

An Element-Free Galerkin (EFG) Meshfree Method Model for Carbon Sequestration

P. Dinesh^{1,2,3}, P.G. Ranjith², M.R. Behera³, N. Muthu⁴

¹IITB-Monash Research Academy, IIT Bombay

Powai 400076, Maharashtra, India

Dinesh.Panneerselvam@monash.edu

²Department of Civil Engineering, Monash University

Melbourne, Victoria 3800, Australia

ranjith.pg@monash.edu

³Department of Civil Engineering, IIT Bombay

Powai 400076, Maharashtra, India

manasa.rb@iitb.ac.in

⁴Department of Mechanical Engineering, IIT Guwahati

Guwahati 781039, Assam, India

nelsonm@iitg.ernet.in

Abstract - The element-free Galerkin (EFG) meshfree method is presented to study the vertically averaged two-phase flow of carbon dioxide (CO₂) and brine during the injection and sequestration of CO₂ in the deep saline aquifer. A local nodal refinement is introduced around the injection well to capture the near-injection well asymptotic pressure solution with lesser nodal density in the domain. The stabilisation parameter study and nodal independence analysis have been performed in the EFG method to fix the stabilisation parameter (τ) and the maximum Courant number (Cr_{max}) respectively, to accurately estimate the pressure and average CO₂ saturation solution without spurious oscillations. The methodology comprises solving two simultaneous partial differential equations (PDE) involving pressure and saturation terms which are obtained by combining mass conservation (continuity equation) and momentum conservation (Darcy's law of multiphase extension) equations. These equations are sequentially solved using the Implicit Pressure and Explicit Saturation (IMPES) solution strategy to obtain the spatial and temporal distribution of aquifer bottom pressure build-up and the average CO₂ saturation and these obtained results will help to study the integrity of seal/caprock and the storage capacity of the aquifer respectively. The computed pressure and average CO₂ saturation profiles are compared and validated with existing approximate mesh-based Finite Element Method (FEM) and XFEM (extended FEM) numerical solutions and analytical solutions, and are found to be in good agreement, thus demonstrating the efficiency of the EFG meshfree methodology.

Keywords: Carbon Sequestration, Element-Free Galerkin (EFG) Meshfree Method, Vertically Averaged Multiphase Flow Model.

1. Introduction

In order to combat global warming and climate change caused by the rising CO₂ level in the atmosphere, a possible solution is geologic CO₂ sequestration (GCS) in which the supercritical CO₂ (ScCO₂) is injected into deep saline aquifers (sandstone) that have brine (dissolved salts more than five percent) as the formation water and shale or mudstone as the caprock. It is believed that GCS enables the storing of a large quantity of CO₂ in the subsurface. Over time, the injected CO₂ will get trapped in the aquifer by means of four stages of trapping mechanisms, namely, 'structural and stratigraphic trapping, residual trapping, solubility trapping and mineral trapping [1]. In order to simulate a complete trapping mechanism, one need to develop fully coupled THMC (Thermo-Hydro-Mechanical-Chemical reaction) three dimensional (3D) multiphase flow model for CO₂ injection. However, developing such a model is highly computationally expensive and its numerical solutions are highly oscillating in nature, which can be minimized by using stabilized FEM [2].

The objective of the present work is based on the first stage, i.e. structural and stratigraphic trapping mechanism, in which the buoyant CO₂ moves towards the bottom of the caprock. When the CO₂ plume starts radially spreading away

from the injection well, CO₂ displaces formation water and accumulates towards the bottom of the caprock. Recently, Ladubec et al. [3] demonstrated the application of XFEM to capture the asymptotic pressure behaviour that occurs near the injection well and used a Streamline Upwind/Finite Element Method/Finite Difference Method (SU-FEM-FDM) to approximate the distribution of CO₂ in the horizontal and sloped aquifer. In the present work, the focus is on solving the coupled PDEs of the vertically averaged multiphase flow model (VAMFM) by using a popular EFG meshless method with consideration of local nodal refinement zone around the injection well, which is very similar to grid refinement in FEM.

To the best of the authors' knowledge, this is the first work that shows the application of meshless methods such as EFG method in solving the vertically averaged multiphase flow model in a horizontal aquifer, with consideration of a local nodal refinement zone around the injection well. The shape functions that have been utilised in the EFG method are based on the moving least-squares (MLS) approximants, which are both consistent and compatible with a higher order continuous polynomial, developed initially for data interpolation [4-6]. Due to this advantage, the EFG method can capture the pressure field with sufficient accuracy closer to the discontinuity (injection well) with a relatively lower nodal density than that of FEM. The superiority of the proposed EFG methodology has been demonstrated by using square and circular shaped horizontal aquifer results and its application of numerical and analytical validation purposes.

2. Vertically Averaged Multiphase Flow Equations

The governing PDE of the vertically averaged multiphase flow model for pressure and saturation equations are developed by combining the mass conservation (continuity equation) for brine and CO₂ that are combined with the momentum conservation (multiphase extension of Darcy's law) equation. Fig. 1 shows the description of the terms involved in the governing equation and its pictorial representation of a conceptual CO₂ sequestration model in the saline aquifer and its defining parameters. The governing equations were obtained using the below several simplifying assumptions and its detailed explanation with derivation that can be found in the literature [3, 7-8].

- Both pore fluids (brine and CO₂) and solid matrix are incompressible;
- Fluid properties such as viscosity and density are constant;
- The sharp-interface exist between the fluids which separate them by gravity and leads to simple linear functions of average saturation (or effective relative permeability) and capillary pressure is zero;
- Vertical pressure variation exists across the depth of the aquifer and
- Thermal, mechanical, and chemical effects are negligible.

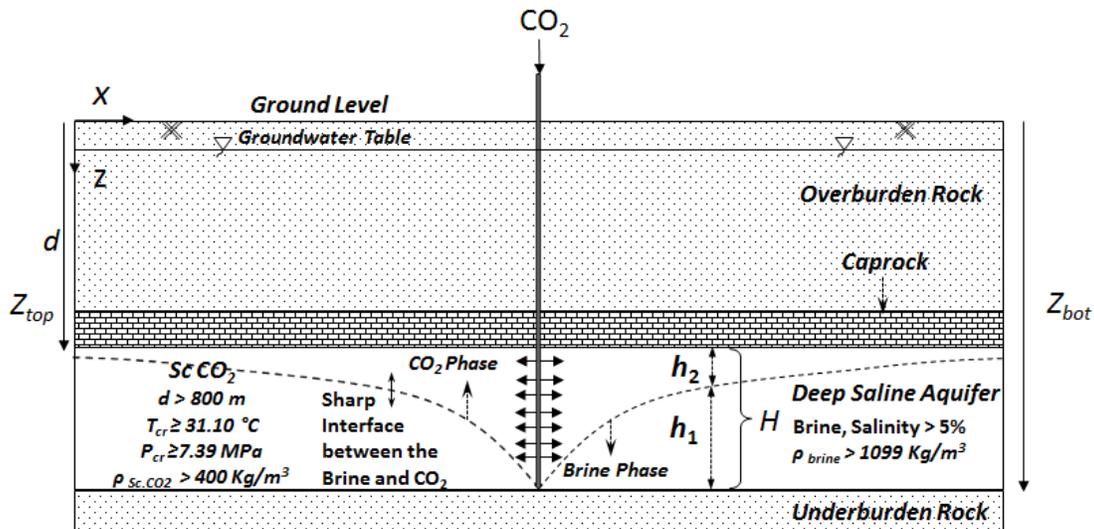


Fig. 1: A conceptual diagram of CO₂ sequestration model with defining parameters.

The mass balance equations for the brine and CO₂ phases in the aquifer are similar to Ladubec et al. [3]. The pressure is obtained by summing the individual phases of mass balance equations and its simplicity results into a single equation without time derivative. The saturation equation is one of the phase (brine phase is used in this study) equation as follows:

$$\phi(1 - S_{res,1}) \frac{\partial h_1}{\partial t} + \nabla \cdot \mathbf{u}_1^r = 0; \quad \mathbf{u}_1^r = -h_1 \frac{k}{\mu_1} (\nabla p_{bot} + \rho_1 g \nabla z_{bot}); \quad (1)$$

$$\left. \begin{aligned} \phi(1 - S_{res,1}) \frac{\partial h_2}{\partial t} + \nabla \cdot \mathbf{u}_2^r &= q_2 = Q_2 \delta(x - x_i); \\ \mathbf{u}_2^r &= -h_2 \frac{kk_{r2}}{\mu_2} (\nabla p_{bot} - \rho_1 g \nabla H + \Delta \rho g \nabla h_2 + \rho_2 g \nabla z_{top}) \end{aligned} \right\} \quad (2)$$

where the subscript 1 and 2 for wetting phase (brine) and non-wetting phase (CO₂), ϕ is the porosity of the aquifer, $S_{res,1}$ is residual saturation of the brine, $h_1(x, y, t)$ is the depth of CO₂ from $Z_{top}(x, y)$, $h_2(x, y, t)$ is the depth of brine from $Z_{bot}(x, y)$, the total aquifer depth is $H = h_1 + h_2$, and $q_2(x, y, t)$ is the source term or recharge rate to account for the injection of CO₂ into the aquifer as a point source, $\delta(x - x_i)$ is the Dirac delta function, $\mathbf{u}_1^r(x, y, t)$ and $\mathbf{u}_2^r(x, y, t)$ are the vertically averaged brine flux and CO₂ flux respectively, using the multiphase extension of Darcy's law, $p_{bot}(x, y, t)$ is the bottom pressure acting on the $Z_{bot}(x, y)$ plane and it is evolved due to the injection of CO₂ into the brine-filled aquifer, k is the intrinsic permeability tensor of the aquifer, μ_1 and μ_2 are the dynamic viscosities of the respective phases, $\Delta \rho = \rho_1 - \rho_2$ is the density difference between brine and CO₂ fluids and g is the acceleration due to gravity. Therefore, by substituting \mathbf{u}_1^r and \mathbf{u}_2^r into the corresponding mass balance equations, we can get the governing mass balance equations for the respective phases and adding Eqs. (1) and (2) gives pressure equation (3) and one of the phase (brine) Eq. (1) gives saturation equation (4) as follows:

$$\begin{aligned} &\nabla \cdot \left(-h_1 \frac{k}{\mu_1} (\nabla p_{bot} + \rho_1 g \nabla z_{bot}) \right) + \\ &\nabla \cdot \left(-h_2 \frac{kk_{r2}}{\mu_2} (\nabla p_{bot} - \rho_1 g \nabla H + \Delta \rho g \nabla h_2 + \rho_2 g \nabla z_{top}) \right) = q_2 \end{aligned} \quad (3)$$

The boundary conditions for the pressure equation can be specified as the Dirichlet boundary condition (specified pressure, p_{bot}) or Neumann boundary condition (specified flux \mathbf{u}_1^r and \mathbf{u}_2^r) throughout the boundary depending upon the type of problem interest. In this study, the specified pressure boundary condition is used throughout the study.

$$\phi(1 - S_{res,1}) \frac{\partial h_1}{\partial t} + \nabla \cdot \left(-h_1 \frac{k}{\mu_1} (\nabla p_{bot} + \rho_1 g \nabla z_{bot}) \right) = 0 \quad (4)$$

The boundary conditions for the saturation equation can be specified as the Dirichlet boundary condition. Initially, the aquifer depth is fully saturated with brine, i.e. ($H = h_1$ and $p_{bot} = \rho_1 g H$ at the time, $t = 0$). The average saturation for brine phase — $S_1 = h_1/H$ and for CO₂ phase — $S_2 = h_2/H$ (i.e. $S_1 + S_2 = 1$ or $h_1 + h_2 = H$).

3. Application of the EFG Method

In this study, a meshless EFG method based on the MLS scheme for VAMFM equations in porous media is developed. Unlike FEM, the element topology is lost in the EFG method. In this EFG method, a background mesh is used for domain integration, and the MLS technique [5] is used to generate nodal shape functions [6]. The support set is used to generate the MLS shape functions to compute the field approximation [9]. Fig. 2 shows the circular domains of influence of a fixed size ($1.75 \times \delta$) where δ is the distance between two adjacent nodes for a square-shaped aquifer domain having 11×11 nodes with the closer view of a triangular integration cells using 7th order polynomial (13 Gauss points).

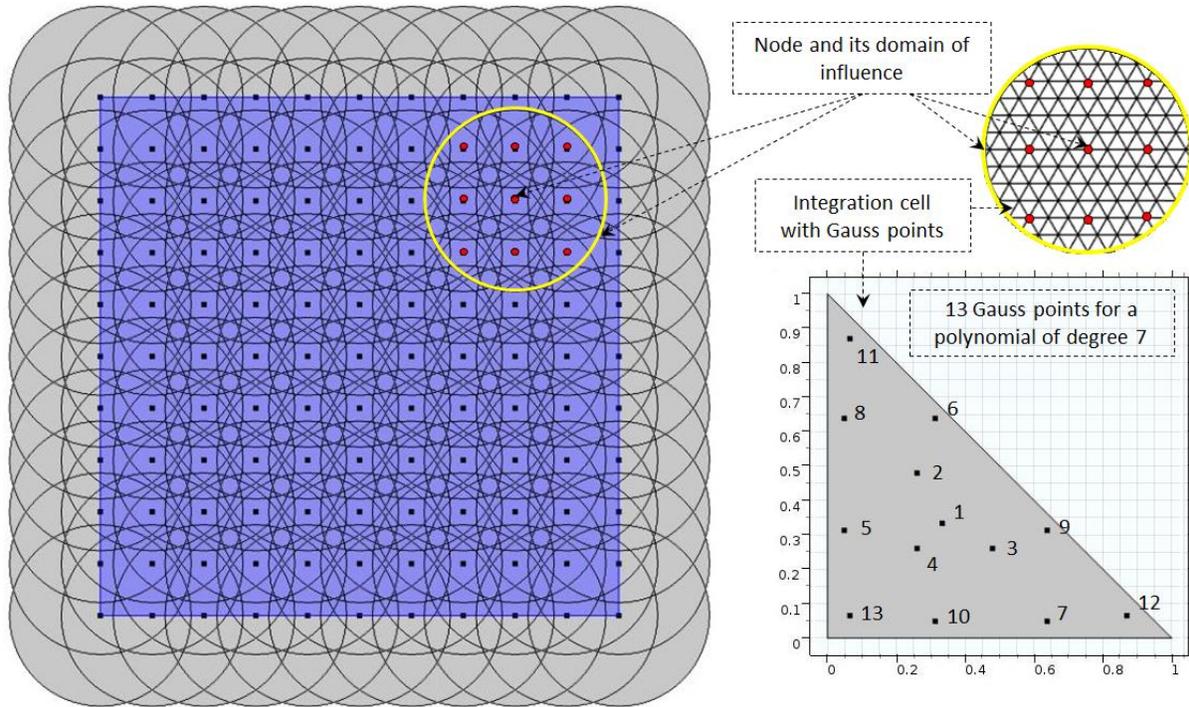


Fig. 2: The domain of influence (DMI) for the field nodes with background integration cells and Gauss points.

The representation of the field variable in the EFG method follows the conventional FEM form. The bottom pressure (p_{bot}) and height of brine (h_1) in the coupled system of PDE equations in the VAMFM can be approximated using the MLS scheme. Let us write the approximation for a general variable, e.g. $\hat{u}(x)$ for $u(x)$, which can be evaluated at a point $x \in \Omega$ as

$$u(x) \approx \hat{u}(x) = \sum_{j=1}^m p_j(x) a_j(x) = p^T(x) a(x) \quad (j = 1, 2, \dots, m), \quad (5)$$

where $P(x)$ is a standard complete polynomial of order m . In this study, a linear basis is used in 2D form, $p^T(x) = [1 \ x \ y]$. The term $a(x)$ is the unknown coefficient vector obtained using the weighted residual principle [5]:

$$a(x) = A^{-1}(x) B_k(x) u_k \quad (6)$$

By substituting the above obtained unknown coefficient into the approximation leads to the MLS based EFG shape function:

$$\hat{u}(x) = \sum_{j=1}^m p^T(x) A^{-1}(x) B_k(x) u_k = \sum_{k=1}^N N_k(x) u_k; \quad N_k(x)_{[1 \times k]} = p^T(x)_{[1 \times 3]} A^{-1}(x)_{[3 \times 3]} B_k(x)_{[3 \times k]}, \quad (k = 1, 2, \dots, N), \quad (7)$$

where N_k is the shape function or basis function of the MLS approximation of node k . In this study bell-shaped Cubic B-spline weight function is used and the matrices $A(x)$ and $B(x)$ are expanded as follows:

$$A(x) = \sum_{k=1}^N W(x-x_k) p(x_k) p^T(x_k) = \sum_{k=1}^N W(x-x_k) \begin{bmatrix} 1 & x_k & y_k \\ x_k & x_k^2 & x_k y_k \\ y_k & x_k y_k & y_k \end{bmatrix}; \quad B_k(x) = W(x-x_k) p(x_k) = W(x-x_k) \begin{pmatrix} 1 \\ x_k \\ y_k \end{pmatrix}, \quad (k = 1, 2, \dots, N) \quad (8)$$

4. Numerical Results

The discrete system of equations is obtained from the spatial and temporal discretization of governing coupled system of weak forms of PDE equations having pressure and saturation terms as it is explained in Ladubec et al. [3] except the substitution of EFG shape function for its FEM formulation. In this work, the pressure (elliptical PDE) and saturation equations (hyperbolic PDE with an added Streamline Upwind artificial diffusion term that counteracts the spurious oscillations occurring in the solution of CO₂ saturation from Galerkin FEM formulation) are discretised both spatially using EFG method and temporally using FDM to obtain discrete system of the equations. Finally, the obtained discrete system of equations is solved by using the IMplicit Pressure and EXplicit Saturation (IMPES) solution strategy as explained by Ladubec et al. [3]. Fig. 3 shows the considered square and circular domain shaped horizontal aquifer problem description with its EFG nodal discretization (41×41 nodes) over the domain and the local nodal refinement zone (15×15 nodes) around the injection well. Table 1 shows the assumed aquifer system and its fluid properties.

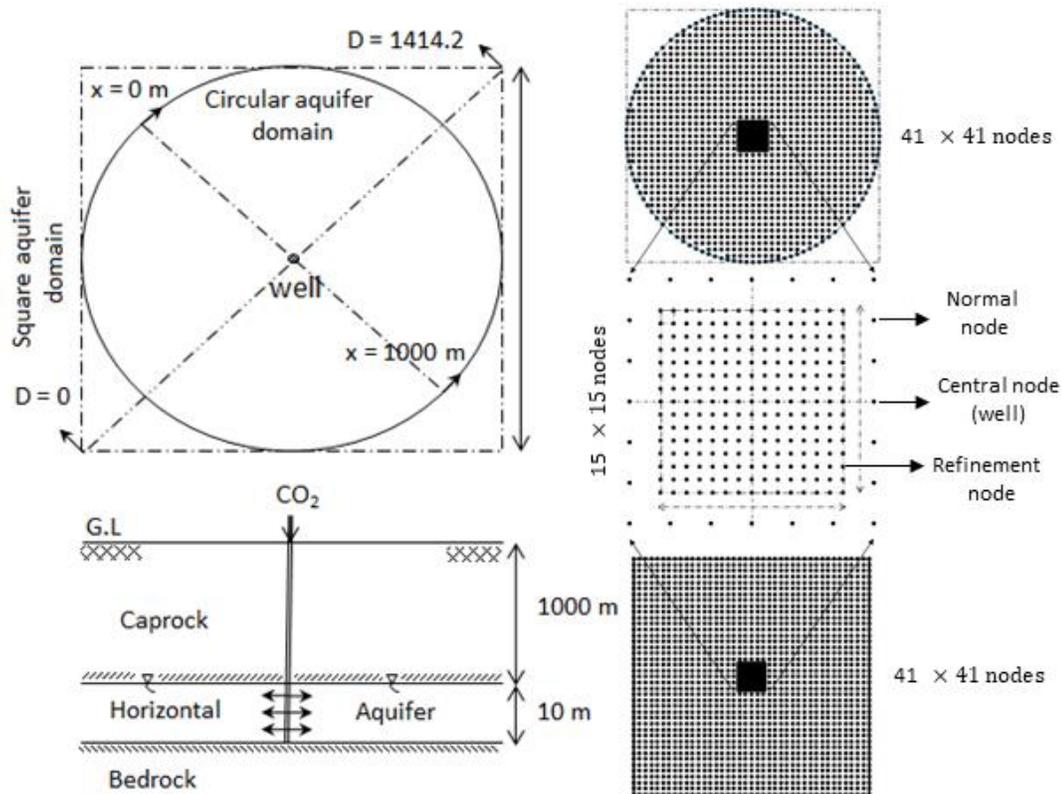


Fig. 3: Set-up of the square and circular shaped horizontal adapted from Ladubec et al. [3] with its EFG nodal discretization.

After performing several numerical experiments for the effect of the stabilization parameter (τ) on the pressure and saturation solution, the optimum τ value ranges from 0.15 to 0.2 for the Table 1 system properties. Fig. 4 shows the performance of EFG mesh (nodal) independent study at $Cr_{\max} = 0.3780$ and $\tau = 0.2$, for the pressure and its relative error at the injection well. The Courant number is defined as $Cr = \frac{\|a\|\Delta t}{\Delta x}$, where $\|a\|$ is, $\|a\| = -\frac{k}{\varphi(1-S_{res,1})\mu_1}(\nabla p_{bot} + \rho_1 g \nabla z_{bot})$ advection velocity, Δt is the size of time step and Δx is the minimum nodal distance between any two adjacent nodes in both the coordinate directions. The remaining notations in the $\|a\|$ term are same as those described in the above Eqs. (1)-(2).

Table 1: System properties for all the case study problems that were adapted from Ladubec et al. [3].

Property	Value	Units	Description
μ_1	5.11e-4	Ns/m ²	Viscosity of brine
μ_2	6.11e-5	Ns/m ²	Viscosity of CO ₂
ρ_1	1099	Kg/m ³	Density of brine
ρ_2	400	Kg/m ³	Density of CO ₂
$S_{res,1}$	0	-	Residual saturation of brine
ϕ	0.15	-	Aquifer porosity
k	1e-15	m ²	Aquifer permeability
$k_{r,2}$	1	-	Relative permeability of CO ₂
Q_2	1600	m ³ /d	Injection rate of CO ₂

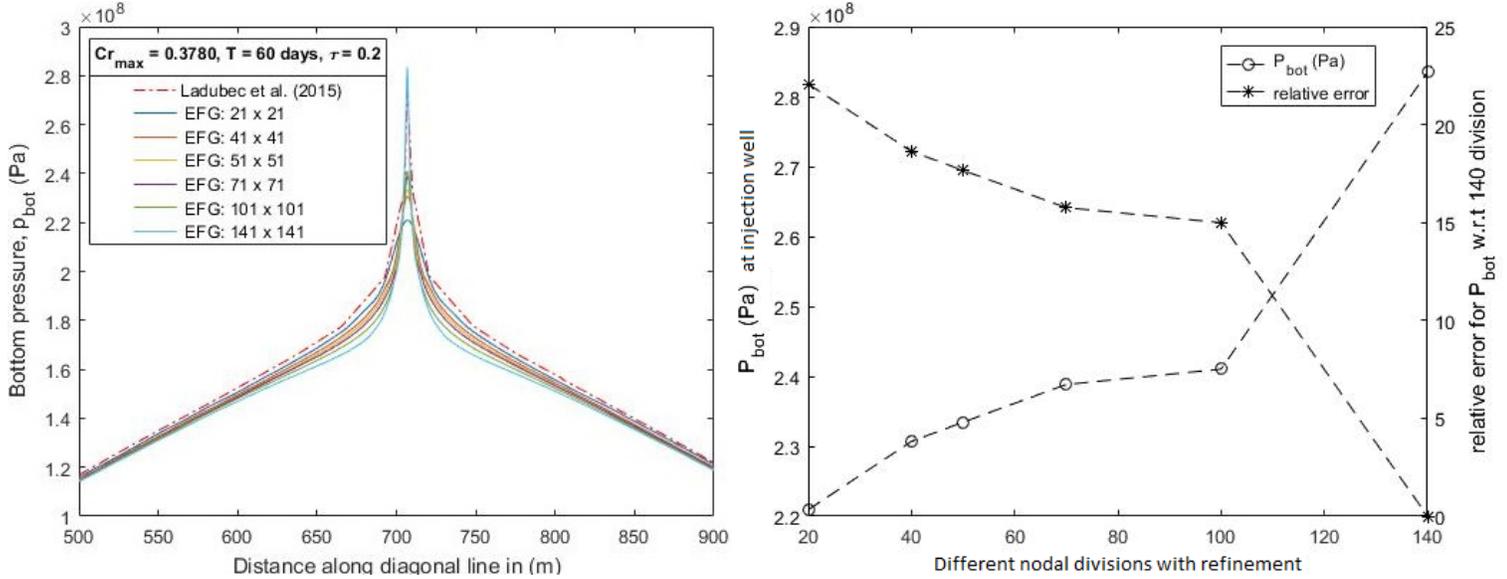


Fig. 4: The pressure solution and its EFG nodal independent analysis at maximum courant number of 0.3780 and τ is 0.2.

4.1. Analytical and Numerical Validation

Nordbotten et al. [10] developed an analytical solution for the CO₂-brine interface by imposing (a) neglecting the gravity term in the flow equation, thus predominating viscous dissipation, and (b) volume balance, (c) gravity override (CO₂ plume travels preferentially along the top) and (c) they minimize energy at the well. The fluid pressure applies over the entire thickness of the aquifer and fluid properties were vertically averaged [11]. Thus, the derivation of present

vertically averaged flow model also follows the very similar assumptions. Under these conditions, the pressure build-up (p_{bot}) and the thickness of the CO₂ (h_2) plume at time t and radial distance r was governed by the Eqs. (9) – (10), as described in [10-11] as follows:

$$p_{bot} - p_o = \frac{Q_2 \mu_1}{2\pi H k} \begin{cases} \ln\left(\frac{R}{r_o}\right) + \sqrt{\frac{\mu_2 \phi \pi H}{\mu_1 V(t)}}(r_o - r_b) + \frac{\mu_2}{\mu_1} \ln\left(\frac{r_b}{r}\right), & r < r_b \\ \ln\left(\frac{R}{r_o}\right) + \sqrt{\frac{\mu_2 \phi \pi H}{\mu_1 V(t)}}(r_o - r), & r_b \leq r < r_o \\ \ln\left(\frac{R}{r}\right), & r \geq r_o \end{cases} \quad (9)$$

$$h_2 = H \frac{\mu_2}{\mu_1 - \mu_2} \left(\sqrt{\frac{\mu_1 Q_2 t}{\mu_2 \phi \pi H r^2}} - 1 \right) \quad (10)$$

where all the notations are same as those described above in Eqs. (1) – (2) except, $p_o = \rho g H$ is the initial aquifer pressure, R is the radial length of circular aquifer domain and r_o and r_b are the radii of the top and bottom of the plume is given as:

$r_b = \sqrt{2Q_2 t / \pi \phi H \Lambda_{21} (e^{2/\Lambda_{21}} - 1)}$, and the dimensionless parameter is given by $\Lambda_{21} = Q_2(\mu_1 - \mu_2) / 2\pi k H^2 g (\rho_1 - \rho_2)$ and that measures the relative importance of viscous and gravity forces.

Fig. 5 shows the developed EFG circular domain model results and its comparison with above described analytical model results. Fig. 6. shows the EFG model results (41×41 nodes) are compared with the respective Ladubec et al. [4] XFEM pressure solution and the Streamline Upwind/Finite Element Method/Finite Difference Method (SU-FEM-FDM) average CO₂ saturation solution (150×150 elements) after 60 days of CO₂ injection in the water-filled deep saline aquifer.

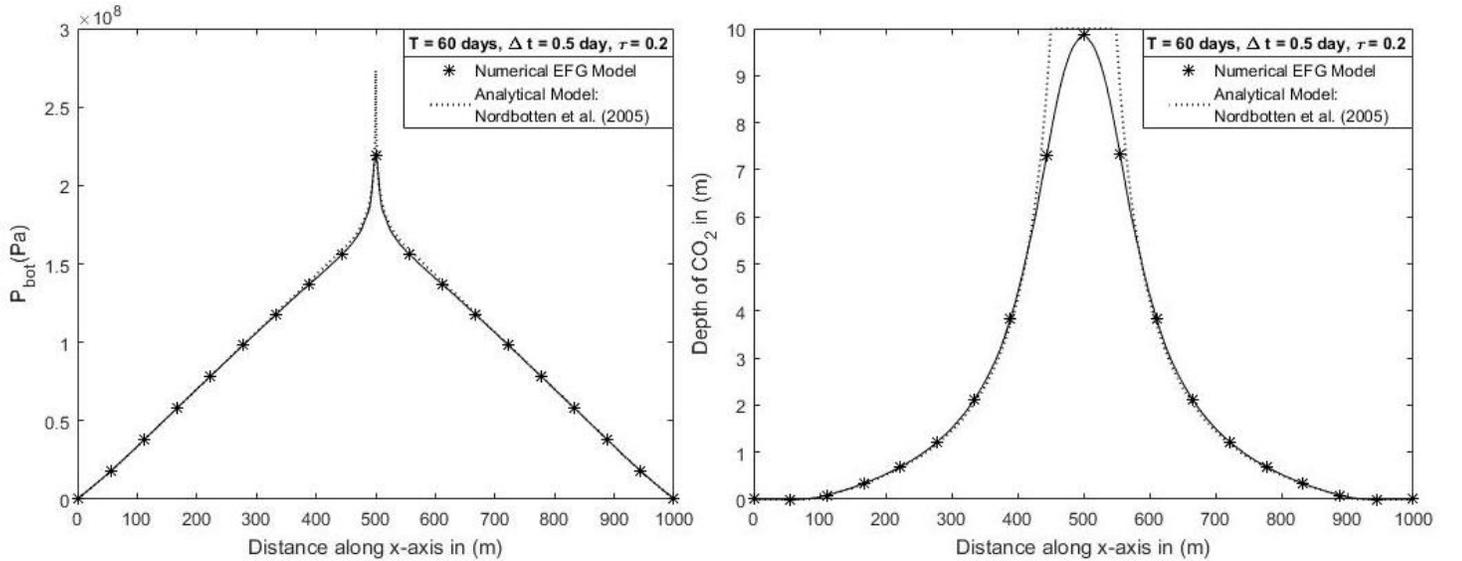


Fig. 5: Comparison of analytical and numerical EFG model for pressure and average CO₂ saturation from circular aquifer domain.

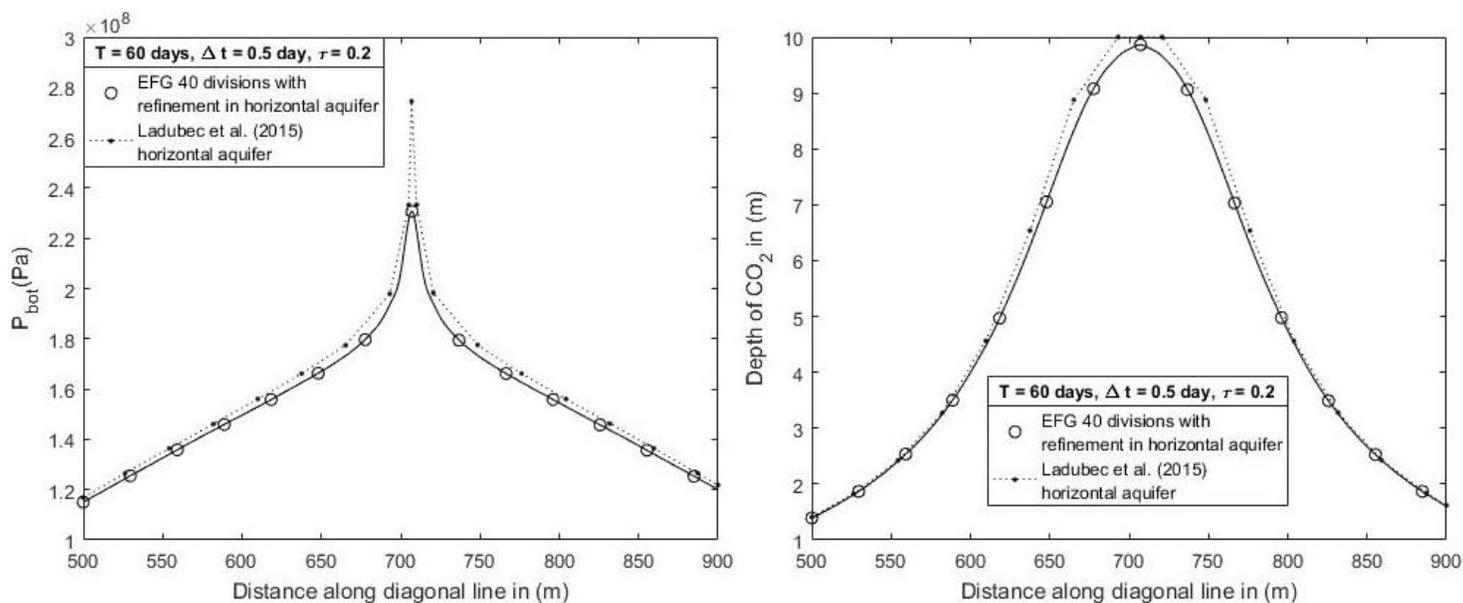


Fig. 6: Comparison of numerical XFEM and EFG model for pressure and average CO₂ saturation from square aquifer domain.

5. Conclusion

The present study demonstrated the application of the EFG method in solving the coupled system of PDEs in the vertically averaged multiphase flow model for carbon sequestration in deep saline aquifers. In order to avoid spurious oscillations occurring in the solution of CO₂ saturation from Galerkin formulation, the nodal independence and the stabilization parameter study procedure were performed to select the maximum Courant number (Cr_{max}) and the optimum stabilization parameter (τ), respectively. The obtained square-shaped horizontal aquifer EFG model pressure and average CO₂ saturation results are compared and validated numerically [3] with Extended Finite Element Method (XFEM) for pressure approximation and Streamline Upwind/Finite Element Method/Finite Difference Method (SU-FEM-FDM) for average CO₂ saturation, respectively. The numerical validation results with Ladubec et al. [3] showed that the application of vertically averaged multiphase flow EFG model was able to capture the 150×150 mesh density of the FEM benchmark results [3] using 41×41 nodal density of the EFG with 15×15 local nodal refinement around the injection well accurately without compromising its computational efforts and demands. Similarly, the obtained circular shaped horizontal aquifer EFG model pressure and average CO₂ saturation results are also compared and validated analytically [10-11] for pressure and saturation approximation by using Eqs. (9) and (10), respectively. Thus, the developed EFG meshfree method for vertically averaged multiphase flow model in carbon sequestration was successfully validated with both numerically and analytically.

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