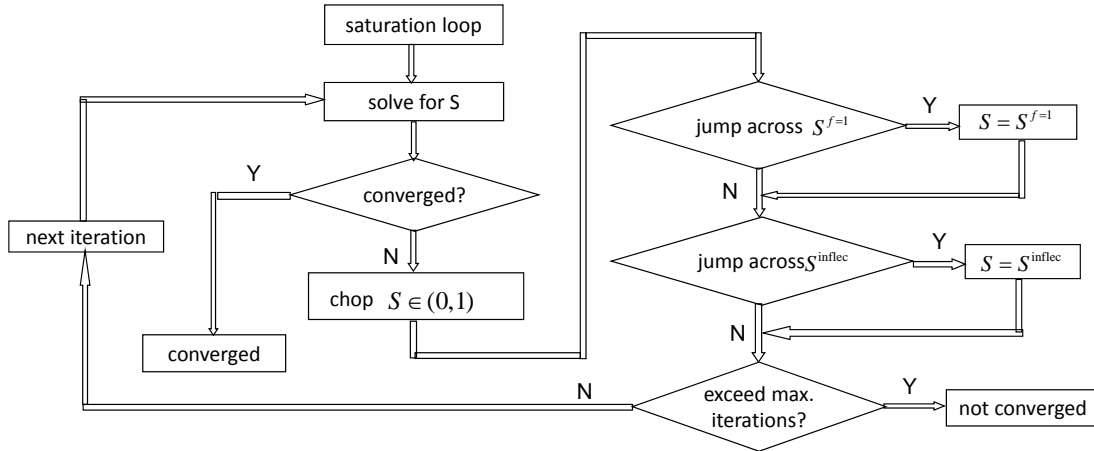


Figure 2: The flow chart of the modified Newton scheme, which accommodate the coupling of viscous, gravitational and capillary forces, for one time step.

The convergence maps of the standard and modified Newton schemes are shown in Figs. 3 and Fig. 4, respectively. The colors in Fig. 3 and 4 depict the number of iterations required until the convergence criteria $|S^{n+1,\nu+1} - S^{n+1,\nu}| < 10^{-5}$ and $|R| < 10^{-4}$ are satisfied. Specifically, dark blue means fast convergence (1 iteration) and dark red means slow convergence (15 iterations); the white region in the phase space $S^{n+1,0} - S^L$ indicates that no convergence is achieved after 200 iterations. Fig. 3 shows that for very small time steps ($c = 0.1$), the standard Newton scheme is convergent, i.e., the convergence map contains no white regions. However, the size of the non-convergence (white) area increases rapidly as the time step size increases ($c = \{1, 10, 100\}$). Fig. 4 shows that the modified Newton scheme is convergent for all the time step sizes, i.e., there is no white region for any time step size.

4.2 Multiple cells problems: 1D domain

Now, we study a 1D nonlinear transport problem. We study the savings in computational cost by using this modified Newton method if convergence is the only criterion and accuracy is not the main concern. We study 1D transport using 80 cells (control-volumes) in the presence of viscous, buoyancy, and capillary forces. We set $N_g = -5$ and $P_e = 0.2$. The initial condition is $S = 0.8$ in the left-half of the domain, and $S = 0.0$ in the right-half of the domain (Fig. 5(b)). The boundary conditions are $S_L = 1.0$ and $S_R = 0.0$. Note that in this case, the capillary model is heterogeneous, with the two capillary curves shown in Fig. 5(a) used for the left and right sub-domain, respectively.

The solutions using the modified Newton scheme are shown in Fig. 5(c). Despite the numerical diffusion due to time truncation errors, the solution with Δt of 500 PVI is quite close to that with Δt of 0.1 PVI. Note that there is a kink in the saturation solution,

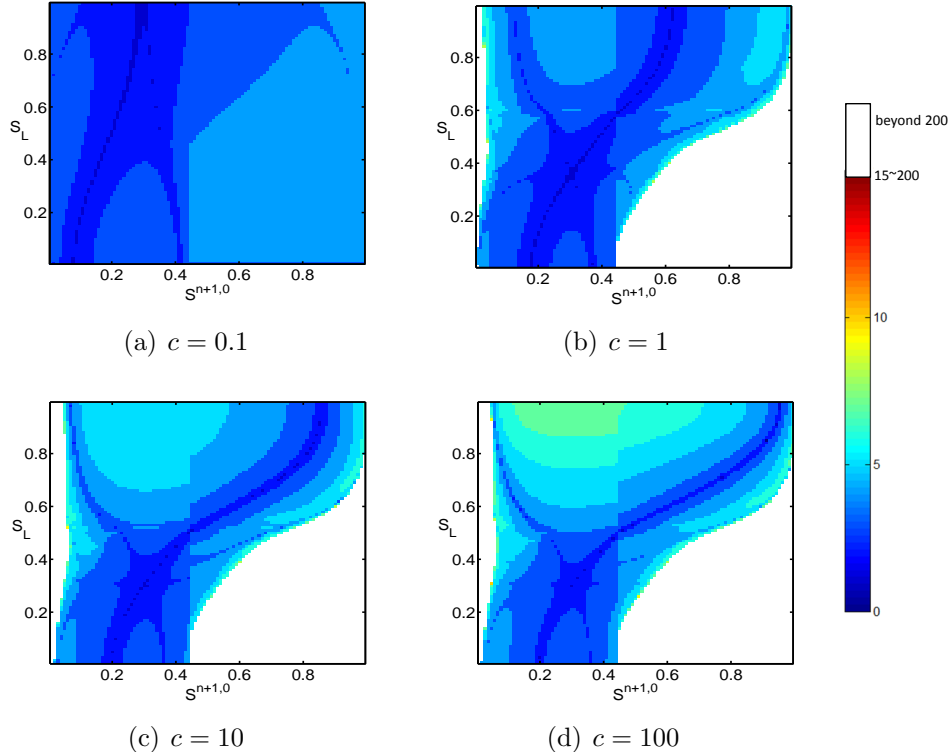


Figure 3: Standard Newton scheme: convergence map for single-cell incompressible viscous, gravitational and capillary flux: (a) $c = 0.1$; (b) $c = 1$; (c) $c = 10$; (d) $c = 100$. $c = \frac{\Delta t}{\Delta x}$. $M^0 = 1$, $N_g = -5$, and $P_e = 0.2$.

which results from the discontinuity in the capillary model. Fig. 6(a) shows that the standard Newton scheme is convergent only for small time steps, i.e. $\Delta t \in \{0.1, 1\}$ or $CFL < 10$, while the modified scheme converges for any time step (up to $\Delta t = 500$ or $CFL \approx 3491$). We compare the number of total iterations in Fig. 6(b), which shows a saving in computational effort of more than one order of magnitude using the modified Newton scheme.

5 CONCLUSIONS

We developed a new nonlinear solver for immiscible two-phase flow where viscous, buoyancy, and capillary forces are significant. The modified Newton solver employs trust-regions of the flux function to guide the Newton iterations and solution updating. This development is a significant generalization of the inflection-point approach of Jenny et al. ([4]), which was proposed for viscous dominated transport. Convergence maps for single-cell problems, which cover the full range of the parameter space of viscous, gravity and capillary forces, demonstrated unconditionally convergence. That is, for a given choice of timestep size, the unique saturation solution is found independently of the initial guess.

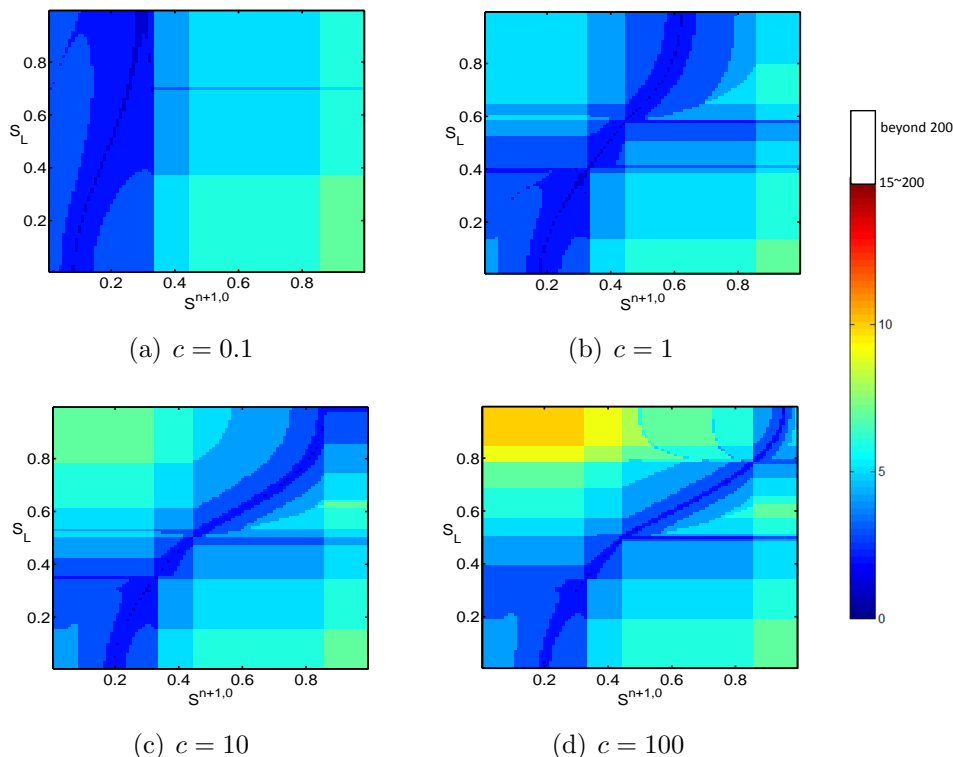


Figure 4: Modified Newton scheme: convergence map for single-cell incompressible viscous, gravitational and capillary flux: (a) $c = 0.1$; (b) $c = 1$; (c) $c = 10$; (d) $c = 100$. $c = \frac{\Delta t}{\Delta x}$. $M^0 = 1$, $N_g = -5$, and $P_e = 0.2$.

In addition, a 1D nonlinear transport problem, which is dominated by buoyancy and capillarity, was studied. It was shown that the modified Newton solver overcomes the often severe limits on time step size associated with existing Newton-based nonlinear solvers.

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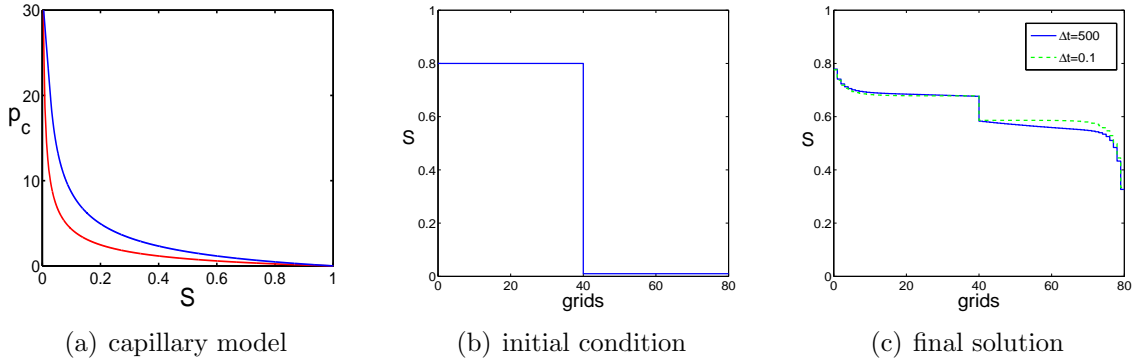


Figure 5: Numerical results with modified Newton scheme: (a) capillary models; (b) initial condition; (c) final solution with $\Delta t = 0.1$ and with $\Delta t = 500$ ($CFL \approx 3491$). $M^0 = 1$, $N_g = -5$ and $P_e = 0.2$.

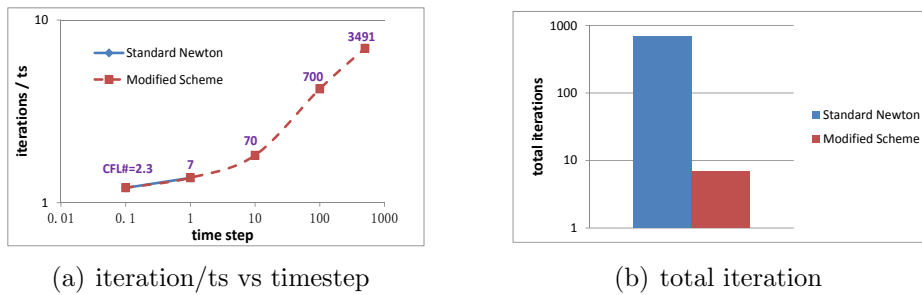


Figure 6: Performance comparison between standard and modified Newton schemes: (a) iterations vs. timestep (with CFL numbers marked on the data); (b) total iterations ($\Delta t = 1$ for standard Newton and $\Delta t = 500$ for modified scheme). $M^0 = 1$, $N_g = -5$ and $P_e = 0.2$.

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