An experimenting field approach for the numerical solution of multiphase flow in porous media

Amgad Salama^{1,*}, Shuyu Sun¹, and Kai Bao²

¹Computational Transport Phenomena Laboratory (CTPL), Division of Physical Sciences and Engineering (PSE), King Abdullah University of Science and Technology (KAUST), Thuwal 23955-6900, KSA

²SINTEF, Department of Applied Mathematics, Forskningsveien 1, 0373, Oslo, Norway

(*Corresponding author: Tel: +966 8080423, E-mail address: amgad.salama@kaust.edu.sa)

Abstract

In this work we apply the experimenting pressure field technique to the problem of the flow of two or more immiscible phases in porous media. In this technique a set of predefined pressure fields are introduced to the governing partial differential equations. This implies that the velocity vector field and the divergence at each cell of the solution mesh can be determined. However, since none of these fields is the true pressure field entailed by the boundary conditions and/or the source terms, the divergence at each cell will not be the correct one. Rather the residue which is the difference between the true divergence and the calculated one is obtained. These fields are designed such that these residuals are used to construct the matrix of coefficients of the pressure equation and the right hand side. The experimenting pressure fields are generated in the solver routine and are fed to the different routines, which may be called physics routines, which return to the solver the elements of the matrix of coefficients. Therefore, this methodology separates the solver routines from the physics routines and therefore results in simpler, easy to construct, maintain and update algorithms.

Key words

Numerical algorithms, multiphase flow in porous media, experimenting pressure field approach, LNAPL and DNAPL transport.

Introduction

The continuum hypothesis as applied to porous media furnishes a suitable framework in which transport phenomena in porous media may be described, Salama and Van Geel (2008-a,b). Under this framework macroscopic field variables are continuous functions of space and time. Such upscaled description allowed the governing laws to be described in the form of partial differential equations. The solution of the governing equations is usually obtained numerically. However, several aspects are unique to the numerical solution of transport phenomena in porous media. Probably, the most important is the fact that, porous media application spans quite large number of scales starting from small scale applications in confined spaces (porous filters, bed reactors, etc.) to large scale applications that could span length scales of kilometers such as groundwater reservoirs, oil and gas fields, etc. Furthermore, porous media are generally highly heterogeneous even at the continuum scale and could also possess directional properties (i.e., anisotropy). The problem could even get more complicated by the fact that many porous media applications involve the flow and transport of multiphase systems. These pose tremendous challenges to numerical schemes and a search for a robust one has never reached a conclusion. Although there have been several attempts to speed up numerical algorithms, they abide to methods to enhance linear equations solvers and iterative schemes. As for the algorithms themselves they are to a large extent standard based on the numerical scheme (finite differences, finite elements, etc.), Blessent et al. (2009). With the advent of high level computer languages (Matlab, Python, etc.) with its inefficient looping techniques, the efforts have been devoted to vectoring the calculations to eliminate loops and to speed up computations, Sun et al. (2012-a), and Salama et al. (2013-a). While, this has significantly enhanced the speed of calculations they remain specific to those languages which require repeating interpretations.

On the other hand, one of the most important and favorable aspect of any numerical scheme is that it should follow the physics of the problem with minimum manipulation of the governing equations. This ensures generating schemes which are maintainable, easy to adopt, update and modify. Unfortunately, many of the numerical schemes depend on manipulating the governing set of equations into reduced forms that are easy to solve. Although this trend is feasible, it often generates equations that are large in size (many terms are involved) and probably higher order expressions are used. Numerical investigation of these reduced equations requires dealing with many terms, which would lead to expressions that are often large, difficult to track and debug. Furthermore, the numerical scheme is often specific to each particular problem. Although there are a number of numerical schemes that simulate the governing equations as they appear (e.g., mixed finite element and its variants), they, apart from their complex formulations, often produce a global system that is usually large (the unknown vector includes both the pressure and velocity). Apparently, for time dependent problems, this larger global system would significantly increase CPU time. Recently, Sun et al. (2012-b) introduced a new methodology in which no to minimal manipulations of the governing equations is required. The benefit of this scheme, apparently, is that the expressions of the discretized governing equations are simpler, easy to adopt, manipulate, maintain and update. In this work, we generalize this technique for single phase flow by adding the effect of velocity boundary conditions. We then apply this method to the more involved problem of multi-phase flow in porous media including light non-aqueous phase liquid (LNAPL) and dense non-aqueous phase liquid (DNAPL) transport. Carbon dioxide sequestration in deep aquifers in supercritical state is investigated as an example of LNAPL, while tetrachloromethane is considered as an example of DNAPL transport.

Single-phase flow

Consider a porous medium domain, Ω bounded by the boundary, Γ , the governing equations describing the flow in this system may be given as:

$$\mathbf{u} = -K\nabla p \quad \text{in } \Omega \quad (1)$$

$$\nabla \cdot \mathbf{u} = q \quad \text{in } \Omega \quad (2)$$

$$p = p^B \quad \text{on } \Gamma_D \quad (3)$$

$$\mathbf{u} \cdot \mathbf{n} = u^B \quad \text{on } \Gamma_N \quad (4)$$

where $\mathbf{u}$ is the velocity, K is the hydraulic conductivity, p is the pressure, p^B and u^B are the pressure and velocity at the boundary, respectively. The traditional numerical solution methodology for this problem is to substitute eq. 1 into eq. 2 to obtain an equation only in the pressure, such that

$$\nabla \cdot (-K\nabla p) = q \quad \text{in } \Omega \quad (5)$$

Applying any numerical scheme on this equation results in a system of algebraic equations which can be written in a matrix form as:

$$Ap = b \quad (6)$$

Solving this system along with the boundary conditions, which are implemented in b , results in the pressure field to be obtained from which the velocity field is obtained using eq. 1. This methodology seems to be simple and straight forward. However, a number of remarks worth investigation: the first is the need to do this extra manipulation of the governing equations to have an equation in only one variable. Although, this may be trivial for this system, for other systems (e.g., multiphase flows) it may be quite involved, as will be apparent later. The second point is that no direct use of eqs. 1 and 2 to obtain the pressure field numerically have been implemented. Only as a post processing to obtain the velocity field, that eq. 1 is used. Therefore, it is clear that the solution methodology does not follow the physics, which suggests that given the pressure, one can

find the velocity and given the velocity, one can find the divergence. Furthermore, the difference expression (in the sense of finite differences method) of eq. 10 can be long, particularly for complex stencils. It is therefore beneficial to separate the physics from the solver as is suggested in this new methodology.

The experimenting pressure field approach

In this section, the essence of the experimenting field approach is highlighted by considering how it is applied to single phase flow problem in porous media. We include the effect of velocity boundary condition and show several aspects related to this method including comparisons between the time to solving the linear system of equation and that taken to constructing the matrix of coefficients. Without loss of generality, we consider the cell-centered finite differences approximation (which is a control volume method over Cartesian grid) of the governing equations. We define a simple 2D problem in a rectangular porous medium domain, $\Omega: (a_1, b_1) \times (a_2, b_2)$, saturated with a fluid that moves as a result of pressure gradient. The approximation is thought over the rectangular mesh defined by $\{x_0, x_1, x_2, \dots, x_i, \dots, x_m\} \times \{y_0, y_1, y_2, \dots, y_j, \dots, y_n\}$. In this set up, the pressure is defined at the center of the cells and the velocity at the center of the edges. As indicated earlier, the numerical solution of eq. 5 produces a set of algebraic equations of the form:

$$\sum_{j=1}^{mn} a_{ij} p_j = q_i \pm c_{\hat{i}} p_{\hat{i}}^B \pm c_{\tilde{i}} u_{\tilde{i}}^B, \quad i = 1, 2, \dots, mn, \quad \hat{i} + \tilde{i} = 1, 2, \dots, 2(m+n) \quad (7)$$

where m and n are the number of segments in x and y -directions respectively, and the indices $\hat{i}$ and $\tilde{i}$ runs over the boundary. That is, when i and j represent boundary cells, the terms $c_{\hat{i}} p_{\hat{i}}^B$ and $c_{\tilde{i}} u_{\tilde{i}}^B$ are nonzero and are zero otherwise. These terms represent the prescribed Dirichlit and Neumann boundary conditions. This system of equations can be written in matrix form as given in eq. 6

this technique it is used to determine the coefficients of the global matrix. In other words if the residue vector is known, one can easily determine all the coefficients of the first column of the global matrix such that

$$a_{11} = res_1 \quad (10)$$

$$a_{21} = res_2, \quad (11)$$

$$\vdots$$

$$a_{mn1} = res_{mn} \quad (12)$$

On the other hand, when the experimenting pressure field is all zeros, the residue calculates the contribution of the boundary conditions. To obtain the residue vector we define the vector function $\mathbf{f}(\mathbf{p}) : \Re^{mn} \rightarrow \Re^{mn}$ such that,

$$\mathbf{f}(\mathbf{p}) = \sum_{j=1}^{mn} a_{ij} p_j \pm c_i p_i^B \pm c_{\bar{i}} u_{\bar{i}}^B \pm q_i, \quad i = 1, 2, \dots, mn \quad (13)$$

If $\mathbf{p}$ is the true pressure field the above function produces the zero vector and if it is not the correct pressure field this function, generally, produces a nonzero vector which we call the residue, $\mathbf{R}$, which may be given as,

$$\mathbf{R} = \nabla \cdot \mathbf{u} - \mathbf{q} \quad (14)$$

where $\nabla \cdot \mathbf{u}$ is the divergence for all the cells given the pressure field, $\mathbf{p}$. In other words for any pressure field, we use Eqs. 1 to obtain the velocity components at the mid cell faces which may be used to calculate the divergence for each cell using Eq. 2. The residual is then calculated from Eq. (14). From Eq. 13, we have,

$$\mathbf{f}(\mathbf{p}) - \mathbf{R} = (\mathbf{0}) \quad (15)$$

or,

$$\sum_{j=1}^{mn} a_{ij} p_j + c_i p_i^B + c_i u_i^B + q_i - R_i = 0, \quad i = 1, 2, \dots, mn \quad (16)$$

Using 14, one obtains

$$\sum_{j=1}^{mn} a_{ij} p_j + c_i p_i^B + c_i u_i^B = (\nabla \cdot \mathbf{u})_i, \quad i = 1, 2, \dots, mn \quad (17)$$

Eq. (17) is valid for any pressure field. Writing Eq. (17) in the form,

$$\sum_{j=1}^{mn} a_{ij} p_j = (\nabla \cdot \mathbf{u})_i - c_i p_i^B - c_i u_i^B, \quad i = 1, 2, \dots, mn \quad (18)$$

Let

$$\mathbf{p}^0 = \mathbf{0}, \text{ or } \mathbf{p}^0 = [0 \ 0 \ \dots \ 0 \ \dots \ 0]_{mn}^T \quad (19)$$

We call this the zeros pressure field which is zero everywhere in Ω . Eq. (18) becomes,

$$c_i p_i^B + c_i u_i^B = (\nabla \cdot \mathbf{u})_i^{\mathbf{p}^0}, \quad i = 1, 2, \dots, mn \quad (20)$$

This produces a vector which is zero except when i represents boundary cells. That is eq 20 determines the contribution of the boundary conditions to the right hand side of eq. 6. Eq. 18, therefore, can be written as

$$\sum_{j=1}^{mn} a_{ij} p_j = (\nabla \cdot \mathbf{u})_i - (\nabla \cdot \mathbf{u})_i^{\mathbf{p}^0} \quad (21)$$

On the other hand, for the pressure field,

$$\mathbf{p}^{\check{j}} = [0 \ 0 \ \dots \ 1 \ \dots \ 0]_{mn}^T, \quad \check{j} = 1, 2, \dots, mn \quad (22)$$

where $\mathbf{p}^{\check{j}}$ is the $\check{j}$ -pressure field which is zero everywhere in Ω except at cell $\check{j}$ which is one.

We, therefore, have

$$a_{i\check{j}} = (\nabla \cdot \mathbf{u})_i^{\mathbf{p}^{\check{j}}} - (\nabla \cdot \mathbf{u})_i^{\mathbf{p}^0}, \quad i = 1, 2, \dots, mn \quad (23)$$

This implies that an $m \times n$ experimenting pressure fields are required in order to construct the matrix

176 of coefficients. The experimenting pressure fields are such that they are one at cell center of interest
177 and zero elsewhere as shown in Fig. 1. It is apparent from this figure that the velocity at the mid-
178 edges of the cell where the pressure is one will only be nonzero. Furthermore the divergence of
179 the four cells surrounding the cell where the pressure is one together with this cell will also be
180 nonzero. All the other cells will not get affected by this pressure field. As will be indicated later,
181 this behavior may be used to speed up the time to construct the matrix of coefficients. From this
182 equation one may be able to construct the coefficient matrix, A , and to obtain the pressure and
183 velocity fields. A flow chart diagram showing the features of this approach is shown in Fig. 2
184 below. It is noteworthy that this approach can work equally well with any numerical scheme in
185 which the local problem is described including control volume, finite element (and its variants,
186 e.g., mixed methods), etc. In mixed finite element (based on RT or BDM spaces), in particular,
187 where both the pressure and velocity fields are solved for simultaneously, the experimenting fields
188 in this case are not only for the pressure but also for the velocity. To sum up, in traditional schemes
189 such local problems are not solved, rather they are used to construct the global system manually.
190 In the experimenting field approach, the local problems are solved to obtain automatically the
191 global system, Salama et. al. (2013-b, 2015). It may seem that constructing the global system
192 manually may not be that difficult which is true for simple lower order systems. In more complex
193 systems involving complicated stencils it can be quite challenging, Salama et. al. (2014). There
194 are two bottle-neck problems worth mentioning in the execution of this approach. The first is
195 common to all numerical schemes and is related to the solution of the matrix equations for which
196 the sparse solvers are the best choice. The second is particular to this methodology and is related
197 to the construction of the matrix of coefficients, A . That is, as indicated earlier, $mn+1$
198 experimenting pressure fields are required to construct the matrix of coefficients and the right hand

199 side vector of the global system, Eq. 9. This problem is even more pronounced if the matrix of
200 coefficients is routinely updated (e.g., in time-dependent problems). However, careful
201 investigation reveals that this could be significantly minimized given the sparsity and the pattern
202 of the coefficient matrix. In other words, for the interior cells, for example, the pressure at the
203 center of a cell affects only the four adjacent cells and therefore only these cells are considered in
204 the calculations of the velocity, the divergence, etc. Based on this idea, the $mn+1$ experimenting
205 pressure fields could shrink to only 10 non-overlapping fields in 2D problems or 28 fields in 3D.
206 This, clearly, offers substantial reduction in the time required to construct the linear system. Figure
207 3 shows schematic of one of the experimenting nine pressure fields for the given mesh. It is also
208 noteworthy that such experimenting field could also be generated for velocity as well and this
209 facilitates solving even more complex problems (e.g., Navier-Stokes). Figure 4 shows schematic
210 of one of the experimenting velocity fields in the x-direction. To compare the time taken to
211 construct the matrix of coefficients with the time taken to solve the linear system, a single phase
212 flow problem has been investigated. The problem defines a square domain of size 50x50 m with
213 the top and bottom boundaries are assigned no flow, the right boundary is pressure boundary
214 condition and, at the left boundary, the flow is allowed at a central window with the rest of the
215 boundary is no flow. The system of equations has been solved using an efficient direct linear solver
216 based on sparse LU factorization, (UMFPACK, Davis 2004) and the simulation has been
217 conducted on a laptop running Mac operating system. Figure 5 shows the pressure contours and
218 velocity vector field of half of the domain. Figure 6 shows a comparison between the times taken
219 to construct the matrix of coefficients with that taken to solve the linear system for different mesh
220 resolutions. It is clear that when the mesh resolution is small, both times are small and are
221 comparable. As the mesh resolution increases, the time to solve the system of equations largely

dominates the execution time. Figure 7 shows the ratio of the time taken to construct the matrix of coefficients with the time taken to solve the linear system of equations for different mesh resolutions. It is again clear that when the mesh is coarse both times are comparable and as the mesh resolution becomes dense the time to solving the linear system dominates. This implies that the time required to automatically constructing the matrix of coefficients only constitute a negligible part of the total execution time of the system.

Application to multiphase flows

For the sake of illustration and to make the discussion simpler without loss of generality, we consider the case of two-phase, immiscible flows in porous media. This has large number of applications including LNAPL (light non-aqueous phase liquids) and DNAPL (dense non-aqueous phase liquids) migration in the subsurface. Generally, both of LNAPLs and DNAPLs are slightly soluble in water and can, therefore, exist in the subsurface as a separate fluid phase immiscible with both water and air. These materials are considered contaminants if they get introduced to groundwater and hence, have been the subject for intensive research and mathematical modeling to highlight their behavior in the subsurface, (e.g., Mercer and Cohen 1990, Hunt et al. 1991, Ahmadi and Quintard 1996, Ataie-Ashtiani et al. 2003, Reynolds and Kuepe 2002, Monteagudo and Firoozabadi 2004, Hoteit and A. Firoozabadi 2006, 2008, to list but a few). LNAPL is characterized by the fact that its density is smaller than the hosting fluid. This initiates an upward buoyancy-driven movement if injected at the bottom of a subsurface water body. Several research work have considered the migration of LNAPL in the subsurface including Blunt et al (1993), Van Geel and Sykes (1994-a,b), Chen et al. (2004), Jessen et al. (2005), Hayek et al. (2009), Celia and Nordbotten (2009), Haest et al. (2010), Zhou et al. (2010), Salama et al. (2012), Negara et al. (2015), to list but a few. In this work, we consider as an example of LNAPL, the injection of

supercritical CO₂ into deep aquifer. At these conditions the compressibility of CO₂ is comparatively small and therefore CO₂ can be treated as an incompressible fluid, (a typical value of supercritical CO₂ compressibility at depths similar to those suggested for CO₂ sequestration is on the order of 10⁻⁹ Pa⁻¹, Law and Bachu 1996, Span and Wagner 1996) On the other hand, DNAPLs are fluids which are denser than the water and are slightly soluble in it. Common types of DNAPLs include a variety of chlorinated solvents such as trichloroethene (TCE) and tetrachloroethene (PCE), etc. Unlike LNAPLs such as petrol and heating oil, DNAPLs have the ability to migrate downward to significant depths below the water table, Sterling et al. (2005). The governing equations for the flow of two-phase, immiscible and incompressible phases in the subsurface may be described as follows:

- Mass conservation equation for both phases

$$\phi \frac{\partial S_n}{\partial t} + \nabla \cdot (\mathbf{v}_n) = q_n, \quad (24)$$

$$\phi \frac{\partial S_w}{\partial t} + \nabla \cdot (\mathbf{v}_w) = q_w, \quad (25)$$

- Darcy's laws

$$\mathbf{v}_n = -K k_{rn}/\mu_n (\nabla p_n - \rho_n g \nabla z) \quad (26)$$

$$\mathbf{v}_w = -K k_{rw}/\mu_w (\nabla p_w - \rho_w g \nabla z) \quad (27)$$

- Constraints relations

$$S_n + S_w = 1 \quad (28)$$

$$p_c = p_n - p_w \quad (29)$$

A number of relationships are required to relate the relative permeability of each phase and the capillary pressure with saturation. These relationships are usually obtained experimentally and therefore we have

$$k_{rn} = k_{rn}(S_n) \quad (30)$$

$$k_{rw} = k_{rw}(S_w) \quad (31)$$

$$p_c = p_c(S_n) \quad (32)$$

For the sake of illustration, we ignore capillarity. Adding Eqs. 24 and 25 and using Eqs. 26 and 27, one obtains an equation of the form

$$\nabla \cdot \mathbf{v}_t = q_t \quad (33)$$

where $\mathbf{v}_t = \mathbf{v}_w + \mathbf{v}_n$ is the total velocity and $q_t = q_w + q_n$ is the source/sink term of the two phases. The above equation reduces to

$$-\nabla \cdot K \frac{k_{rw}}{\mu_w} (\nabla p - \rho_w \mathbf{g}) - \nabla \cdot K \frac{k_{rn}}{\mu_n} (\nabla p - \rho_n \mathbf{g}) = q_t \quad (34)$$

And upon some manipulations one gets

$$-\nabla \cdot K \lambda_t \nabla p + \nabla \cdot K (\rho_w \lambda_w + \rho_n \lambda_n) \mathbf{g} = q_t \quad (35)$$

where $\lambda_t = \lambda_w + \lambda_n = \frac{k_{rw}}{\mu_w} + \frac{k_{rn}}{\mu_n}$ is the total mobility with λ_w and λ_n are the mobility of the wetting and non-wetting phases, respectively. The non-wetting phase velocity can be expressed as:

$$\mathbf{v}_n = f_n \mathbf{v}_t - f_n \lambda_w (\rho_w - \rho_n) K \mathbf{g} \quad (36)$$

where f_n is the fractional flow of the non-wetting phase, $f_n = \lambda_n / \lambda_t$. In the IMPES scheme Eq. 9 is used to obtain the pressure field given the saturation from the previous time step, thus

$$-\nabla \cdot K \lambda_t^k \nabla p^{k+1} + \nabla \cdot K (\rho_w \lambda_w^k + \rho_n \lambda_n^k) \mathbf{g} = q_t \quad (37)$$

This equation generates a linear system of equations which can be written in matrix form as

$$A^k p^{k+1} = b^k \quad (38)$$

To update the saturation one needs to decide which saturation equation to use for saturation update. If the saturation equation based on the non-wetting phase, for example, is chosen, one updates the saturation using

$$\frac{\partial S_n}{\partial t} + \nabla \cdot f_n[\mathbf{v}_t - \lambda_w(\rho_w - \rho_n)K\mathbf{g}] = q_n \quad (39)$$

where $f_w = f_w(S_w) = \lambda_w/\lambda_t$ is the fractional flow of the wetting phase. It is apparent by looking into eqs. 36, 37, and 39, how long and complex the corresponding finite difference expressions would be. Furthermore, they are not very much following the sequence of the basic physical laws which makes their interpretation not easy unless they are post processed to obtain the basic variables. In the framework of the experimenting pressure field approach, only equations 24-29 are used. The matrix of coefficients that is used to obtain the pressure field is generated within the solver routine as is described in the following section. It is noteworthy that the upwind scheme is used when calculating the phase velocity. In this scheme the new pressure and gravity difference is checked to determine the direction of the phase velocity and based on this direction the value of relative permeability is chosen, Moortgat et al. (2011).

The experimenting pressure field approach as applied to the problem of two-phase flow in porous media

As explained earlier, applying this technique to the problem of two-phase flow in porous media is very straightforward and follows the following procedures:

- 1- The velocity components as given in equations 21 and 22 are discretized assuming the pressure field is known.
- 2- Applying a set of experimenting pressure fields (i.e., $mn+1$) with the first field $\mathbf{p}^0 = [0 \ 0 \ 0 \ \dots 0]^T$ and the subsequent mn fields as $\mathbf{p}^j = [0 \ 0 \ 0 \ \dots 0 \ 1 \ 0 \ \dots 0]^T$ and for each of these fields the velocity components are obtained (i.e., $\mathbf{u}_\alpha, \mathbf{u}_\beta$).
- 3- For each of the obtained velocity fields, the divergence of velocity in each cell is calculated (i.e., $\nabla \cdot \mathbf{u}_\alpha, \nabla \cdot \mathbf{u}_\beta$).
- 4- Add the two divergence to obtain $\nabla \cdot \mathbf{u}_\alpha + \nabla \cdot \mathbf{u}_\beta$
- 5- Find the residue, $R = [\nabla \cdot (\mathbf{u}_\alpha + \mathbf{u}_\beta)]^{\mathbf{p}^j} - (\tilde{q}_\alpha + \tilde{q}_\beta) - [\nabla \cdot (\mathbf{u}_\alpha + \mathbf{u}_\beta)]^{\mathbf{p}^0}$
- 6- From the above equation, the matrix of coefficients can be constructed which upon solution

determines the correct pressure field.

7- Knowing the pressure field, the velocity field can be obtained

8- The saturation is then updated using the time dependent saturation equation

A flow chart to highlight the different processes involved in this technique is shown in Fig. 8. In this flow chart, the purple box collects all the physics of the problem including conservation laws. The solver part includes the experimenting pressure field generator (p_a) which is used to construct the matrix of coefficients. These are a set of $mn+1$ pressure fields that operate on the conservation laws and the residue is used to construct the components of the matrix of coefficients. After constructing the matrix of coefficients, the linear system of equations is solved using sparse linear solver. As indicated earlier, the time taken to construct the matrix constitutes negligible part of the total time of solving the system.

Numerical examples and discussion

Several examples on the use of the experimenting pressure field technique on single phase flow in porous media can be found in Sun et al., 2012-b. In order to verify our numerical model, a comparison study is conducted for the case of 1D Buckley-Leverett (1942) problem in a homogeneous medium ignoring capillary pressure. Buckley-Leverett problem is a first order hyperbolic transport equation that is used to model two-phase flow in porous media. The solution of the 1D Buckley-Leverett equation when both the capillary pressure and gravity are ignored has the form

$$S(x, t) = S(x + ut) \quad (40)$$

where u is the velocity of the front (function of saturation), t is the time and x is the distance along the 1D domain. In this work a 1D horizontal domain of length 300 m, initially saturated with oil (non-wetting) is considered. Water (the wetting phase) is injected with a constant flow rate of

5x10⁻⁴ PV/day at the left hand side end to displace oil to the other end. The porosity is assumed 0.2, the permeability $K=100$ mD, the viscosity ratio is assumed one and the relative permeability relation with effective saturation is assumed quadratic. The residual saturation of both the water and the oil are assumed 0.01 and 0.2 respectively. Figure 9 shows saturation contours of the water phase after 100, 300, and 500 days, respectively, from which it is clear that the water phase is advancing from left to right. In Fig. 10 the analytical solution and the cell-centered finite difference (CCFD), which is obtained using a uniform mesh of 100 cells, is shown. It is clear that, apart from some numerical dispersion across the sharp interface, the solution, generally, conforms to the analytical solution.

The other two examples which are used to demonstrate the generalization of the experimenting pressure field approach to the problem of multiphase flows in porous media investigate the transport of LNAPL and DNAPL into an initially water-saturated porous medium domain. For this sake, a rectangular porous medium domain of dimensions 250m x 50m is considered, Fig. 11. The domain is initially assumed fully saturated with water. Two examples are considered; the first example is concerned with LNAPL migration in which supercritical CO₂ is injected at the bottom left corner of the rectangular domain. Whereas, the second example is concerned with the migration of DNAPL that, in this example, is injected at the top left corner of the domain. In the first example we consider flooding in the interval between 0 m and 5 m of the West boundary. In this scenario, velocity boundary condition of 10⁻⁵ m/s is assigned at the boundary of the injection cells while the entire east boundary is assigned a constant head. The whole north and south boundaries are considered impermeable. The permeability field is assumed homogeneous in the entire domain. To simulate these scenarios, we consider the following relationships for the relative

permeability with saturations (for the case of CO₂ sequestration problem) as suggested in Hayek et al., 2009. These are:

$$S_{e\alpha} = \frac{S_{\alpha} - S_{r\alpha}}{1 - S_{r\alpha} - S_{r\beta}} \quad (58)$$

$$k_{r\alpha}(S_{e\alpha}) = S_{e\alpha}^2 [1 - (1 - S_{e\alpha})^{\frac{2+\lambda}{\lambda}}] \quad (59)$$

$$k_{r\beta}(S_{e\alpha}) = (1 - S_{e\alpha})^{\frac{2+3\lambda}{\lambda}} \quad (60)$$

$$p_c = p_c^0 (1 - \frac{S_{\alpha}}{1 - S_{r\beta}} + b_c)^{-m_c} \quad (61)$$

where $S_{r\alpha}$ and $S_{r\beta}$ are the residual permeability of the α and β phases, respectively, λ, m_c, b_c and p_c^0 are constants (their values are given as: $\lambda = 0.333$, $b_c = 0.0001$, $m_c = 3.0$, and $p_c^0 = 10,000$). The absolute permeability is taken as 10 mD and the porosity is assumed 0.3. The injected phase is assumed at saturation of unity at the injection boundary and the initial saturation in the domain is assumed residual with a sufficiently small value of one percent. For the LNAPL migration example, Fig. 12 shows the CO₂ plume history in terms of saturation propagation with time. Apparently CO₂ plume is buoyantly lifted upwards due to the density contrast between supercritical CO₂ and water. When the plume reaches the cap rock, it moves laterally. In this figure only part of the lateral length is shown. To the contrary, DNAPL migration is downward as a result of the higher density it has compared with water. When it reaches the impervious layer, it moves laterally as shown in Fig. 13.

Conclusions

A new methodology to implement numerical techniques to the equations governing transport phenomena in porous media has been developed. The methodology follows the governing

381 equations as suggested by the physics of the problem with minimal manipulations. This produces
382 an algorithm which is easy to use, implement, maintain, and update. That is, while, traditional
383 techniques manipulate the governing equations so that a unified equation/s is obtained which is/are
384 reduced to a matrix form, whose entries are obtained within the algorithm, in this method, the
385 matrix of coefficient are constructed automatically within the solver. Furthermore, no need to
386 discretize a unified equation/s is required. Rather, the equations as suggested by the physics are
387 discretized which produces simpler algebraic equations. This is done by introducing a set of
388 predefined experimenting pressure fields which are used to determine the corresponding velocity
389 and divergence of velocity fields. These fields are then used to construct the matrix of coefficients
390 that is needed to construct the correct pressure field. This technique has been applied to the
391 simulation of LNAPL (in this work it is CO₂) and DNAPL (in this work trichloromethane) in the
392 subsurface. The time incurred to construct the matrix of coefficients is found to be negligibly small
393 compared with the time required to solving the linear system of equations.

References

- Ahmadi, A., and M. Quintard. 1996. Large-scale properties for two-phase flow in random porous media. *J. Hydrology*, 1983, no. 1-2: 69-99.
- Ataie-Ashtiani, B., M. Hassanizadeh, O. Oung, F.A. Weststrate, and A. Bezuijen. 2003. Numerical modeling of two-phase flow in geocentrifuge, *Environmental Modeling & Software*, 18: 231-141.
- Blessent, D., R. Therrien, R., K. MacQuarrie. 2009. Coupling geological and numerical models to simulate groundwater flow and contaminant transport in fractured media. *Computers & Geosciences*, 35, no. 9: 1897-1906.
- Blunt, M., F. J. Fayers, and F. M. Orr. 1993. Carbon dioxide in enhanced oil recovery. *Energy Conversion and Management*, 34, no. 9-11: 1197-1204.
- Buckley S, Leverett M., 1942, Mechanism of fluid displacement in sands. *Trans AIME*, 146: 187–96.
- Celia, M.A., M. Nordbotten. 2009. Practical Modeling Approaches for Geological Storage of Carbon Dioxide. *Groundwater*, 47, no. 5: 627-638.
- Chen, Z., G. Huan, and B. Li. 2004. An improved IMPES method for two-phase flow in porous media. *Transport in porous media*, 54, no. 3: 361-376.
- Chen, Z., G. Huan, and Y. Ma, (ed). 2006. Computational methods for multiphase flows in porous media. *SIAM*, Philadelphia.
- Davis, T.A. 2004. A column pre-ordering strategy for the unsymmetric-pattern multifrontal method, *ACM T. Math. Software*, 30: 165–195
- Gerhard, J.I., T. Pang, and B. H. Kueper. 2007. Time Scales of DNAPL Migration in Sandy Aquifers Examined via Numerical Simulation. *Groundwater*, 45, no. 2: 147–157.
- Haest, P. J., R. Lookman, I. Van Keer, J. Patyn, J. Bronders, M. Joris, J. Bellon, F. De Smedt. 2010. Containment of groundwater pollution (methyl tertiary butyl ether and benzene) to protect a drinking-water production site in Belgium. *Hydrogeology J.*, 18, no. 8: 1917-1925.
- Hayek, M., E. Mouche, and C. Mügler. 2009. Modeling vertical stratification of CO₂ injected into a deep layered aquifer. *Advances in Water Resources*, 32, no.3: 450-462.
- Hoteit, H., and A. Firoozabadi. 2006. Compositional modeling of discrete-fractured media without transfer functions by the discontinuous Galerkin and mixed methods. *SPE J.*, 11, no. 3: 341-352.
- Hoteit, H., and A. Firoozabadi. 2008. Numerical modeling of two-phase flow in heterogeneous permeable media with different capillarity pressures. *Adv. Water Res.*, 31, no. 1: 56–73.

- Hunt, J.R., N. Sitar, and K.D. Udell. 1991. Nonaqueous Phase Liquid Transport and Cleanup, *Water Res. Research*, 24, no.8.
- Jessen, K., A. R. Kavscek, and F.M. Orr. 2005. Increasing CO₂ storage in oil recovery. *Energy Conversion and Management*, 46, no. 2: 293-311.
- Law, D.H.S. and S. Bachu. 1996. Hydrogeological and numerical analysis of CO₂ disposal in deep aquifers in the Alberta sedimentary basin. *Energy Conversion & Management*. 37, no. 6-8: 1167–1174.
- Mercer, J.W. and R.M. Cohen. 1990. A Review of Immiscible Fluids in the Subsurface: Properties, Models, Characterization and Remediation, *J. of Cont. Hydrology*, 6.
- Monteagudo, J. E. P., A. Firoozabadi. 2004. Control-volume method for numerical simulation of two-phase immiscible flow in two- and three-dimensional discrete-fractured media, *Water Resources Research*, 40: W0740.
- Moortgat, J., S. Sun, and A. Fairoozabadi. 2011. Compositional modeling of three-phase flow with gravity using higher-order finite element methods. *Water Resources Research*, 47, no. 5: W05511
- Reynolds, D.A. and B.H. Kuepe. 2002. Numerical Examination of the Factors Controlling DNAPL Migration Through a Single Fracture. *Groundwater*, 40, no. 4: 368-377.
- Salama, A. and P. J. Van Geel. 2008-a. Flow and Solute Transport in Saturated Porous Media: 1. The Continuum hypothesis. *J. Porous Media*, 11, no. 4: 403-413.
- Salama, A. and P. J. Van Geel. 2008-b. Flow and Solute Transport in Saturated Porous. Media: 2. Violating the Continuum Hypothesis. *J. Porous Media*, 11, no. 5: 421-441.
- Salama, A., S. Sun, M. F. El-Amin. 2013-a. An Efficient Implicit-Pressure/Explicit-Saturation-Method-Based Shifting-Matrix Algorithm To Simulate Two-Phase, Immiscible Flow in Porous Media With Application to CO₂ Sequestration in the Subsurface. *SPE Journal*, 13, no. 6: 1092-1101.
- Salama, A., S. Sun, and M. Wheeler. 2014. Solving global problem by considering multitude of local problems: application to flow in anisotropic porous media using the multipoint flux approximation. *J. Computational and Applied Mathematics*, 267: 117-130.
- Salama, A., S. Sun, M. F. El Amin. 2015. Investigation of thermal energy transport from an anisotropic central heating element to the adjacent channels: A multipoint flux approximation. *Annals of Nuclear Energy*, 76: 100-112.
- Span, R. and W. Wagner. 1996. A new equation of state for carbon dioxide covering the fluid region from the triple-point temperature to 1100 K at pressures up to 88 MPa. *Journal of Physical and Chemical Reference Data* 25, no. 6: 1509–1595.

- 484 Sterling, S.L., B.L. Parker, J.A. Cherry, J.H. Williams, J. W. Lane Jr, and F. P. Haeni. 2005.
485 Vertical Cross Contamination of Trichloroethylene in a Borehole in Fractured Sandstone,
486 *Groundwater*, 43, no. 4: 557–573.
- 487
- 488 Sun, S., A. Salama, and M. F. El-Amin. 2012-a. Matrix-oriented implementation for the numerical
489 solution of the partial differential equations governing flows and transport in porous media.
490 *Computers & Fluids*, 68: 38–46.
- 491
- 492 Sun, S., A. Salama, and M. F. El-Amin. 2012-b. An Equation-Type Approach for the Numerical
493 Solution of the Partial Differential Equations Governing Transport Phenomena in Porous Media.
494 *Procedia Computer Science*, 9: 661-669.
- 495
- 496 Van Geel, P.J., and J.F. Sykes. 1994a. Laboratory and model simulations of a LNAPL spill in a
497 variably-saturated sand, 1. Laboratory experiment and image analysis techniques. *Journal of*
498 *Contaminant Hydrology* 17: 1–25.
- 499
- 500 Van Geel, P.J., and J.F. Sykes. 1994b. Laboratory and model simulations of a LNAPL spill in a
501 variably-saturated sand, 2. Comparison of laboratory and model results. *Journal of Contaminant*
502 *Hydrology* 17: 26–53.
- 503
- 504 Zhou, Q., J. T. Birkholzer , E. Mehnert, Y.-F. Lin, K. Zhang. 2010. Modeling Basin- and Plume-
505 Scale Processes of CO₂ Storage for Full-Scale Deployment, *Groundwater*, 48, no. 4: 494–514.

0 •	0 •	0 •	0 •
0 •	1 •	0 •	0 •
0 •	0 •	0 •	0 •
0 •	0 •	0 •	0 •

Fig. 1 Experimenting pressure field

Fig. 2 Flow chart of the Experimenting pressure field methodology

1 •	0 •	0 •	1 •
0 •	0 •	0 •	0 •
0 •	0 •	0 •	0 •
1 •	0 •	0 •	1 •

Fig. 3 One of the nine Experimenting pressure fields

→ 0	→ 0	→ 0	→ 0	→ 0
→ 0	→ 0	→ 0	→ 0	→ 0
→ 0	→ 0	→ 1	→ 0	→ 0
→ 0	→ 0	→ 0	→ 0	→ 0

Fig. 4 One of the Experimenting velocity fields

Fig.5 Pressure contours and velocity vectors for the single phase example

Fig. 6 Time taken to construct the matrix versus to solve the linear system

Fig. 7 Ratio of the time taken to construct the matrix versus the time taken to solve the linear system

Fig. 8 A flow chart diagram for the use of the experimenting pressure field technique to the problem of two-phase flows in porous media

(a) After 100 day

(b) After 300 days

Fig. 9 Water saturation at the time: (a) $t = 100$ days (b), and $t = 300$ days (c)

Fig. 10 Solution of the Buckley-Leverett problem with quadratic relative permeability with viscosity ratio of unity

Fig. 11: A schematic of the computational domain and the boundary conditions

(a) After 1 year

(b) After 2 years

(c) After 3 years

(d) After 4 years

(e) After 6 years

(f) After 8 years

Fig. 12 CO₂ plume migration into water-saturated porous medium domain (part of the domain is shown)

(a) After 6 months

(b) After 1 years

(c) After 2 years

(d) After 3 years

(e) After 4 years

(f) After 4.5 years

Fig. 13 DNAPL plume migration with time (part of the domain is shown)