
Article:
Baù, D., Cody, B.M. and González-Nicolás, A. (2015) An iterative global pressure solution for the semi-analytical simulation of geological carbon sequestration. Computational Geosciences, 19 (4). 781 - 789. ISSN 1420-0597

https://doi.org/10.1007/s10596-015-9489-4

An Iterative Global Pressure Solution for the Semi-Analytical Simulation of Geological Carbon Sequestration

Domenico Baù[1], Brent M. Cody[2] and Ana González-Nicolás[3]

Computational Geosciences - DOI 10.1007/s10596-015-9489

Published online 03 May 2015: http://link.springer.com/article/10.1007/s10596-015-9489-4.

[1] Department of Civil and Structural Engineering, University of Sheffield, Sheffield, S1 3JD, UK
[2] Natural Resources Consulting Engineers Inc., Fort Collins, 80524, USA
[3] Department of Civil and Environmental Engineering, Colorado State University, Fort Collins, 80523, USA

An Iterative Global Pressure Solution for the Semi-Analytical Simulation of Geological Carbon Sequestration

Domenico Baù, Brent M. Cody and Ana González-Nicolás

Abstract Successful large-scale implementation of geological CO_2 sequestration (GCS) will require the preliminary assessment of multiple potential injection sites. Risk assessment and optimization tools used in this effort typically require large numbers of simulations. This makes it important to choose the appropriate level of complexity when selecting the type of simulation model. A promising multiphase semi-analytical method proposed by [40] to estimate key system attributes (i.e. pressure distribution, CO_2 plume extent, and fluid migration) has been found to reduce computational run times by three orders of magnitude when compared to other standard numerical techniques. The premise of the work presented herein is that the existing semi-analytically leakage algorithm proposed by [40] may be further improved in computational efficiency by applying a fixed point type iterative global pressure solution to eliminate the need to solve large sets of linear equations at each time step. Results show that significant gains in computational efficiency are obtained with this new methodology. In addition, this modification provides the same enhancement to similar semi-analytical algorithms that simulate singe-phase injection into multi-layer domains.

Keywords: Semi-Analytical Modeling; Iterative Methods; Geological Carbon Sequestration; Injection Site Assessment

1 Introduction

Geological CO_2 sequestration (GCS) has the potential to greatly reduce greenhouse gas loading to the atmosphere while cleaner, more sustainable energy solutions are developed. However, displaced brine or sequestered CO_2 may intrude into and adversely affect shallow groundwater resources. Brine leakage would increase aquifer salinity, while CO_2 intrusion may cause secondary effects, such as the mobilization of hazardous inorganic constituents present in aquifer minerals and changes in pH values. These risks must be fully understood and minimized before project implementation.

It is thus often beneficial to use faster, though less accurate, leakage estimation models to perform the large quantities of model simulations required for preliminary GCS planning, site selection, optimization, and sensitivity analysis. In addition, inherent subsurface uncertainties often necessitate the need for stochastic methods, further increasing the quantity of simulations needed. The direct use of other multi-phase multi-layer numerical methods in the initial planning stage is typically prohibited by both the high computational cost per simulation and the significant effort involved in building and calibrating a custom model for each potential injection site. In response to these obstacles, analytical and semi-analytical methods have been developed which greatly reduce simulation complexity and computational run times.

Several attempts have been made to analytically quantify the hydraulic communication between aquifers separated by leaky aquitard layers [19,20,21,30]. In addition, several other authors have presented analytical or semi-analytical solutions used to estimate subsurface pressure distributions and fluid flux across layer boundaries resulting from leaky wells [24,25]. For example, [29] introduced fluid and matrix compressibility to the similarity solutions governing single-well CO_2 injection presented in [33], while [43] presented a single-phase semi-analytical solution for large scale injection-induced pressure perturbation and leakage in a laterally bounded aquifer-aquitard system. Also, a semi-analytical model estimating multi-phase fluid flux through a single caprock perforation was developed by [27] to determine optimal injection intervals based upon trapping effects for secure CO_2 storage in saline aquifers and [5,9,10] presented and applied a single-phase semi-analytical model for both forced and diffuse leakage in a multi-layer system. Finally, [4] combined solutions presented by [21], [38], and [42] to create a semi-analytical solution for approximating the area of potential impact from a single CO_2 injection well.

However, while other semi-analytical algorithms provide insight regarding specific processes (e.g. diffuse leakage[10]), this work focuses upon the multi-phase subsurface flow model proposed by [40] and further

developed by [7] because it is the only semi-analytical model able to simulate multi-phase flow in domains having multiple injection wells and multiple aquifer and aquitard (i.e. caprock) layers.

An analytical algorithm was developed by [38] for estimating the pressure distribution and leakage for single-phase injection (e.g. injection of brine into a brine filled domain of aquifer) into a domain having multiple passive wells and multiple aquifer-aquitard layers. This algorithm creates a set of linear equations describing the pressure distribution throughout the domain by superimposing pressure changes caused by each source or sink in each aquifer. The general algorithm presented in [38] in conjunction with the development of a multiphase pressure response function [33,34,35,38] has led to a semi-analytical CO_2 leakage algorithm, presented in [40] and expounded upon in [7] and [36], which estimates both brine and CO_2 flux across confining layers resulting from the injection of CO_2. While there are multiple pathways for the leakage of sequestered CO_2 from subsurface storage reservoirs (e.g. geological discontinuities, caprock permeability, etc.), [40] assumes that hydrocarbon exploration and production boreholes created preferential flow paths in the domain [2,3,12,14,18,28,32]. This assumption appears reasonable as the existing caprock had successfully held the recently produced hydrocarbons for many millennia prior to production [37].

Stochastic techniques for preliminary GCS site assessment (e.g. injection scheme optimization, risk analysis, and sensitivity analysis, etc.) require large numbers of simulations. Therefore, it is important to be continually developing the efficiency of simulation tools. Herein, a fixed point type iterative global pressure solution modification to the semi-analytical CO_2 leakage algorithm [7,36,40] is presented and explored. This work first includes a detailed description of the original semi-analytical leakage algorithm then presents the methodology for applying the proposed modification. Following this is a description of the hypothetical test case and a discussion regarding the accuracy and computational efficiency results. Finally, we conclude with suggestions of cases when usage of this modification would be essential.

2 Methodology

A thorough understanding of the existing semi-analytical leakage algorithm's methodology is needed before describing potential modifications. Therefore, the first part of this section provides a detailed description of work presented in [40] and [7].

2.1 The Estimating Leakage Semi-analytically (ELSA) Algorithm

Referred to as Estimating Leakage Semi-analytically (ELSA) when used by [31] to estimate the maximum probable leakage along abandoned oil wells, this semi-analytical algorithm estimates both brine and CO_2 flux through permeable caprock locations resulting from GCS. Permeable caprock locations are conceptualized as segments of abandoned wells and represent cylindrical portions of the aquitard layers having non-negligible permeability values. These are referred to as 'passive wells' and are assumed to be the only pathways for fluid flux between aquifer layers. Users of this model are able to specify the number of injection wells (M), passive wells (N), and aquifer/aquitard layers (L), as well as their respective spatial locations and hydrogeological parameters when characterizing the domain.

The domain is structured as a stack of aquifer/aquitard layers perforated by injection and passive wells. Aquifers are assumed to be horizontally level, homogenous, and isotropic. Aquitards are assumed to impermeable, except where perforated by passive wells. Injection wells are able to inject into any layer. Initially, fluid is not flowing through any of the passive wells because the entire domain is assumed to be saturated with brine at hydrostatic pressure. Additional assumptions made by this model include: 1) Aquifers exhibit horizontal flow; 2) Capillary pressure is negligible resulting in a sharp fluid interface; 3) CO_2 plume thickness at any given location is assumed to be the maximum plume thickness from all sources in the aquifer; 4) Pressure response from sources and sinks are superimposed in each aquifer; and 5) the injectivity of the formation remains constant. Several of these processes are important [9,11,13,15,17,22,26]

and should be included [6,16,23,39] when model accuracy is more important that efficiency (e.g. during final project design).

At the start of injection, aquifer fluid pressures throughout the domain begin to change resulting in pressure differentials across aquitards and fluid flux through passive wells. It is therefore very important to understand aquifer fluid pressure response resulting from changes in the mass storage of CO_2 and brine. A pressure response function for the injection of CO_2 into a brine filled confined aquifer was derived in [33]. Reference [7] expresses this radial overpressure response, Δp, at the bottom of a confined aquifer for a single well injecting CO_2 as:

$$\Delta p = p - p_0 = \Delta p'(\rho_b - \rho_c)gH \tag{1}$$

where p_0 and p are the initial and resulting fluid pressures at the bottom of the aquifer, ρ is fluid density, g is gravitational acceleration, H is aquifer thickness, and subscripts b and c denote phase types brine and CO_2, respectively. In addition, $\Delta p'$ is a dimensionless function defined as:

$$\Delta p'(\chi) = \begin{cases} 0, & \chi \geq \psi \\ -\frac{1}{2\Gamma}\ln\left(\frac{\chi}{\psi}\right) + \Delta p'(\psi), & \psi > \chi \geq 2\lambda \\ \frac{1}{\Gamma} - \frac{\sqrt{\chi}}{\Gamma\sqrt{2\lambda}} + \Delta p'(2\lambda) + F(h'), & 2\lambda > \chi \geq \frac{2}{\lambda} \\ -\frac{1}{2\lambda\Gamma}\ln\left(\frac{\chi\lambda}{2}\right) + \Delta p'\left(\frac{2}{\lambda}\right), & \frac{2}{\lambda} > \chi \end{cases} \tag{2}$$

where,

$$\chi = \frac{2\pi H\varphi(1 - S_b^{res})r^2}{Q \cdot t} \tag{3}$$

$$\Gamma = \frac{2\pi(\rho_b - \rho_c)gkH^2}{\mu_b Q} \tag{4}$$

$$\psi = \frac{4.5\pi H\varphi k(1 - S_b^{res})}{\mu_b c_{eff} Q} \tag{5}$$

$$h' = \frac{h(\chi)}{H} = \frac{1}{\lambda - 1}\left(\frac{\sqrt{2\lambda}}{\sqrt{\chi}} - 1\right) \tag{6}$$

$$F(h') = \frac{-\lambda}{\lambda - 1}\left[\mathrm{h}' - \frac{ln[(\lambda - 1)h' + 1]}{\lambda - 1}\right] \tag{7}$$

In Equations (2-7), B is aquitard thickness, h is CO_2 plume thickness, h*'* is the ratio of CO_2 plume thickness to aquifer thickness, S_b^{res} is the residual saturation of the brine, t is the injection duration, k is the aquifer permeability, μ is the dynamic viscosity, φ is the aquifer porosity, Q is the total volumetric well flux, c_{eff} is the effective compressibility of the fluid and solid matrix, and r is the radial distance from the CO_2 source or sink. Also, *F(h')* is an offset term related to the vertical pressure distribution [7] and the mobility ratio is defined as $\lambda = \lambda_c/\lambda_b$, where $\lambda_\alpha = k_{r,\alpha}/\mu_\alpha$ and $k_{r,\alpha}$ is the relative permeability of phase α (α = b for brine or α = c for CO_2).

ELSA uses Equation (1) to determine the pressure distribution throughout the aquifer, then applies a multiphase version of Darcy's law to determine each flow rate, $Q_{\alpha\,j,l}$, for each phase α across each confining layer l (l=1,2,..,L) for each passive well j (j=1,2,..,N):

$$Q_{\alpha\,j,l} = \pi r_{pw\,j,l}^2 \frac{k_{r,\alpha\,j,l} k_{pw\,j,l}}{\mu_\alpha B_l}\left(p_{j,l-1} - \rho_\alpha g B_l - g\rho_\alpha H_{l-1} - p_{j,l}\right) \tag{8}$$

In Equation (8), $r_{pw_{j,l}}$ is the passive well radius and $k_{pw_{j,l}}$ is the permeability for passive well j (j=1,2,..,N) and aquitard layer l.

Equation (1) differs significantly from the solution derived by [42] for single phase flow in that estimated pressure responses are non-linear with respect to the injection flow rate. Also, unlike single phase flow, CO_2 plume locations and thicknesses must be known when determining fluid saturations and relative permeabilities found in passive well pathways. ELSA overcomes these problems by linearizing Equation (1) using Green's functions and applying time stepping to approximate the changing pressure distribution, passive well fluxes, and CO_2 plume locations and thicknesses over the injection duration. For each time step, the following linear equation is written for each passive well in each aquifer.

$$p_{i,l} = p_{0_l} + \sum_{iw=1}^{M} G_{i,iw,l} Q_{iw,l} + \sum_{j=1}^{N} G_{i,j,l}\{Q_{j,l} - Q_{j,l+1}\} + F(h'_{max})(\rho_b - \rho_c)gH \qquad (9)$$

where i (i=1,2,..,N) denotes the passive well at which pressure is being solved, l (l=1,2,..,L) denotes aquifer layer, and iw (iw=1,2,..,M) and j (j=1,2,..,N) denote the injection and passive well, respectively, whose flux is causing pressure change at well i. Green's functions are defined by the partial derivatives:

$$G_{i,j,l} = \frac{\partial(\Delta p_{i,l})}{\partial Q_{avg_{j,l}}} \qquad (10)$$

Reference [40] describes the Green's functions defined by Equation (10) as representations of "the sensitivity of the pressure field for a given source or sink". These are obtained analytically by calculating the partial derivative of Equation (1) with respect to the average flux, $Q_{avg_{j,l}}$, of a given injection or passive

well. For each time step, Green's function coefficients, $G_{i,j,l}$, are evaluated using the previous time step's flow rates.

As shown by the denominator of Equation (3), for each time step, the semi-analytical algorithm presented in [40] and [7] estimates the total pressure change from the start of simulation, rather than the incremental pressure change over the time step, at well i (i=1,2,..,N) resulting from fluid flux at well j (j=1,2,..,N), by multiplying the current time step's passive well flow rate by a Green's function constant calculated using the average flow rate over all previous time steps. The CO_2 pressure response function from [38] is derived for sources or sinks having a constant flow rate. However, passive well fluxes occur as a response to pressure differentials across caprock layers and therefore change over the injection duration. In response, [36] proposed a volume preserving approximation of the convolution integral. This is implemented by estimating the pressure change from each passive well flux as the product of the well's Green's function constant and its average flow rate:

$$\Delta p_{i,j,l} = G_{i,j,l} \cdot Q_{avg}^{(t)}{}_{j,l} \tag{11}$$

Therefore, Equation (9) is rewritten with respect to Q_{avg}:

$$p_{i,l} = p_{0_l} + \sum_{iw=1}^{M} G_{i,iw,l} Q_{avg}{}_{iw,l} + \sum_{j=1}^{N} G_{i,j,l} \left\{ Q_{avg}{}_{j,l} - Q_{avg}{}_{j,l+1} \right\} + F(h'_{max})(\rho_b - \rho_c) g H \tag{12}$$

In Equation (12) volumetric flow rate is equal to total fluid mass transferred through passive well segment, $M_{j,l}^{(t)}$, divided by the effective fluid density, ρ_{eff}, divided by the time, t.

$$Q_{avg}{}_{j,l}^{(t)} = M_{j,l}^{(t)} / \rho_{eff} t \tag{13}$$

where the subscript eff denotes 'effective'. Effective fluid densities are needed in this case because $M_{j,l}^{(t)}$ may be composed of both CO_2 and brine. The total fluid mass transferred from the start of injection through the current time step between aquifers by a passive well segment is defined as:

$$M_{j,l}^{(t)} = M_{j,l}^{(t-\Delta t)} + \Delta t \cdot 0.5 \left(Q_{j,l}^{(t-\Delta t)} + Q_{j,l}^{(t)} \right) \rho_{eff} \tag{14}$$

where $M_{j,l}^{(t-\Delta t)}$ is total fluid mass transferred by the well segment during all previous time steps, Δt is the time step duration, and $0.5 \left(Q_{j,l}^{(t-\Delta t)} + Q_{j,l}^{(t)} \right) \rho_{eff}$ is the average mass flux over the current time step. Substituting Equation (14) into Equation (13) gives:

$$Q_{avg}{}_{j,l}^{(t)} = \left[M_{j,l}^{(t-\Delta t)} + 0.5 \Delta t \left(Q_{j,l}^{(t-\Delta t)} + Q_{j,l}^{(t)} \right) \rho_{eff} \right] / \rho_{eff} t \tag{15}$$

Subtracting the bottom layer's average flow rate by the top layer's average flow rate gives:

$$Q_{avg}{}_{j,l} - Q_{avg}{}_{j,l+1} = c_2 (Q_{j,l} - Q_{j,l+1}) + c_1 \tag{16}$$

where c_1 and c_2 are defined as:

$$c_1 = \frac{M_{j,l}^{(t-\Delta t)} - M_{j,l+1}^{(t-\Delta t)} + 0.5 \Delta t \left(Q_{j,l}^{(t-\Delta t)} - Q_{j,l+1}^{(t-\Delta t)} \right) \rho_{eff}}{\rho_{eff} t} \tag{17}$$

$$c_2 = \frac{0.5\Delta t}{t} \tag{18}$$

Finally, substituting Equation (16) into Equation (12) gives the pressure equation for the modified method:

$$\begin{aligned} p_{i,l} = p_{0,l} + \sum_{iw=1}^{M} \left[G_{i,iw,l} Q_{iw,l}\right] \\ + \sum_{j=1}^{N} \Bigg[c_2 G_{i,j,l} \Bigg\{ \pi {r_{pw}}_{j,l}^{2} k_{j,l} \frac{k_{r,eff,j,l}}{\mu_{eff} B_l} \big(p_{j,l-1} - \rho_b g B_l - g H_{l-1}(\rho_b - \rho_b h'_{i,l-1} \\ + \rho_c h'_{i,l-1}) - p_{j,l}\big) \\ - \pi {r_{pw}}_{j,l+1}^{2} k_{j,l+1} \frac{k_{r,eff,j,l+1}}{\mu_{eff} B_{l+1}} \big(p_{j,l} - \rho_b g B_{l+1} - g H_l(\rho_b - \rho_b h'_{i,l} + \rho_c h'_{i,l}) \\ - p_{j,l+1}\big) \Bigg\} + c_1 G_{i,j,l} \Bigg] + F(h'_{max})(\rho_b - \rho_c) g H \end{aligned} \tag{19}$$

It is now possible to isolate unknown pressure terms $p_{i,l}$, $p_{j,l-1}$, $p_{j,l}$, and $p_{j,l+1}$. Equation (19) is written for each passive well i (i=1,2,..,N) at the bottom of each aquifer l (l=1,2,..,L) resulting in a linear system of N*L equations and unknowns. Solving this set of linear equations provides fluid pressures, $p_{i,l}$, at each passive well at each layer.

Once pressures are known throughout the domain, Equation (8) is used to explicitly calculate passive well segment fluxes for the current time step. The time step is then advanced and the process is repeated until the full simulation duration is reached. Mass storage changes in each layer, $\Delta M_{\alpha,l}$, may be determined for both CO_2 (α = c) and brine (α = b) by calculating the product of fluid density, ρ_α, injection duration, t_{inj}, and the sum of average passive well segment flow rates, $Q_{\alpha,avg}$:

$$\Delta M_{\alpha,l} = \rho_\alpha t_{inj} \sum_{iw=1}^{M} Q_{avg}{}_{iw,l} + \rho_\alpha t_{inj} \sum_{j=1}^{M+N} \left[Q_{\alpha,avg}{}_{j,l} - Q_{\alpha,avg}{}_{j,l+1} \right] \quad (20)$$

2.2 The Iterative Global Pressure Solution (IGPS) Modification

The number of unknown variables, hence the number of linear equations, is equal to the product of the number of passive wells and the number of aquifer layers (N*L). Domains having large numbers of passive wells and/or layers produce very large sets of linear equations and resulting in significantly higher simulation run times. An iterative fixed point [41] approach is proposed here to increase computational efficiency by solving the global pressure solution. In addition, this method is able to solve nonlinear sets of equations, therefore eliminating the need to linearize the pressure response equation. In the following methodology, iter denotes iteration index, $\mathbf{Q_{avg}}$ and $\mathbf{Q}$ are vectors of average and current time step passive well flow rates with a size of [N*L], $\mathbf{p}$ is a vector of fluid pressures at the bottom of each aquifer at each passive well with a size of [N*L], and $\mathbf{\Omega_1}$ and $\mathbf{\Omega_2}$ are sets of parameters and independent variables, other than $\mathbf{Q}$ and $\mathbf{p}$, for Equation (1) and Equation (8), respectively:

$$\mathbf{\Omega}_1 \equiv \left\{ \rho_c, \rho_b, g, \mathbf{H}, \lambda, \pi, \boldsymbol{\varphi}, S_b^{res}, \mathbf{r}, t, \mathbf{k}, \mu_b, c_{eff} \right\} \quad (21)$$

$$\mathbf{\Omega}_2 \equiv \left\{ \pi, \mathbf{r}_{pw}, \mathbf{k}_{r,c}, \mathbf{k}_{r,b}, \mathbf{k}_{pw}, \mu_c, \mu_b, \mathbf{B}, \rho_c, \rho_b, g, \mathbf{H} \right\} \quad (22)$$

where $\mathbf{H}$, $\boldsymbol{\varphi}$, and $\mathbf{k}$ are vectors of aquifer thicknesses, porosities, and permeabilities, respectively, with size [L], $\mathbf{B}$ is a vector of aquitard thicknesses with size [L+1], $\mathbf{r}$ is an array of radial distances with size [M+N] x [M+N], and $\mathbf{r}_{pw}$, $\mathbf{k}_{pw}$, $\mathbf{k}_{r,c}$, and $\mathbf{k}_{r,b}$ are arrays of passive well radii, permeabilities, and relative permeabilities of the CO_2 and brine phases, respectively, with size [N] x [L+1]. The following is the procedure for the IGPS modification.

1. Use the initial assumption that passive well flow rates for the current time step remain constant from the previous time step:

$$\mathbf{Q}(t)^{(iter=0)} = \mathbf{Q}(t - \Delta t) \tag{23}$$

2. Use Equation (13) to determine average passive well flux rates then apply the non-linear Equation (1) to calculate the global pressure distribution by superimposing pressure changes from both assumed passive well flow rates and known injection well flow rates at each passive well in each aquifer:

$$\mathbf{p}(t)^{(iter)} = \mathbf{p}\left(\mathbf{\Omega_1}, \mathbf{Q}_{\text{avg}}(t)^{(iter-1)}\right) \tag{24}$$

3. Calculate new passive well flow rates using this new pressure distribution and Equation (8):

$$\mathbf{Q}(t)^{(iter)} = \mathbf{Q}\left(\mathbf{\Omega_2}, \mathbf{p}(t)^{(iter)}\right) \tag{25}$$

4. Repeat steps 2 and 3 until the maximum relative error, ε, between the preceding and current iteration's flow rate becomes smaller than a prescribed error tolerance coefficient, $\varepsilon_{\max}$:

$$\varepsilon = max\left\{\left|\frac{{Q_{1,1}}^{(iter+1)} - {Q_{1,1}}^{(iter)}}{{Q_{1,1}}^{(iter+1)}}\right|, \cdots, \left|\frac{{Q_{j,l}}^{(iter+1)} - {Q_{j,l}}^{(iter)}}{{Q_{j,l}}^{(iter+1)}}\right|, \cdots, \left|\frac{{Q_{N,L}}^{(iter+1)} - {Q_{N,L}}^{(iter)}}{{Q_{N,L}}^{(iter+1)}}\right|\right\} \leq \varepsilon_{max} \tag{26}$$

As seen in Equation (24), IGPS uses average flux rates when calculating pressure changes. However, because it does not require the linearization of the pressure solution, Equations (9-12) and (14-19) are not used in conjunction with IGPS. Two additional parameters are implemented when applying this

modification to ensure time step convergence stability. First, a maximum passive well flow rate, $Q_{pw,max}$, is specified to dampen artificially high-magnitude pressure differentials calculated from either large time step intervals or closely-spaced passive well positions. Secondly, a relaxation factor, ω, between preceding and current iterative passive well flow rates is specified to reduce the likelihood of divergent oscillations:

$$\mathbf{Q}^{(iter)} = \omega\mathbf{Q}^{(iter)} + (1-\omega)\mathbf{Q}^{(iter-1)} \tag{27}$$

This work has found that setting $Q_{pw,max}$ equal to one tenth the volumetric injection rate and ω between to 0.1 and 0.5 has resulted in algorithm stability.

3 Results and Discussion

CO_2 leakage estimation and simulation run times are compared for the original and proposed semi-analytical leakage algorithm. A continuous CO_2 injection rate of 50 kg/s is simulated through one injection well (M = 1) into the lower of two 20 m thick aquifers (L = 2) separated by one 20 m thick aquitard. All aquifers have k = 100 mD, λ = 5, S_b^{res} = 30%, c_{eff} = 4.6 x 10^{-10} m^2/N, and φ = 10%. The bottom of the lower aquifer is set to a depth of 2000 m. Parameter values for the domain include g = 9.81 m/s^2, ρ_b = 1000 kg/m^3, ρ_c = 600 kg/m^3, μ_b = 0.5 mPa s, and μ_c = 0.05 mPa s. All passive wells have a radius, r_{pw}, equal to 0.2 m.

Sets of linear equations are solved by LU decomposition with partial pivoting using the DGESV solver available in the optimized linear algebra package LAPACK [1]. This general solver is needed because the matrix characterizing our linear set of equations is non-sparse and non-symmetrical. A computer having a 2.4 GHz Intel® Core™ i7 processor with 8 GB of installed memory is used for all simulations. Multiple identical runs are performed to ensure computational run time consistency.

Time saving measures (e.g. neglecting far or low mass flux sources) should be included when practically implementing this semi-analytical leakage model. However, these are not used in the following comparisons to maintain run time consistency. In addition, this work makes the assumption that Equation (1) accurately estimates pressure changes resulting from a single well injecting CO_2 into a confining aquifer and accepts the numerical validation presented by [33]. While the modifications presented above alter the implementation of the pressure solution, its fundamental form, defined by Equation (1), remains the same. Also, the upconing solution [34] and *F'* offset term defined above with Equation (7) are neglected for the purpose of simplifying the following analyses.

Figure 1 shows the plan and elevation views of a hypothetical injection domain created for all following analyses. Passive well Cartesian coordinates were uniformly randomly generated to be within a 50 km by 50 km domain centered with respect to the injection well.

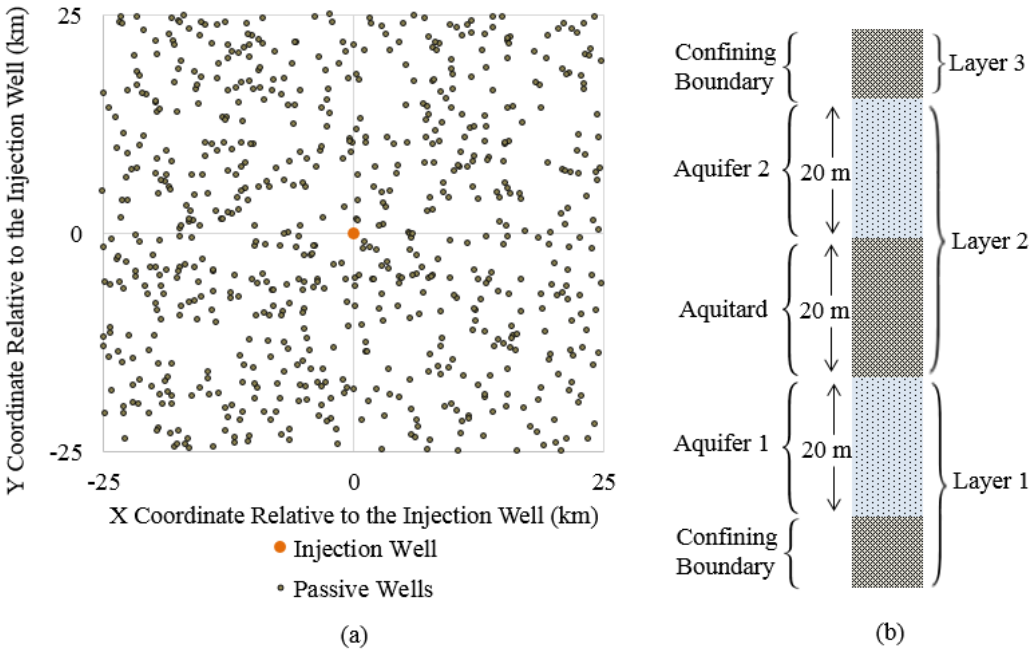


Figure 1: (a) Plan view of the domain showing locations of all 700 passive wells. (b) Elevation view of the domain showing layer locations and thicknesses.

All passive wells permeabilities, k_{pw}, were randomly generated having a 50% chance of being either "intact" or "degraded" [31]. Passive well permeabilities were assumed to be 0.1 mD for "intact" passive wells and 1000 mD for "degraded" passive wells.

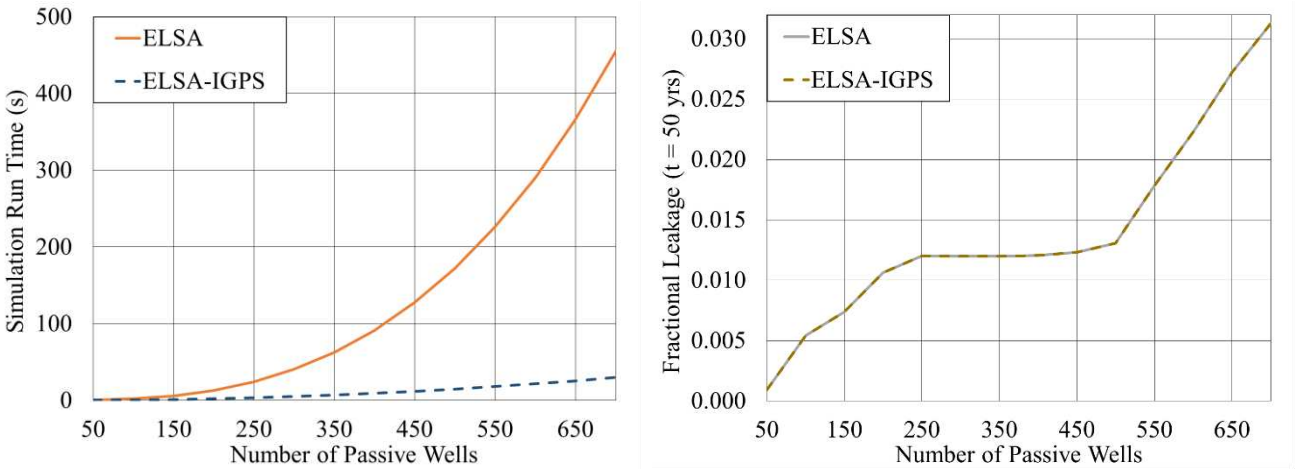
The average number of iterations required for time step convergence is dependent upon the values chosen for the number of time steps (nts), ε_{max} and ω. Acceptable parameter values of nts, ε_{max}, and ω were determined through a preliminary convergence analysis then perturbed to investigate effects upon both the number of iterations required at each time step and fractional leakage estimation. The results shown below in Table 1 were found for the randomly generated domain presented above with 50 passive wells simulated.

Table 1. Convergence sensitivity relating to parameters nts, ε_{max}, and ω.

ε_{max}	Average Iterations Required at Each Time Step				Fractional Leakage (/)			
	nts = 150		nts = 200		nts = 150		nts = 200	
	ω = 0.3	ω = 0.5	ω = 0.3	ω = 0.5	ω = 0.3	ω = 0.5	ω = 0.3	ω = 0.5
10^{-6}	2.00	2.00	2.00	2.00	9.418×10^{-4}	9.418×10^{-4}	9.420×10^{-4}	9.420×10^{-4}
10^{-7}	2.33	2.78	2.00	2.29	9.418×10^{-4}	9.418×10^{-4}	9.420×10^{-4}	9.420×10^{-4}
10^{-8}	6.01	4.57	5.05	4.11	9.418×10^{-4}	9.418×10^{-4}	9.420×10^{-4}	9.420×10^{-4}
10^{-9}	9.57	6.42	8.64	6.03	9.418×10^{-4}	9.418×10^{-4}	9.420×10^{-4}	9.420×10^{-4}

On average, few iterations are required for convergence. Simulations requiring a smaller ε_{max} value or having a lessor specified nts or ω value are typically shown to require more iterations for convergence. A greater nts value causes a more finely time discretization and, thus, less adjustment at each time step. Lower ω values are more stable but result in slower convergence rates. It is interesting to note that, for the parameter ranges chosen, ε_{max} and ω did not noticeably affect fractional leakage estimation. Fractional leakage is found to be slightly higher with a greater nts.

The randomly generated domain presented above is also used to quantify the accuracy and efficiency of the iterative global pressure solution (IGPS) modification. From convergence testing, values of 150, 10^{-6}, and 0.3 are chosen for nts, ε_{max} and ω, respectively. The only changing variable is the number of passive wells simulated, ranging between 50 and 700 in increments of 50. Figure 2 shows a comparison of simulation run times and fractional leakage at the end of the 50 year injection period versus the number of passive wells for the ELSA and ELSA-IGPS algorithms. These results show that there are negligible differences in CO_2 leakage estimation between the ELSA and ELSA-IGPS algorithms while the IGPS modification greatly decreases computational expense. The average observed difference in fractional leakage between the two algorithms is infinitesimal while computational cost is reduced by approximately one order of magnitude.



(a) (b)

Figure 2: Comparison of (a) simulation run time and (b) fractional leakage at the end of the 50 year injection period versus the number of passive wells between the ELSA and ELSA–IGPS algorithms

Leakage mass estimations are very similar between the two methods because both use the same pressure response equation to estimate the pressure distributions throughout the domain. Simulations run times are drastically reduced using the IGPS modification because the problem is solved explicitly within each iteration. In addition, computational efficiency savings increase with the number of passive wells modeled.

Figure 3 shows the ratio of simulation run time between the ELSA and ELSA-IGPS algorithms versus the number of passive wells included in the domain.

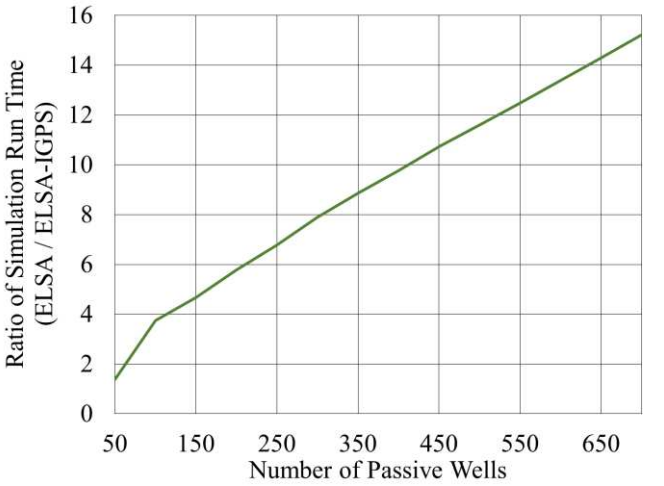


Figure 3: Ratio of ELSA to ELSA-IGPS simulation run time versus the number of passive wells

4 Conclusions

This work has led to an important modification of the semi-analytical CO_2 leakage algorithm presented by [40]. A fixed point type iterative global pressure solution (IGPS) has been proposed as a method to determine the global pressure solution, thereby eliminating the need to solve large linear sets of equations. The average number of iterations required for time step convergence was found to be dependent upon the values chosen for the number of time steps (nts), prescribed error tolerance coefficient (ε_{max}), and relaxation parameter (ω). Values for these parameters were perturbed showing that simulations requiring a smaller ε_{max} value or having a lessor specified nts or ω value are typically shown to require more iterations for convergence at each timestep.

This IGPS method was found to significantly increase computational efficiency. The average difference in fractional leakage between the two algorithms was found to be very small with the computational cost decreasing on average by approximately one order of magnitude. From the results obtained, the simulation

of domains having large quantities of passive wells or aquifer layers would greatly benefit by using the IGPS modification. In addition, this modification would be extremely beneficial when large numbers or simulations need to be performed such as in the cases of stochastic analysis or optimization.

Acknowledgements This study was supported by the U.S. Department of Energy (DOE), National Energy Technology Laboratory (NETL) Office, under Grant DE-FE0001830. The views expressed herein are those of the authors and do not necessarily reflect the official opinions or position of the DOE-NETL.

References

1. Anderson E., Bai Z., Bischof C., et al.: LAPACK Users Guide: Third Edition. Society for Industrial and Applied Mathematics, Philadelphia. (1999)
2. Avci C.: Evaluation of flow leakage through abandoned wells and boreholes. Water Resour Res 30:2565–2578 (1994)
3. Bachu S., Bennion D.B.: Experimental assessment of brine and/or CO_2 leakage through well cements at reservoir conditions. Int J Greenh Gas Control 3:494–501 (2009)
4. Bandilla K.W., Kraemer S.R., Birkholzer J.T.: Using semi-analytic solutions to approximate the area of potential impact for carbon dioxide injection. Int J Greenh Gas Control 8:196–204 (2012)
5. Birkholzer J.T., Cihan A., Zhou Q.: Impact-driven pressure management via targeted brine extraction—Conceptual studies of CO_2 storage in saline formations. Int J Greenh Gas Control 7:168–18 (2012)
6. Buscheck T.A., Sun Y., Chen M., et al.: Active CO_2 reservoir management for carbon storage: Analysis of operational strategies to relieve pressure buildup and improve injectivity. Int J Greenh Gas Control 6:230–245 (2012)
7. Celia M.A., Nordbotten J.M., Court B., et al.: Field-scale application of a semi-analytical model for estimation of CO_2 and brine leakage along old wells. Int J Greenh Gas Control 5:257–269 (2011)
8. Chen Z., Huan G., Ma Y.: Computational methods for multiphase flows in porous media. Society for Industrial and Applied Mathematics, Philadelphia. (2006)

9. Cihan A., Birkholzer J.T., Zhou Q.: Pressure buildup and brine migration during CO_2 storage in multilayered aquifers. Ground Water 51:252–67 (2013)

10. Cihan A., Zhou Q., Birkholzer J.T.: Analytical solutions for pressure perturbation and fluid leakage through aquitards and wells in multilayered-aquifer systems. Water Resour Res (2011) doi: 10.1029/2011WR010721

11. Court B., Bandilla K.W., Celia M.A., et al.: Applicability of vertical-equilibrium and sharp-interface assumptions in CO_2 sequestration modeling. Int J Greenh Gas Control 10:134–147 (2012)

12. Crow W., Carey J.W., Gasda S., et al.: Wellbore integrity analysis of a natural CO_2 producer. Int J Greenh Gas Control 4:186–197 (2010)

13. Doster F., Nordbotten J.M., Celia M.A.: Impact of capillary hysteresis and trapping on vertically integrated models for CO_2 storage. Adv Water Resour 62:465–474 (2013)

14. Duguid A., Butsch R.J., Loizzo M., Stamp V.: Collection of baseline wellbore cement data in multiple wells in the same field. Energy Procedia 4:5130–5137 (2011)

15. Gasda S., Nordbotten J.M., Celia M.A.: The impact of local-scale processes on large-scale CO_2 migration and immobilization. Energy Procedia 4:3896–3903 (2011)

16. Gasda S.E., Nordbotten J.M., Celia M.A.: Vertical equilibrium with sub-scale analytical methods for geological CO_2 sequestration. Comput Geosci 13:469–481 (2009)

17. Gasda S.E., Nordbotten J.M., Celia M.A.: Application of simplified models to CO_2 migration and immobilization in large-scale geological systems. Int J Greenh Gas Control 9:72–84 (2012)

18. Gasda S.E., Nordbotten J.M., Celia M.A.: Determining effective wellbore permeability from a field pressure test: a numerical analysis of detection limits. Environ Geol 54:1207–1215. doi: 10.1007/s00254-007-0903-7 (2007)

19. Hantush M.S.: Modification of the theory of leaky aquifers. J Geophys Res 65:11:3717-3725 (1960)

20. Hantush M.S.: Nonsteady flow to flowing wells in leaky aquifers. J Geophys Res 64:1043–1052 (1959)

21. Hantush M.S., and Jacob C.E.: Nonsteady radial flow in an infinite leaky aquifer, Am. Geophys. Union Trans., 36: 95-100 (1955)

22. Heße F., Prykhodko V., Attinger S.: Assessing the validity of a lower-dimensional representation of fractures for numerical and analytical investigations. Adv Water Resour 56:35–48 (2013)

23. Huang X, Bandilla K.W., Celia M.A., Bachu S.: Basin-scale modeling of CO_2 storage using models of varying complexity. Int J Greenh Gas Control 20:73–86 (2014)

24. Hunt B.: Flow to a well in a multiaquifer system. Water Resour Res 21:1637–1641 (1985)

25. Javandel I., Witherspoon P.: A semianalytical solution for partial penetration in two-layer aquifers. Water Resour Res 16:1099–1106 (1980)

26. Juanes R., MacMinn C.W., Szulczewski M.L.: The Footprint of the CO_2 Plume during Carbon Dioxide Storage in Saline Aquifers: Storage Efficiency for Capillary Trapping at the Basin Scale. Transp Porous Media 82:19–30 (2009)

27. Kumar N., Bryant S.L.: Semi-analytical model to determine perforation interval for secure CO_2 storage in saline aquifers. Energy Procedia 1:3071–3078 (2009)

28. Lacombe S., Sudicky E.: Influence of Leaky Boreholes on Cross-Formational Groundwater Flow and Contaminant Transport. Water Resour (1995)

29. Mathias SA, Hardisty P.E., Trudell M.R., Zimmerman R.W.: Approximate Solutions for Pressure Buildup During CO_2 Injection in Brine Aquifers. Transp Porous Media 79:265–284 (2008)

30. Neuman S., Witherspoon P.: Applicability of current theories of flow in leaky aquifers. Water Resour. Res. 5: 817-829 (1969)

31. Nogues J., Court B., Dobossy M., et al.: A methodology to estimate maximum probable leakage along old wells in a geological sequestration operation. Int J Greenh Gas Control 7:39–47 (2012)

32. Nogues J., Nordbotten J., Celia M.: Detecting leakage of brine or CO_2 through abandoned wells in a geological sequestration operation using pressure monitoring wells. Energy Procedia 4:3620–3627 (2011)

33. Nordbotten J., Celia M.: Semianalytical solution for CO_2 leakage through an abandoned well. Environ Sci Technol 39:602–611 (2005)

34. Nordbotten J., Celia M.: An improved analytical solution for interface upconing around a well. Water Resour Res 42:1–10. (2006a)

35. Nordbotten J., Celia M.: Similarity solutions for fluid injection into confined aquifers. J Fluid Mech 561:307–327. (2006b)

36. Nordbotten, J., Celia M.: Geological Storage of CO_2, Wiley. (2012)

37. Nordbotten J., Celia M., Bachu S.: Analytical solutions for leakage rates through abandoned wells. Water Resour Res 40:1–10. (2004)

38. Nordbotten J., Celia M., Bachu S.: Injection and storage of CO_2 in deep saline aquifers: Analytical solution for CO_2 plume evolution during injection. Transp Porous media 58:339–360 (2005)

39. Nordbotten J., Flemisch B.: Uncertainties in practical simulation of CO_2 storage. Int J Greenh Gas Control 9:234–242 (2012)

40. Nordbotten J., Kavetski D., Celia M., Bachu S.: Model for CO_2 leakage including multiple geological layers and multiple leaky wells. Environ Sci Technol 43:743–749 (2009)

41. Takahashi W.: Nonlinear Functional Analysis: Fixed Point Theory and Its Applications, Yokohama Publishers, Yokohama (2000)

42. Theis C.V.: The relation between the lowering of the piezometric surface and the rate and duration of discharge of a well using groundwater storage, Am. Geophys. Union Trans., 16: 519-524 (1935)

43. Zhou Q., Birkholzer J., Tsang C.: A semi-analytical solution for large-scale injection-induced pressure perturbation and leakage in a laterally bounded aquifer–aquitard system. Transp Porous Media 78:127–148 (2009)