

Imperial College of Science, Technology and Medicine
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Discontinuous Pressure Approximations for Modeling Multiphase Flow in Complex Porous Media

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Abstract

The control volume finite element (CVFE) method provides a flexible framework for modeling multiphase flow in complex porous media domains. This method employs two meshes—the element mesh and the control volume mesh—to represent the flow field and the transport solution, respectively. In the presence of material heterogeneity, the dual-mesh approach introduces inconsistency due to the control volume construction spanning element boundaries. This inconsistency leads to inaccuracies in the transport solution, which are further exacerbated when encountering sharp material interfaces or discontinuities.

In this thesis, two approaches are developed for addressing the inconsistency challenge exhibited in the CVFE method. First, the hybrid control volume finite element (HyCVFE) method is developed. This approach combines the best features of continuous and discontinuous approximations within a single framework. It applies an efficient, continuous approximation in subdomains with homogeneous or smoothly varying material properties, while exclusively using a discontinuous approximation along subdomain boundaries. The control volumes constructed by this approach are restricted within each subdomain, ensuring accurate transport solutions. The method is validated and demonstrated to outperform other CVFE approximations in the presence of heterogeneity, requiring minimal computational overhead for embedding discontinuities.

The second developed approach is based on a single mesh control volume finite element (SM-CVFE) method. The discretization of the proposed new element pair allows for a one-to-one mapping between the element mesh and control volume mesh. This ensures correct representation of material property between adjacent elements, leading to accurate saturation distributions. The approach is shown to naturally honor geo-statistically mapped material properties. Further extensions to the SM-CVFE framework are described, demonstrating the method’s superiority in capturing 3D multiphase flow solutions without exhibiting mesh sensitivity.

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Statement of originality

I, Jumanah Al Kubaisy, hereby declare that this thesis, entitled "Discontinuous Pressure Approximations for Modeling Multiphase Flow in Complex Porous Media," is entirely my own work, except where clearly indicated. To my knowledge

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Journal publications

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Chapter 1

Introduction

1.1 Motivation and Objectives

Accurate and efficient numerical methods for modeling coupled physical processes are essential components for sustainable environmental practices and economic prosperity. They are indispensable for understanding and predicting flow dynamics and transport patterns in subsurface models. Those tools complement the design and execution phases of many applications including the management of groundwater, energy and other natural resources, as well as contaminant remediation techniques.

The current subsurface formations are the culmination of sediment deposition spanning millions of years, shaped by a series of natural forces, from tectonic movements to volcanic eruptions. Historically, subsurface models often simplified the inherent complexity of these systems due to the associated uncertainty in characterization and limitations in computational power for data processing. However, there is now a growing interest in achieving a more accurate representation of complex subsurface features and material heterogeneities. This includes mapping features such as faults, facies transitions, layering, and the presence of fractures [Nelson, 2001], that introduce temporal and spatial effects with variable scales on the flow field [Matthäi et al., 2007; Matthäi et al., 2010].

Traditional flow simulation tools employ gridding approaches based on Cartesian grids, corner point geometries, or perpendicular bisection (PEBI or Voronoi) grids. Cartesian grid blocks utilize a straightforward numerical approximation such as the two-point flux approximation, but they fall short in accurately representing geological features [Helne-
mann et al., 1991; Jackson et al., 2015]. To accommodate various heterogeneous features, Cartesian grid blocks require using fine meshes globally, which can result in severe inefficiency. Using corner point geometries [K. Ponting, 1989] provide a more flexible meshing scheme but can compromise mesh orthogonality [Helne-
mann et al., 1991; Jackson et al., 2015]. As a consequence, dealing with non-k-orthogonal grids require more sophisticated approximation methods, such as the multi-point flux approximation (MPFA) scheme [Aa-
vatsmark et al., 1994; Aavatsmark et al., 1996; Aavatsmark et al., 1996] which can suffer from deteriorating convergence [Aavatsmark et al., 2007]. Voronoi grids that are gener-
ated via PEBI algorithm [Helne-
mann et al., 1991] are known for flexible geometries in 2D while implementing TPFA Mlacnik et al. [2006]. The 3D representations of the model are projected using the constructed 2D plane in order to ensure the orthogonality of the mesh along the third dimension [Mlacnik et al., 2006]. However, this limit their geometrical flexibility for capturing complex 3D domains.

Control volume finite element methods are well established for modeling coupled flow and transport in complex porous domains using unstructured meshes [Durlofsky, 1993; Fung et al., 1992; Geiger et al., 2004]. The flow field is resolved on the element mesh with petro-
physical properties mapped onto elements, while the control volumes necessary to ensure mass conservative transport solution are constructed by a dual mesh spanning element boundaries [Geiger et al., 2004; Jackson et al., 2015; Gomes et al., 2017; Salinas et al., 2018]. However, the control volumes that span element boundaries introduce non-physical leakage in the numerical solution of transported fields such as saturation, concentration or temperature. The leakage of the solution is exacerbated for sharp element-to-element variations in the material properties. A common practice to overcome non-physical leakage while using conventional CVFE approaches is based on refinement of the mesh where

material properties vary abruptly. As fine elements would in turn shrink the control volume dual mesh near the discontinuities resulting in a reduction of the mass leakage. More recently, Salinas et al. [2018] proposed an alternative CVFE approach that employed high order, fully discontinuous element pair and prevented the control volumes from spanning different regions. As a trade-off to improved accuracy, this method require prohibitively many more degrees of freedom.

This work focuses on investigating and developing numerical techniques for modeling multiphase flow within complex porous media systems. The primary objectives are three-folds

- Addressing the inherent challenge of control volume finite element (CVFE) methods to accurately capture transport solutions in the presence of material heterogeneities.
- Creating an efficient formulation capable of modeling multiphase flow in complex porous media domains. Efficiency here is defined by the ability to achieve optimal balance between computational requirement and mesh resolution.
- Ensuring the developed approach yields monotone, stable solutions for both flow and transport variables. The success of the formulation is demonstrated through a series of challenging numerical experiments, including scenarios with abrupt interfaces (material discontinuities), complex geometries in porous media, and substantial differences in element sizes between neighboring elements.

Chapter 2

Background

2.1 Introduction

Numerical methods provide powerful tools for solving partial differential equations governing physical processes. As modeling scenarios grow more complex representing real-world applications, those approaches offer the primary means to approximate dynamic variables in space and time. Numerical methods that couple physical processes, i.e. flow and transport in porous media, are used in many applications across various domains ranging from underground CO_2 storage [Kelemen et al., 2019] to groundwater modeling [Neretnieks, 1980; Forsyth, 1991; Karatzas, 2017] and contaminant transport assessment [Karatzas, 2017; Banaei et al., 2021].

We first review the governing equations that serve as the mathematical description of porous media flow and transport in Section 2.2. Then Section 2.3 briefly describes classical key methods for solving multiphase flow problems and highlight their differences. Finally, we shed some light on more nuanced methods developed to handle challenging models, particularly those that incorporate abrupt material interfaces and complex geometrical features.

2.2 Governing equations

Consider Darcy's law that describes fluid flow through porous media. The total fluid Darcy velocity ($\mathbf{v}_t$) is given by

$$\mathbf{v}_t = -\lambda_t \mathbf{K} \cdot \nabla p, \quad (2.1)$$

where $\mathbf{K}$ and ∇p are the permeability tensor and the pressure gradient, respectively. Here the gravity and capillary forces are neglected. For a two phase system, the total mobility (λ_t) is the summation of the wetting phase mobility (λ_w) and the non-wetting phase mobility (λ_{nw}) as

$$\lambda_t = \frac{k_{r,w}(S_w)}{\mu_w} + \frac{k_{r,nw}(S_w)}{\mu_{nw}}, \quad (2.2)$$

Here k_r is the relative permeability, that is a function of the saturation S_w , and μ is the fluid viscosity. The subscripts w and nw denote the wetting and non-wetting phases, respectively. The continuity equation of the incompressible system is given by

$$\nabla \cdot \mathbf{v}_t = q_t, \quad (2.3)$$

where q_t denotes a source term. Now consider the fractional flow form of the mass balance equation for the wetting phase

$$\phi \frac{\partial S_w}{\partial t} + \nabla \cdot (f_w \mathbf{v}_t) = q_w, \quad (2.4)$$

where ϕ is the porosity of the medium, S_w is the wetting phase saturation, t is time and q_w is a source term for the wetting phase. The fractional flow of phase α (f_α) is given by

$$f_\alpha = \frac{\lambda_\alpha}{\lambda_t}. \quad (2.5)$$

We solve the mass balance equation for the unknown saturation subject to

$$S_w + S_{nw} = 1, \quad (2.6)$$

in order to constrain the total volume fraction.

2.3 Numerical methods for coupled flow and transport in porous media

We are interested in numerical methods that discretize the computational domain and subsequently transform partial differential equations into equivalent algebraic systems. These systems can then be solved to yield approximations of primary variables. Several methods have been developed and adopted for modeling multiphase flow in porous media. In this section, we cover the shortcomings of some classical methods with limitations in accuracy to preserve heterogeneous features and realistic geological representations.

2.3.1 Finite difference and finite volume methods

In the finite difference method, the solution is estimated at a discrete set of points $(x_1, x_2, \dots, x_{N+1})$. This numerical approach leverages Taylor series expansions to derive differential operators, allowing the transformation of the underlying differential equation into a system of algebraic equations [LeVeque, 2007]. The resulting algebraic problem is represented as:

$$\mathbf{A}u = b, \tag{2.7}$$

where $\mathbf{A}$ captures the discretized form of the differential operators, u is the vector of unknowns representing the approximate solution at discrete points, and b captures the discretized form of the source terms or boundary conditions, see Aziz and Settari [1979]; LeVeque [2007] for additional details.

The finite volume method, on the other hand, computes the solution within control volumes that partition the domain into discrete blocks rather than a set of points. Each control volume (CV) has its associated faces and reflect distinct properties within the

block [Aziz and Settari, 1979]. The approach employs integral formulation of conservation laws to derive discrete equations for each control volume [Aziz and Settari, 1979]. Green's theorem is used to convert the integral over the control volume and the central difference handles the spatial derivative terms [Aziz and Settari, 1979]. The finite volume approach is most closely associated with the physical meaning of the conservation equation and, in practice, it is the preferred approach given the symmetry of its assembled matrices in addition to the method being suitable for material balance calculations [Aziz and Settari, 1979]. The approach is extensively used in many practical and industrial applications [Lie, 2019]. In the remaining part of this section, we emphasize relevant aspects of classical FV methods pertinent to this work and recognize that there have been recent advancements in FV methods that extend beyond the scope of this study. For a comprehensive description of finite difference and finite volume methods see Forsythe and Wasow [1960], Henrici [1962], Saul'yev [1964], Wendroff [1968], Lapidus and Seinfeld [1972], and Ames [1977].

The governing equations describing coupled systems of flow and transport have been traditionally solved using finite difference methods on structured meshes [Aziz and Settari, 1979; Douglas, 1983] or finite volume methods on both structured or unstructured meshes [Narasimhan and Witherspoon, 1976]. When using the FV method for the flow model, the primary unknown for solving the global model is the pressure. The flux continuity principle is then applied such that the flux over a CV interface (Γ_i) is

$$\text{flux}_{\Gamma_i} = - \int_{\Gamma_i} (\lambda_{t,i} K_h \nabla p) \cdot \mathbf{n} d\Gamma_i, \quad (2.8)$$

where $\lambda_{t,i}$ is the approximation of the total mobility on the interface, K_h is the harmonic permeability of the control volumes CV_a and CV_b as shown in Fig 2.1a. ∇p is the pressure gradient of the control volumes. Therefore, in the classical implementation of FV method, two control volumes are used to construct continuous fluxes. This approach is referred to as the two-point flux approximation (TPFA). The convergence of the TPFA scheme is only guaranteed for K-orthogonal grids [Lie, 2019], i.e. grids based on the alignment between

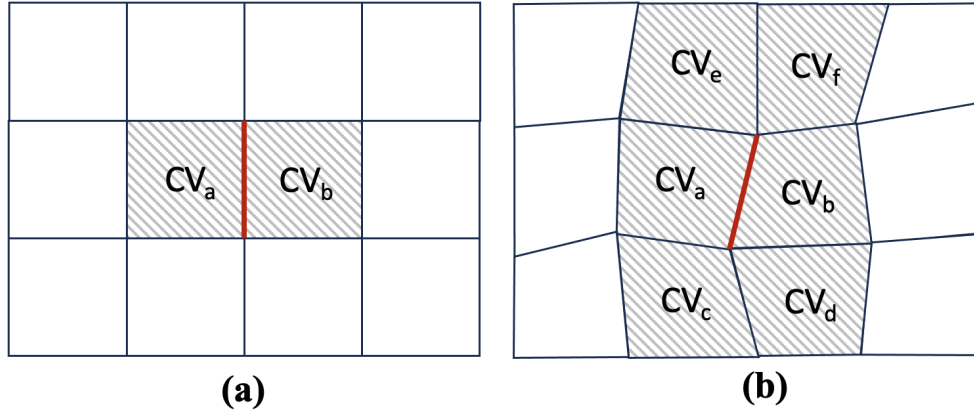


Figure 2.1: In the FV method, the continuity of flux over the red interface is computed from the solution of the shaded control volumes in two types of grids: **(a)** The two-point flux approximation for K-orthogonal grids. **(b)** The multi-point flux approximation for general quadrilateral grids.

principal axes of the permeability tensor with the computational grid [Edwards, 2002]. However, when employing the TPFA scheme on non-k-orthogonal grids, significant grid orientation effects are observed [Wu and Parashkevov, 2009] due to the lack of consistency associated with the approximation [Lie, 2019].

In general, grid orientation effects introduce inaccuracies into the numerical solution due to the misalignment between the computational grid with the principle directions of the permeability tensor [Lie, 2019]. There have been significant efforts investigating grid orientation effects in the literature [e.g., Aavatsmark, 2007; Wu and Parashkevov, 2009] and others that aim to reduce its effects [Helnemann et al., 1991; Gunasekera et al., 1997; Mlacnik et al., 2006].

The generalization of TPFA for any quadrilateral grids was later developed [Aavatsmark et al., 1994; Aavatsmark et al., 1996; Aavatsmark et al., 1996], the approach known as multi-point flux approximation (MPFA). Fig 2.1b shows the additional neighboring cells contributing to the flux calculation of the interface (Γ_i). A variation of the MPFA was also developed independently by G. Edwards and F. Rogers [1994; Edwards and Rogers [1998]. Some of the drawbacks associated with the MPFA are the additional compu-

tational requirements, convergence issues of the approximation [Eigestad and Klausen, 2005; Aavatsmark et al., 2007], non-monotonicity, and limitation to accommodate strong anisotropic permeability fields [Chen et al., 2008; Samier and Masson, 2017]. Consequently, extensive efforts have been dedicated to investigating the monotonicity and convergence of MPFA [e.g., Aavatsmark et al., 2008, 2007; Aavatsmark and Eigestad, 2006; Klausen and Winther, 2006; Keilegavlen et al., 2009; Nordbotten et al., 2007; Nordbotten and Eigestad, 2005; Nordbotten and Aavatsmark, 2005].

Over the past two decades, variations of FV methods have emerged to incorporate fine-scale features into coarse grid models (e.g., multiscale finite volume method by Jenny et al. [2003]). The approach employs a multi-point discretization scheme to capture the fine-scale flow field. Further development of the formulation to accommodate multiphase flow models can be found in the works of Jenny et al. [2006a]; Lunati and Jenny [2006]; Zhou and Tchelepi [2012], as well as extensions to unstructured grids by Møyner and Lie [2013, 2014].

2.3.2 Finite element method

The finite element (FE) method stands as a powerful numerical technique employed in numerous applications. Two approaches associated with the FE method are the variational principle and the Galerkin weighting method; for additional details and differences between the approximations, refer to Zienkiewicz and Taylor [2002]. Both approaches transform the strong form of the problem to the weak form by multiplying with a test function and subsequent integration. The variational principle is essentially based on a minimization concept where the solution is sought in a function space, often minimizing an energy functional [Zienkiewicz and Taylor, 2002]. The minimization process leads to an approximation of the solution to the original partial differential equation (PDE) problem.

On the other hand, the Galerkin method (or the method of weighted residuals) is the general, widely used approach in the FE method [Zienkiewicz and Taylor, 2002; Hughes,

1987] and is relevant to this work. Once the weak form is established, the FE method works by discretizing the domain into a set of elements. Then the solution (u) is approximated by

$$u \approx \hat{u} = \sum_{i=1}^n a_i \phi_i(x), \quad (2.9)$$

here $\hat{u}$, n , a , and ϕ are the solution approximation, the number of degrees of freedom, the unknown coefficients, and the basis function, respectively (see Zienkiewicz et al. [2005] for additional details). The basis function (ϕ) is a locally supported piecewise polynomial. Two types of FE methods are of interest in this work: the Galerkin (Bubnov-Galerkin) approach and the Petrov-Galerkin approach.

In the Bubnov-Galerkin (or simply Galerkin) finite element method, the applied basis functions also serve as the test (or weighting) functions. This often results in symmetric matrices with desirable properties for solving in various solution algorithms [Huyakorn and Pinder, 1983; Zienkiewicz and Taylor, 2002]. On the other hand, the Petrov-Galerkin approach works by applying a different shape function to the test function. This enables the approach to be tailored to specific features of the problem, such as modeling discontinuities in the flow or rapidly changing solutions (e.g., see Burns et al. [2005]; Mizukami and Hughes [1985]).

2.3.3 Control volume finite element method

The control volume finite element (CVFE) method is inherently flexible for modeling multiphase flow and transport in such complex porous media, and is well documented in the literature [Forsyth, 1991; Fung et al., 1992; Durlofsky, 1993, 1994; Bastian and Helmig, 1999; Edwards, 2002; Geiger et al., 2004; Paluszny et al., 2007; Schmid et al., 2013; Jackson et al., 2015; Gomes et al., 2017; Salinas et al., 2018; Tran et al., 2020]. The approach combines the finite element method that resolves flow for elliptic or parabolic problems on geometrically complex, unstructured meshes with the stable and mass conservative finite volume method for resolving the parabolic, with hyperbolic characteristic, transport

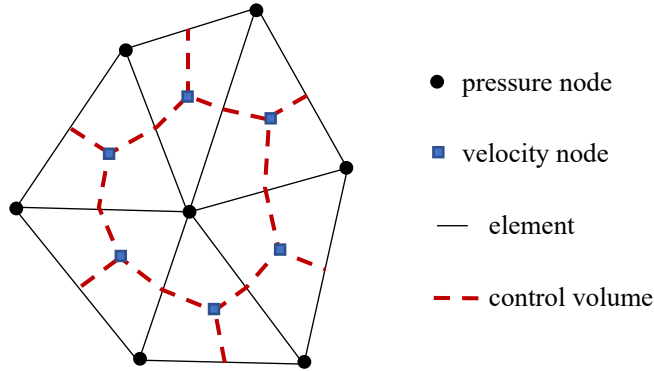


Figure 2.2: The discretization of the flow variables using the classical (CVFE) method.

problem [Durlfisky, 1993; Geiger et al., 2004]. In the CVFE approach, the discretization of primary flow and transport variables is based on two meshes, the element (primary) mesh and the control volume (dual) mesh. The variables of the flow model are the velocity and pressure; where the element pair representation using the classical CVFE is $P_{0,DG} - P_1$. This element pair denotes a low-order discontinuous Galerkin velocity approximation and a first-order Lagrangian pressure approximation, see section 2.3.6 for additional details. The element mesh describes the material properties that can vary element-wise (i.e. permeability) while the control volumes are centered on the vertices of the elements [Fung et al., 1992; Geiger et al., 2004; Jackson et al., 2015]. The fluxes within an element, lying on the control volume boundaries, are continuous by construction of the approach. Fig. 2.2 highlights the control volume mesh along with the discretization of the flow variables on the element mesh. One challenge associated with the approach involves capturing accurate saturation solution for control volumes spanning element boundaries when those elements contain contrasting material properties (i.e. they lie on either side of a sharp boundary such as a fracture wall). The shared control volumes that span these elements result in non-physical mass leaking across the boundary, contaminating the multiphase transport solution [Edwards, 2006; Salinas et al., 2018]. Consequently, the heterogeneous model is not honored.

A variant of the CVFE method, the finite element finite volume (FE-FV) method, is widely used [e.g., Huber and Helmig, 2000; Matthäi et al., 2007; Paluszny et al., 2007]. Unlike the CVFE method, the FE-FV approach only considers pressure as the primary flow unknown. However, it is important to note that this approach faces similar leakage issues due to its utilization of two different meshes for capturing the flow and transport processes.

2.3.4 Mixed finite element method

The family of mixed finite element (MFE) methods offers a flexible approach to simulate flow in heterogeneous subsurface domains [Chavent et al., 1984, 1990; Chavent and Roberts, 1991; Durlofsky, 1994; Helmig and Huber, 1998]. In the MFE method, the flow variables are estimated using an element-wise constant approximation for pressure and the lowest order Raviart-Thomas (RT) approximation for velocity (Fig. 2.3). Since the fluxes are continuous between elements, the transport is resolved on the same element mesh, ensuring a mass conservative solution [Durlofsky, 1994]. The main drawbacks of the approximation are (i) the increased computational cost: it requires between 1.5 to 4 times the degrees of freedom (DoF) used by the CVFE method [Durlofsky, 1994; Geiger et al., 2004] and (ii) the indefinite matrices assembled by the set of equations [Durlofsky, 1994]. The mixed-hybrid finite element (MHFE) method addresses the latter issue by the introduction of additional trace variables [Mosé et al., 1994; Chavent and Roberts, 1991]. More recently, the mimetic finite difference (MFD) method [Brezzi et al., 2005a,b] extended the MHFE approach to discretize any polygonal shape by the numerical evaluation of the shape function [Abushaikha and Terekhov, 2020]. The development of the MFD method for flow in porous media applications is described by several authors [Nilsen et al., 2012; Zhang and Abushaikha, 2019a,b; Abushaikha and Terekhov, 2020; Nardean et al., 2021].

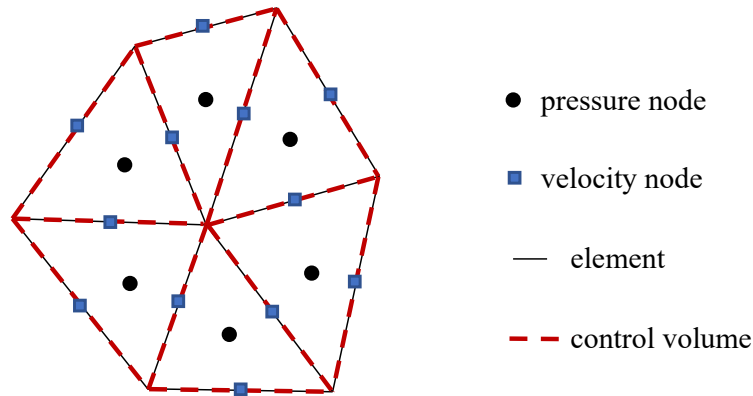


Figure 2.3: The discretization of the flow variables using the mixed finite element (MFE) method.

2.3.5 Discontinuous Galerkin methods

The Discontinuous Galerkin (DG) method offers a flexible numerical framework. Unlike the classical, continuous Galerkin method, DG allows for discontinuities in the solution across element boundaries. Essentially, each element is associated with its own set of basis functions, and the solution is approximated by piece-wise polynomials within each element [Collis et al., 2000]. DG methods are unique given the distinct treatment of inter-element boundaries. The method introduces numerical fluxes that capture the information exchanged between neighboring elements [Hughes et al., 2000]. This flux conservative approach ensures a robust handling of discontinuities and allows for high order accuracy in approximating complex solutions [Cockburn et al., 2000].

The resemblance between DG and FV methods lies in their treatment of elements or control volumes. DG can be described as a hybrid of finite volume and finite element methods, as it employs the element-wise polynomial approximations, a feature of finite element methods while incorporating the flux-based conservation approach characteristic of the finite volume method [Collis et al., 2000; Hughes et al., 2000]. This combination makes DG particularly effective in capturing sharp gradients and discontinuities in the

solution while maintaining the advantages of both finite element and finite volume approaches [Hughes et al., 2000]. For a comprehensive review of the DG methods see the work of Cockburn et al. [2000]; Cockburn [2003]; Li [2006].

The interior penalty (IP) method, introduced by [Douglas and Dupont, 1976; Wheeler, 1978], represents an early milestone in the development of Discontinuous Galerkin (DG) methods. The theoretical foundation for the IP method on non-uniform meshes and its associated error estimates were established by Arnold [1982]. Subsequent advancements in the application of the DG approach to single-phase flow in porous media using unstructured meshes can be found in the work of Rivière et al. [2000].

2.3.6 Element pair representations

The representation of the finite element variables are commonly reported by the polynomial order of approximation in the element, $P_n - P_m$, where the subscripts n and m denote the polynomial orders of velocity and pressure, respectively. We make the distinction when employing discontinuous Galerkin approximation by using the subscript *DG* following the polynomial order, similar notation used by Cotter et al. [2009], otherwise the approximation is assumed continuous. The stability analysis of the element pair of velocity and pressure variables has been the focus of Ladyzhenskaya [1969], Babuska [1971], and Brezzi [1974]. In theory, the LBB condition is an inf-sup condition necessary to ensure the well-posedness of discrete saddle point problem, in this case, resulting from Galerkin method discretization [Malkus, 1981]. In other words, if we consider the algebraic system of equation for an incompressible fluid flow given by

$$\begin{bmatrix} \mathbf{A} & \mathbf{B} \\ \mathbf{C} & \mathbf{0} \end{bmatrix} \cdot \begin{bmatrix} \mathbf{v}_t \\ p \end{bmatrix} = \begin{bmatrix} b_1 \\ b_2 \end{bmatrix} \quad (2.10)$$

where $\mathbf{v}$ and $\mathbf{p}$ are the vectors of unknowns in the system. By employing the projection-based method, we eliminate $\mathbf{v}$ from the first equation, giving

$$(\mathbf{CA}^{-1}\mathbf{B})p^{n+1} = (\mathbf{CA}^{-1}b_1) - b_2. \quad (2.11)$$

The equation shows that $\mathbf{A}$ needs to be non-singular, ensuring that the corresponding term $(\mathbf{CA}^{-1}\mathbf{B})$ remains non-singular. To prevent singularity in this context, the essential stability condition is:

$$N_p \geq N_v \quad (2.12)$$

where N_p and N_v are the number of unknowns of pressure (p) and velocity (v) in the system, respectively [Zienkiewicz et al., 2005]. The element pair $(P_{1,DG} - P_2)$ with a linear discontinuous Galerkin velocity approximation and a quadratic continuous pressure approximation was proven to meet the LBB stability condition in the work of Cotter et al. [2009] and Sollie et al. [2011].

2.3.7 Fluid velocities

In order to solve for the transport equation for multiphase flow problems, accurate and mass conservative fluxes are constructed from the velocity approximation. In the literature, two finite element formulations are commonly used; the first is based on mixed element formulation. The approach computes the pressure at the barycenter of the elements and then construct continuous fluxes on the mid-point of each edge [Chavent and Jaffre, 1986]. The other approach, used by the CVFE method, includes velocity approximation continuous at the control volume interfaces in each element, while being discontinuous between the elements. This approach ensures mass conservation of the solution over each control volume [Durlinsky, 1994].

2.3.8 Alternative formulations

Several methods have been developed to reduce or eliminate the numerical mass leakage; mass leakage is defined here as the non-physical mass transferred into the low permeability region as a result of control volume spanning heterogeneous subdomain boundaries. Fig. 2.4a shows the control volumes spanning element boundaries resulted from employing the CVFE method in the presence of material discontinuity. The interface control volume finite element (ICVFE) method, proposed by Abushaikh et al. [2015], globally applies the pressure discretization on the element edges rather than the element vertices in order to reduce the size of the overlap across elements. The control volumes constructed by this approach span at most two adjacent elements, see Fig. 2.4b. The method is effective in reducing numerical leakage; however, it does not eliminate the issue entirely and is numerically expensive.

Salinas et al. [2018] employed a fully discontinuous pressure discretization. In the Salinas et al. [2018] method, the element pair $P_{2,DG} - P_{1,DG}$ is used where the velocity and pressure are approximated using discontinuous Galerkin of second order and first order, respectively. The control volumes in this discretization are discontinuous across all element edges (Fig. 2.4c). The technique is effective in preventing numerical leakage without mesh refinement at discontinuities. The drawback of this approach is that it is numerically expensive as a result of the global duplication of pressure and velocity nodes and the higher order velocity approximation required to ensure stability. Thus, the method requires solution of prohibitively large system of equations. We note that the current development of this approach [Salinas et al., 2018] in the Imperial College Finite Element Reservoir Simulation (IC-FERST) is non-monotone and requires further investigation.

Nick and Matthäi [2011] presented a discontinuity finite element finite volume method (DFEFVM) that was initially developed for single phase flow and passive solute transport. The approach prevented control volume overlap across discontinuous interfaces by incorporating additional pressure nodes while using the continuous approach elsewhere.

The method was later extended by Tran et al. [2020] to capture capillary barriers in two phase flow problems. Strong coupling of pressure nodes across capillary discontinuities is carried out as a pre-processing step by modifying the system of equations based on the likelihood of fluid movement across the interface. Furthermore, they employed an interface condition, described by van Duijn and de Neef [1998], to determine the saturation along the capillary barrier. The approach targeted capillary interface coupling at discontinuities and has not been generalized further.

2.3.9 Grid effects and mesh quality

The mixed finite element method is consistent, i.e. does not suffer from the grid orientation effects associated with TPFA, on non-k-orthogonal grids since the flow formulation is based on the discretization of both pressure and velocity fields [Lie, 2019]. The same underlying principle applies to the flow model solved in the CVFE method and, therefore, grid orientation effects are not relevant for the CVFE approach.

The flexibility offered by unstructured grids while using the MFE method and the CVFE method enables capturing complex geometries. However, a drawback of unstructured meshes involve the occurrence of irregular cell geometries with high aspect ratios [Lie, 2019]. The convergence and performance of the FE solver is therefore impacted by the mesh quality as the conditioning of the pressure matrix depends on the size and shape of elements [Shewchuk, 2002b]. Significant efforts were devoted to generating good quality meshes [e.g., Shewchuk, 1996, 2002b; Erten and Üngör, 2009; Erten and Üngör, 2009; Si, 2015]. Shewchuk [2002b] established error bounds and element quality measures that influence the accuracy and performance of linear FE approximations on triangular and tetrahedral elements. An alternative formulation proposed by Salinas et al. [2017], the double control volume finite element method, addresses the high aspect ratio effects in the finite element flow model.

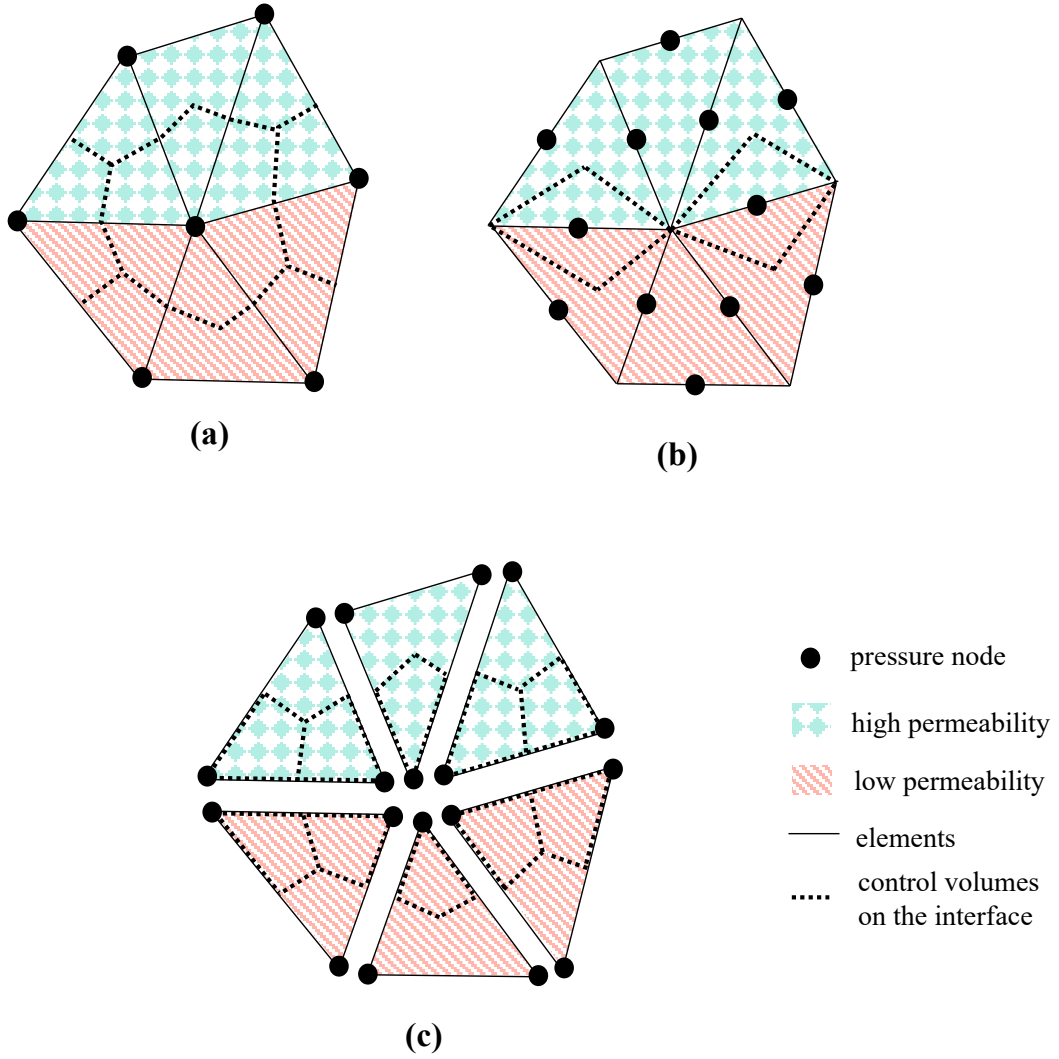


Figure 2.4: Discretization of the control volume mesh in the presence of material discontinuity: (A) the classical control volume finite element (CVFE) method [Fung et al., 1992]. (B) Interface CVFEM by Abushaikha et al. [2015]. (C) Discontinuous element pair $P2_{DG} - P1_{DG}$ by Salinas et al. [2018].

Chapter 3

A hybrid pressure approximation

The work presented in this chapter has been published in the Journal of Computational Physics:

Al Kubaisy, J., Salinas, P., Jackson, M.D., 2023. *A hybrid pressure approximation in the control volume finite element method for multiphase flow and transport in heterogeneous porous media*. Journal of Computational Physics 475, 111839.

3.1 Introduction

The control volume finite element (CVFE) method [Fung et al., 1992] applies a continuous pressure approximation (P_1) globally in the domain. While efficient, this approximation falls short in accurately representing abrupt material boundaries, leading to solutions that fail to capture accurate solutions. This limitation arises from the control volume mesh construction, spanning element boundaries and resulting in the averaging of material properties and computed quantities. In contrast, the discontinuous element pair used in Salinas et al. [2018] introduced a discontinuous pressure discretization ($P_{1,DG}$) that proved effective in capturing solution discontinuities. This specific pressure discretization prevented control volumes from spanning element boundaries.

The objective of this chapter is to formulate a hybrid control volume finite element (Hy-CVFE) method. This approach selectively applies a discontinuous pressure approximation along the boundaries of contrasting material sub-domains, while the continuous approximation is employed in the rest of the domain where material properties are homogeneous or smoothly varying. The method is designed to effectively and accurately capture multiphase flow in highly heterogeneous sub-domains with contrasting material properties, without compromising the robustness of the numerical approximation or significantly increasing computational costs compared to the classical CVFE method.

Section 3.2 details the mathematical derivation of the hybrid approach for the coupled multiphase flow and transport equations and then describes the solution method and other approximations employed in the implementation of the HyCVFE method. We validate the method and demonstrate its effectiveness with numerical experiments in Section 3.3.

3.2 Method

3.2.1 Finite element method for flow equations

The finite element method is used to solve the flow problem. First, the computational domain Ω is partitioned into a set of n_d sub-domains, $\{\Omega_d\}_{d \in [1, n_d]}$ (Fig. 3.1). Each sub-domain (Ω_d) defined by its homogeneous or smoothly varying material properties, following the approach of Jacquemyn et al. [2019] and Osman et al. [2021], and triangulated into $n_{d,e}$ elements such that $(\mathcal{T}_d = \cup_{e=1}^{n_{d,e}} \Omega_e)$ using a constrained conforming Delaunay triangulation Shewchuk [2002a]. We use the element pair $P_{0,DG} - P_{1,H}$ to discretize velocity and pressure. The velocity vector is approximated using a discontinuous element-wise representation. The pressure approximation is hybrid by having a continuous, first order polynomial representation within each sub-domain (Ω_d), but a discontinuous representa-

tion along the boundaries of the sub-domain (Γ_d) (Fig. 3.1). Let

$$\mathbf{v}_t(\mathbf{x}) = \sum_{j \in \Omega} \Phi_j(\mathbf{x}) v_{t,j}, \quad (3.1)$$

and

$$p_d(\mathbf{x}) = \sum_{j \in \Omega_d} \Psi_j(\mathbf{x}) p_j, \quad \forall d \in [1, n_d] \quad (3.2)$$

be the approximations of the total velocity and pressure fields. $\Phi(\mathbf{x})$ and $\Psi(\mathbf{x})$ are the basis functions of velocity and pressure, respectively, while v_t and p are the unknown coefficients. The hybrid approach is applied on the sub-domain boundaries by incorporating additional pressure nodes that separate the sub-domains (Fig. 3.1 (a-b)). Consequently, the nodes are continuous within each sub-domain and the discontinuous pressure approximation is applied only between the sub-domains to establish the global flow model. Fig. 3.1 (b-c) emphasizes the differences between the discretization employed here in the proposed HyCVFE method and the discontinuous method of Salinas et al. [2018]. In the latter approach, the velocity and pressure degrees of freedom placed on the element boundaries are duplicated for neighboring elements (Fig. 3.1c). Moreover, the approach of Salinas et al. [2018] employed a second order discontinuous velocity approximation that was necessary to ensure stable solutions.

Discretization of Darcy's equation

The weak form of Eqn. (2.1) is obtained by weighting with the test function $\Phi_{\mathbf{i}}$, derived from the same space as the velocity basis functions, and integrating over the domain

$$\int_{\Omega} \Phi_{\mathbf{i}} \cdot \mathbf{v}_t \, d\Omega + \int_{\Omega} \Phi_{\mathbf{i}} \cdot (\lambda_t \mathbf{K} \cdot \nabla p) \, d\Omega = 0. \quad (3.3)$$

Equivalently, the domain (Ω) is decomposed of n_d sub-domains, given by

$$\sum_{\Omega_d \in \Omega} \left[\int_{\Omega_d} \Phi_{\mathbf{i}} \cdot \mathbf{v}_t \, d\Omega_d + \int_{\Omega_d} \Phi_{\mathbf{i}} \cdot (\lambda_t \mathbf{K} \cdot \nabla p) \, d\Omega_d \right] = 0. \quad (3.4)$$

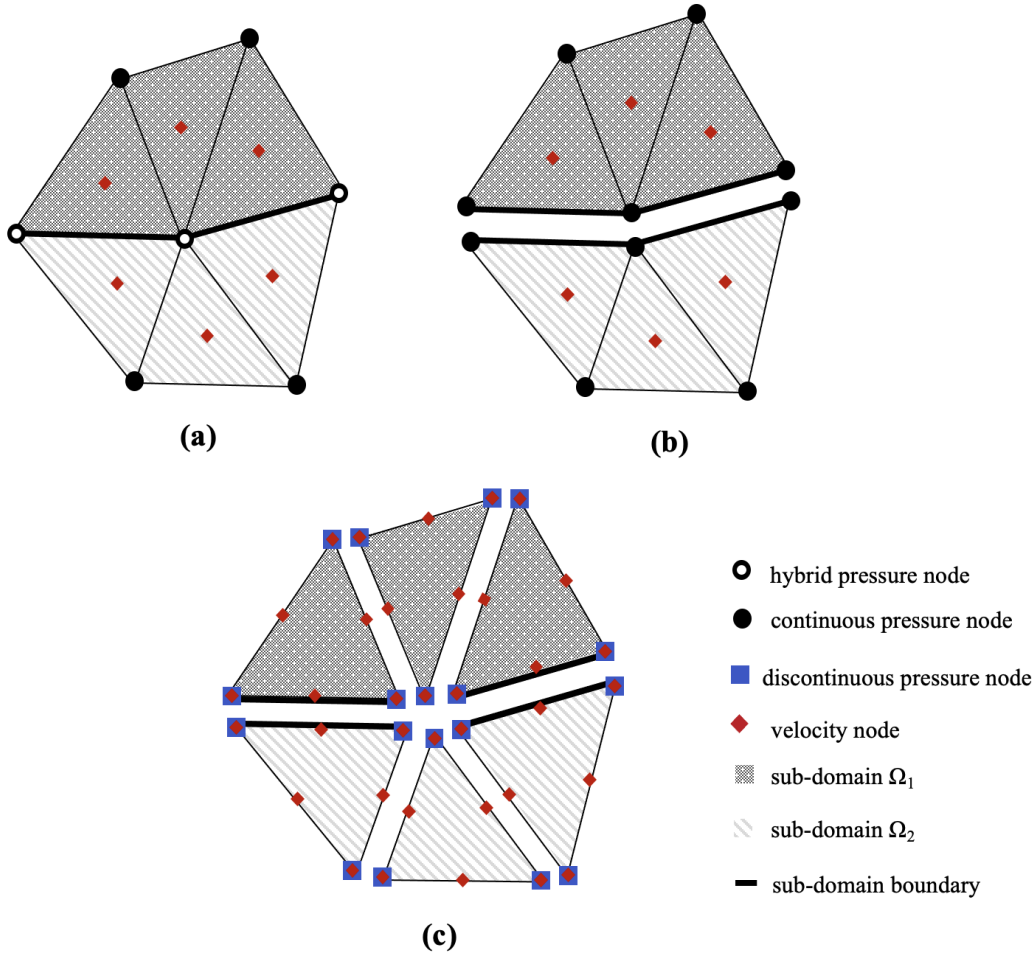


Figure 3.1: (a) Discretization of pressure and velocity on a mesh using the HyCVFE method with two sub-domains Ω_1 and Ω_2 . Emphasis is placed on the hybrid pressure nodes lying on the sub-domain boundary. (b) Internal splitting of the hybrid pressure nodes along the sub-domain boundary. A continuous pressure approximation is applied within each sub-domain while the necessary discontinuous approximations are used to establish the connections between sub-domains. (c) Discretization of the pressure and velocity using the high order discontinuous method of Salinas et al. [2018].

where the term accounting for capillarity and gravitational forces is neglected. Applying integration by parts on the second term, yields

$$\sum_{\Omega_d \in \Omega} \left[\int_{\Omega_d} \Phi_i \cdot \mathbf{v}_t \, d\Omega_d - \int_{\Omega_d} \nabla \left(\Phi_i \cdot \lambda_t \mathbf{K} \right) p \, d\Omega_d + \int_{\Gamma_d} \left(\Phi_i \cdot \lambda_t \mathbf{K} p \right) \cdot \mathbf{n} \, d\Gamma_d \right] = 0. \quad (3.5)$$

In order to accommodate the pressure discontinuity between sub-domains in the approximation, we apply integration by parts one more time on the second term. This approach is adapted from Salinas et al. [2018] and applied exclusively on Γ_d

$$\begin{aligned} \sum_{\Omega_d \in \Omega} \left[\int_{\Omega_d} \Phi_i \cdot \mathbf{v}_t \, d\Omega_d + \int_{\Omega_d} \left(\Phi_i \cdot \lambda_t \mathbf{K} \right) \cdot \nabla p \, d\Omega_d - \int_{\Gamma_d} \left(\Phi_i \cdot \lambda_t \mathbf{K} \tilde{p} \right) \cdot \mathbf{n} \, d\Gamma_d \right. \\ \left. + \int_{\Gamma_d} \left(\Phi_i \cdot \lambda_t \mathbf{K} p \right) \cdot \mathbf{n} \, d\Gamma_d \right] = 0. \end{aligned} \quad (3.6)$$

where p and $\tilde{p}$ in the last two terms on the left hand side correspond to the pressure nodes that share the same coordinates on the discontinuous interface (Γ_d). We substitute the finite element approximations for the velocity and pressure, Eqns. (3.1) and (3.2), and apply the finite element triangulation ($\mathcal{T}_d$) over each sub-domain

$$\begin{aligned} \sum_{\Omega_d \in \Omega} \left[\sum_{\Omega_e \in \Omega_d} \sum_{j=1}^{n_{d,v}} \int_{\Omega_e} \Phi_i \cdot \Phi_j v_{t,j} \, d\Omega_e + \sum_{\Omega_e \in \Omega_d} \sum_{k=1}^{n_{d,p}} \int_{\Omega_e} \left(\Phi_i \cdot \lambda_t \mathbf{K} \right) \cdot \nabla \Psi_k p_k \, d\Omega_e \right. \\ \left. + \sum_{\Gamma_e \in \Gamma_d} \sum_{k=1}^{n_{e,p}} \oint_{\Gamma_e} \left(\Phi_i \cdot \lambda_t \mathbf{K}_h \Psi_k (p_k - \tilde{p}_k) \right) \cdot \mathbf{n} \, d\Gamma_e \right] = 0, \end{aligned} \quad (3.7)$$

where $n_{d,v}$, $n_{d,p}$, and $n_{e,p}$ are the number of velocity nodes in sub-domain Ω_d , the number of pressure nodes in sub-domain Ω_d , and the number of hybrid pressure nodes on the discontinuous interface (Γ_d), respectively. $\mathbf{K}_h$ denotes the harmonic average of the permeability on the discontinuous interface (Γ_d), Ω_e is the element, and Γ_e is the element boundary. Eqn. (3.7) describes the system of equations of all the sub-domains that are coupled by hybrid pressure nodes across their shared interfaces (Γ_d). The last term on the left-hand side in Eqn. (3.7) is nonzero for the hybrid nodes such that $\tilde{p}$ is the hybrid pressure node of p that lies on the sub-domain boundary.

Discretization of the continuity equation

Our approach to discretize the continuity equation on the control volume dual mesh follows Jackson et al. [2015]; Gomes et al. [2017]. Fig. 3.2 highlights the construction of control volumes along the sub-domain boundaries (Γ_d). The hybrid pressure nodes provide restricted control volumes, with limited support, to their respective sub-domains. Consequently, no two adjacent sub-domains share a control volume. We derive the weak form of Eqn. (2.3) by weighting with the test function Ψ_i , from the space of the pressure basis functions, and integrating over the domain (Ω)

$$\sum_{\Omega_d \in \Omega} \left[\int_{\Omega_d} \Psi_i \nabla \mathbf{v}_t \, d\Omega_d - \int_{\Omega_d} \Psi_i q_t \, d\Omega_d \right] = 0. \quad (3.8)$$

Substituting the finite element approximation to the weak form gives

$$\sum_{\Omega_d \in \Omega} \left[\sum_{\Omega_{cv} \in \Omega_d} \sum_{j=1}^{n_{d,v}} \int_{\Omega_{cv}} \Psi_i \nabla \Phi_j v_{t,j} \, d\Omega_{cv} - \sum_{\Omega_{cv} \in \Omega_d} \int_{\Omega_{cv}} \Psi_i q_t \, d\Omega_{cv} \right] = 0. \quad (3.9)$$

with Ω_{cv} representing the control volume. Applying the divergence theorem on the first term yields

$$\begin{aligned} \sum_{\Omega_d \in \Omega} \left[\sum_{\Gamma_{cv} \in \Omega_d \setminus \Gamma_d} \sum_{j=1}^{n_{d,v}} \int_{\Gamma_{cv}} \Psi_i (\Phi_j v_{t,j}) \cdot \mathbf{n} \, d\Gamma_{cv} + \sum_{\Gamma_{cv} \in \Gamma_d} \sum_{j=1}^{n_{d,v}} \int_{\Gamma_{cv}} \Psi_i (\Phi_j \tilde{v}_{t,j}) \cdot \mathbf{n} \, d\Gamma_{cv} \right. \\ \left. - \sum_{\Omega_{cv} \in \Omega_d} \int_{\Omega_{cv}} \Psi_i q_t \, d\Omega_{cv} \right] = 0, \end{aligned} \quad (3.10)$$

where $\tilde{v}_{t,j}$ and Γ_{cv} denote the harmonic permeability-weighted velocity on the discontinuous interface (Γ_d), and the control volume boundary. Here, we separated the internal fluxes of the sub-domain from the external fluxes (Fig. 3.3). The second term in Eqn. (3.10) is non-zero for control volumes that lie on the sub-domain boundaries, contributing to external fluxes. The term ensures continuity of the fluxes across the global domain.

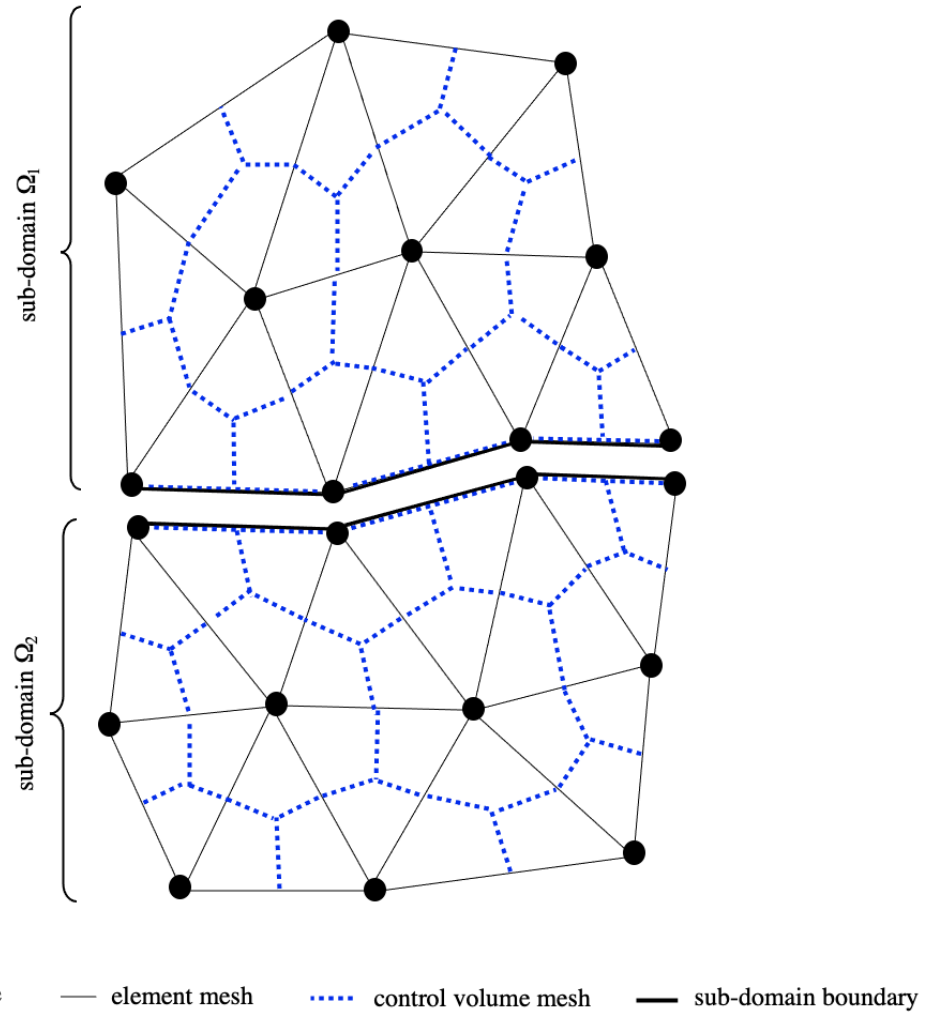


Figure 3.2: The dual mesh construction in the presence of hybrid pressure nodes. The control volumes are separated along the discontinuous interface.

3.2.2 Formulation of the transport equation

Finite-volume discretization

We discretize the mass balance equation in space over each control volume and in time using forward Euler, then apply the divergence theorem to obtain the surface integral of the velocity term in Eqn. (2.4). Since the fractional flow term is a function of saturation that can be nonlinear (a quadratic or even a cubic function), we linearize the term (f_α) in the saturation equation, see Eqn. (2.2) and (2.5). Finally, the linearized integral-form of the transport equation for the wetting phase is given by

$$\begin{aligned} \int_{\Omega_{cv}} \frac{\phi(S_{w,cv}^{n+1} - S_{w,cv}^n)}{\Delta t} d\Omega_{cv} = & - \oint_{\Gamma_{cv}} \left(f_{w,cv}^n \mathbf{v}_t^{n+1} + \frac{\partial f_{w,cv}}{\partial S_{w,cv}} \bigg|_n (S_{w,cv}^{n+1} - S_{w,cv}^n) \mathbf{v}_t^{n+1} \right) \cdot \mathbf{n} d\Gamma_{cv} \\ & + \int_{\Omega_{cv}} q_w d\Omega_{cv}, \end{aligned} \quad (3.11)$$

where Δt is the time step size and the superscripts n and $n + 1$ denote the current and next time steps, respectively. Eqn. (3.11) describes the mass balance equation of the wetting phase applied to any control volume in the domain to approximate the saturation (S_w).

3.2.3 Solution method

We couple the flow and transport equations using an Implicit Pressure Explicit Saturation (IMPES) scheme. This approach is appropriate in the context of CVFE methods due to the sequential nature of the formulation combined with the ease of implementation for testing and validation. In our implementation, the pressure and velocity are obtained implicitly by solving the finite element flow problem while keeping the saturation field unchanged. Then the saturation is updated explicitly on the control volume mesh [Durlinsky, 1993; Geiger et al., 2004]. The explicit time stepping only guarantees stability

for sufficiently small time steps, when the Courant–Friedrichs–Lewy (CFL) number does not exceed unity [Aziz and Settari, 1979].

Implicit pressure solution

Consider the global system of equations assembled from the force-balance given by Darcy’s law and the continuity equation, Eqn. (3.7) and (3.10), respectively. The algebraic system can be written as

$$\begin{bmatrix} \mathbf{A} & \mathbf{B} \\ \mathbf{C} & \mathbf{0} \end{bmatrix} \cdot \begin{bmatrix} \mathbf{v}_t^{n+1} \\ p^{n+1} \end{bmatrix} = \begin{bmatrix} b_1 \\ b_2 \end{bmatrix} \quad (3.12)$$

$\mathbf{A}$ is the mass matrix and in this specific formulation is a diagonal matrix. $\mathbf{B}$ and $\mathbf{C}$ are the stiffness matrix and the divergence-free velocity operator, respectively. Both of these are composed of two terms. The stiffness matrix ($\mathbf{B}$) is composed of the last two terms on the LHS of Eqn. (3.7). The second term has a block diagonal structure for each sub-domain, while the third is the jump-term attributing to fill-ins in the off block-diagonal structure. Similarly, $\mathbf{C}$ is composed of the first two terms on the LHS of Eqn. (3.10). The first term accounts for internal fluxes within each sub-domain, while the second term accounts for external fluxes between sub-domains ensuring continuity of the model.

The coupling term in the flow equation is the total mobility (λ_t), described in Eqn. (2.2), that must be updated in the stiffness matrix ($\mathbf{B}$) prior to solving the flow unknowns for each time step. The saturation-dependence of the relative permeability introduces strong non-linearities in the formulation [Aziz and Settari, 1979]. In the proposed method, we approximate it using upstream weighted values to maintain stable and physical solutions. The velocity and pressure can be solved simultaneously using this formulation. We use a projection-based method to eliminate the velocity unknown and solve first for the pressure, similar to the approach used in Jackson et al. [2015] and Salinas et al. [2018]. The velocity is then determined from the first row in Eqn. (3.12) by substituting the pressure solution.

Interface approximations

When updating the saturation using Eqn. 3.11, we consider two fluxes (Fig. 3.3): the internal flux between control volumes within the same sub-domain, and the external flux between control volumes in different elements in neighboring sub-domains (Fig. 3.3). Internal fluxes are straightforward to compute since the control volume interface is internal to the element and the flux is constructed to be continuous within each element. To establish consistent external flux approximations, we refer to the discretization of the continuity equation, Eqn. (3.10), which computes the velocity using the harmonic average at sub-domain boundaries ($\tilde{\mathbf{v}}_t$) given by

$$\tilde{\mathbf{v}}_t = \frac{1}{2} \left(\mathbf{K}_h \mathbf{K}_{e_1}^{-1} \mathbf{v}_{t,e_1} + \mathbf{K}_h \mathbf{K}_{e_2}^{-1} \mathbf{v}_{t,e_2} \right), \quad (3.13)$$

where $\mathbf{K}_h$, $\mathbf{K}^{-1}$, and $\mathbf{v}_t$ are the harmonic weighted permeability, the inverse of the element's permeability, and the element's velocity, respectively. The approximation described here is similar but not identical to the one used by Gomes et al. [2017] and Salinas et al. [2018]. We differ by not incorporating the weighted volumes in the flux approximation. Our numerical experiments show that this approximation provides locally mass conservative scheme. The fractional flow term (f_w) and its partial derivative with respect to saturation $\left(\frac{\partial f_w}{\partial S_w} \right)$ are approximated, similar to the total mobility term described earlier, by using upstream weighted values.

3.3 Numerical experiments

We first verify the steady state pressure solution for single phase flow in experiment 3.3.1. We next validate and establish the convergence of the HyCVFE formulation for two phase flow using the Buckley-Leverett problem in experiment 3.3.2. We then demonstrate the advantages of the proposed method compared to the classical CVFE method and the discontinuous method of Salinas et al. [2018] using three heterogeneous experiments.

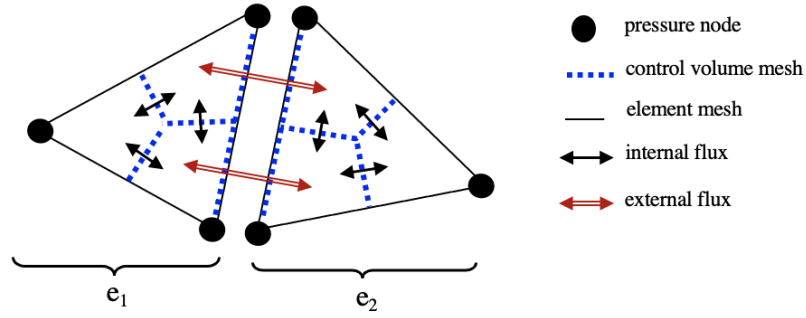


Figure 3.3: Types of fluxes in the hybrid model. The single and double arrows highlight internal fluxes within an element and external fluxes through discontinuous interface connecting e_1 with e_2 , respectively.

Experiments 3.3.3 and 3.3.4 consider two phase flow in a single fracture model, and an embedded box model, that were used previously [Abushaikh et al., 2015; Salinas et al., 2018]. The final experiment, 3.3.5, represents a highly challenging example in which two phase flow is focused into a fracture tip embedded in a low permeability domain.

We report the degrees of freedom in the numerical examples using

$$DoF_{CVFE} = N_p + N_v + N_s, \quad (3.14)$$

for the continuous method where N_p , N_v , N_s are the pressure, velocity, and saturation degrees of freedom. For the hybrid method we use

$$DoF_{HyCVFE} = \sum_{\Omega_d \in \Omega} (n_{d,p} + n_{d,v} + n_{d,s}), \quad (3.15)$$

where $n_{d,p}$, $n_{d,v}$, and $n_{d,s}$ are the pressure, velocity, and saturation degrees of freedom in sub-domain Ω_d . In single phase flow problems, the saturation degrees of freedom in Eqn. (3.14) and Eqn. (3.15) are neglected. In multiphase numerical experiments, we use the Brooks-Corey model [Brooks and Corey, 1964] that describes the relative permeability curves by

$$k_{rw}(S_w) = \left(\frac{S_w - S_{w,r}}{1 - S_{w,r} - S_{nw,r}} \right)^{n_w}, \quad (3.16)$$

Table 3.1: Summary of numerical experiment setup for the HyCVFE method

	Numerical experiments				
	3.3.1	3.3.2	3.3.3	3.3.4	3.3.5
Length of domain in x direction (L_x)	1.	1.	1.	1.	1.
Length of domain in y direction (L_y)	0.05	0.05	0.25	1.	0.5
Porosity (ϕ)	0.1	0.1	0.1	0.1	0.1
Corey exponent of wetting phase (n_w)	N/A	2.	2.	2.	2.
Corey exponent of non-wetting phase (n_{nw})	N/A	2.	2.	2.	2.
Wetting phase residual saturation ($S_{w,r}$)	N/A	0.2	0.2	0.2	0.2
Non-wetting phase residual saturation ($S_{nw,r}$)	N/A	0.3	0.3	0.3	0.3
Permeability ratio ($\mathbf{K}_{high}/\mathbf{K}_{low}$)	2.	N/A	10^4	10^4	10^6
Viscosity ratio (μ_{nw}/μ_n)	N/A	2.	2.	2.	2.

and

$$k_{rnw}(S_w) = \left(\frac{1 - S_w - S_{nw,r}}{1 - S_{w,r} - S_{nw,r}} \right)^{n_{nw}}, \quad (3.17)$$

where the superscript n is the Corey exponent, and $S_{\alpha,r}$ is the residual saturation of phase α . The parameters for each model are provided in Table 3.1 and the DoF requirements for the numerical experiments are shown in Table 3.2. We adapt the approach used by Salinas et al. [2018] to compare the fraction of mass leakage (ϵ_{max}) obtained using different approximations. The normalised mass leakage ϵ_{max} measures the undesired change in wetting phase saturation due to leakage and is defined as

$$\epsilon_{max} = \frac{\sum_{i \in \Omega_{low}} (S_{w,i} - S_{w,r,i}) \Omega_{cv,i}}{\sum_{i \in \Omega_{low}} \Omega_{cv,i}} \quad (3.18)$$

where Ω_{low} refers to the low permeability sub-domain into which numerical mass leakage is of concern.

We note that the implementation of the described formulation of the HyCVFE approach is not integrated into IC-FERST. Instead, it is developed in a prototype Python code

Table 3.2: Comparison of the DoF requirements and the overhead for using the HyCVFE approach.

Numerical experiment	DoF_{CVFE}	$DoF_{Hy-CVFE}$	Overhead (%)
3.3.1	443	446	0.67
3.3.2	N/A	N/A	N/A
3.3.3	2912	3060	5.
3.3.4	966	1006	4.1
3.3.5	874	920	5.2

detailed in Appendix A.2. Several reasons explain this implementation choice. First, the formulation for multiphase flow in porous media utilized in IC-FERST is fundamentally based on Fluidity, and discussed in Jackson et al. [2015]; Salinas et al. [2015]; Gomes et al. [2017]. Fluidity is an open source, general purpose, multiphase computational fluid dynamics code. Consequently, the existing IC-FERST frameworks within IC-FERST establish a solution method based on resolving the flow unknowns of pressure (P is a scalar), and the velocity of each phase (for two-phase systems $\mathbf{v}_w$ and $\mathbf{v}_{nw}$ are vectors), and the transport unknowns including the volume fraction for each phase (for two-phase systems S_w and S_{nw} are scalars). This choice of unknowns in IC-FERST framework is computationally very expensive. Second, we recall from Section 2.3.8 that the implementation of Salinas et al. [2018] in IC-FERST yields non-monotone saturation solutions and requires further investigation. We recognize that the numerical experiment described here could have benefited from direct comparisons with Salinas et al. [2018] formulation. Unfortunately, addressing the non-monotonic solutions exhibited in the multiphase solutions of Salinas et al. [2018] in IC-FERST extends well beyond the objectives of this thesis.

Since this work serves as a proof of concept, we find that a different choice of primary unknowns offers flexibility and can benefit from classical formulations, i.e., the fractional flow form in Eqn. (2.5) that describes how each phase contributes to the total flow and using the constraint of volume fraction in Eqn. (2.6), thereby reducing the number of

unknowns. It is worth mentioning that references to Salinas et al. [2018] numerical experiments are directly captured from the literature (Fig. 3.8b). Meanwhile, cross-plot comparisons of $DoF_{Salinas\ et\ al. [2018]}$ (computed as $N_p + N_v + N_s$) requirements (Fig. 3.8c, 3.10b, and 3.12b) are based on the primary flow and transport unknowns described in this work for consistency, which are restricted to $P, \mathbf{v}_t, S_w$ unknowns. Hence, for each triangular 2D element, the $DoF_{Salinas\ et\ al. [2018]}$ per element is 18 (in the cross-plots) instead of 30 (in IC-FERST).

3.3.1 Steady-state pressure

We validate the pressure solution for single phase flow in a heterogeneous porous medium in the presence of hybrid pressure nodes. The permeability field projected onto the finite element mesh is shown in Fig. 3.4(a); the high permeability sub-domain to the right has twice the permeability of the low permeability subdomain to the left (Table 3.1). The HyCVFE method mesh is decomposed into two sub-domains such that hybrid pressure nodes are placed at $x = 0.5$. DoF_{CVFE} and DoF_{HyCVFE} required to solve the flow model are 443 and 446, respectively. Fig. 3.4(b) compares the pressure profile along the horizontal axis for the two methods with 40 elements along the x-axis ($n_x = 40$). The pressure drop in the higher permeability region to the right correctly corresponds to half the slope of the pressure drop exhibited in lower permeability region to the left. The exact solution of the pressure is given by

$$\text{pressure} = \begin{cases} -\frac{8}{3}x + 1 & x \leq 0.5 \\ -\frac{4}{3}x + \frac{1}{3} & x > 0.5 \end{cases} \quad (3.19)$$

here x denotes the dimensionless distance. The hybrid pressure nodes yield the correct pressure approximation at the discontinuity, $x = 0.5$. The convergence of the pressure solution for the CVFE and the HyCVFE methods are compared against the exact solution in Table 3.3 for several mesh resolutions. The L^1 -norm of HyCVFE pressure solution is

Table 3.3: Convergence of the pressure in numerical experiment 3.3.1

	n_x	DoF	L^1 -norm	ROC
CVFE	40	443	0.002094778	-
	80	883	0.001111908	0.918253463
	160	1763	0.000565433	0.978009389
HyCVFE	40	446	2.12923E-10	-
	80	886	2.4283E-10	-
	160	1766	2.41503E-10	-

many orders of magnitude lower than the classical CVFE method and is not influenced by mesh resolution. In the case of CVFE method, the rate of convergence (ROC) is linear. This numerical experiment demonstrates that the proposed HyCVFE method provides pressure solution with improved accuracy than the classical CVFE method in the presence of discontinuity.

3.3.2 Buckley-Leverett problem

We validate the coupled flow and transport solution of the HyCVFE method against the semi-analytical Buckley-Leverett solution [Buckley and Leverett, 1942]. The model setup is as follows. In the absence of gravity and capillary forces, the homogeneous medium is initially saturated with the non-wetting phase, which is then displaced by the wetting phase. For validation purposes, we introduce multiple discontinuous interfaces in the homogeneous medium to test the hybrid pressure nodes, resulting in 8 sub-domains. Fig. 3.5a shows the two-dimensional mesh used in this numerical example with 40 elements along the x-axis. The dashed red lines represent discontinuous interfaces at which control volumes do not span element boundaries. The numerical saturation solution after 0.2 pore volumes injected (PVI), obtained using the classical CVFE and our HyCVFE approach are shown in Fig. 3.5. The saturation obtained using our HyCVFE method is in good agreement with the classical CVFE. The corresponding pressure distribution deviates

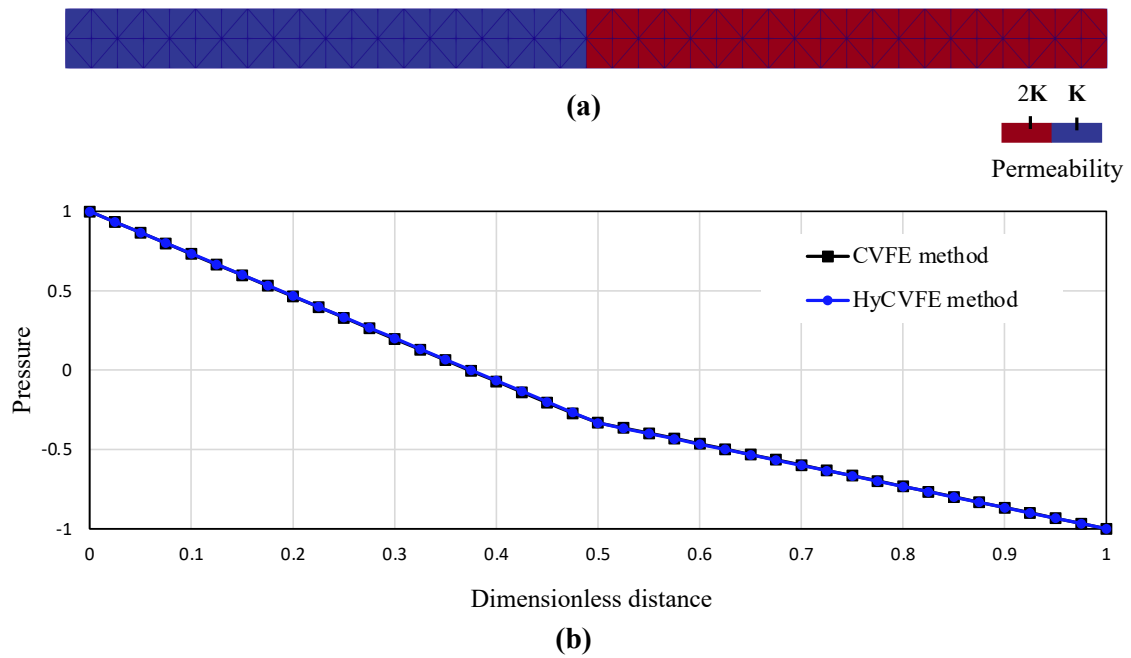


Figure 3.4: Steady-state pressure experiment (3.3.1): **(a)** The heterogeneous permeability field on the finite element mesh. **(b)** Comparison of the pressure distribution along the horizontal axis for the CVFE and the HyCVFE methods. Hybrid pressure nodes yield the correct pressure solution at discontinuities.

from a linear gradient in the interval $x \in [0, 0.5]$ due to the quadratic relative permeability curves. Again, the CVFE and HyCVFE results are in good agreement.

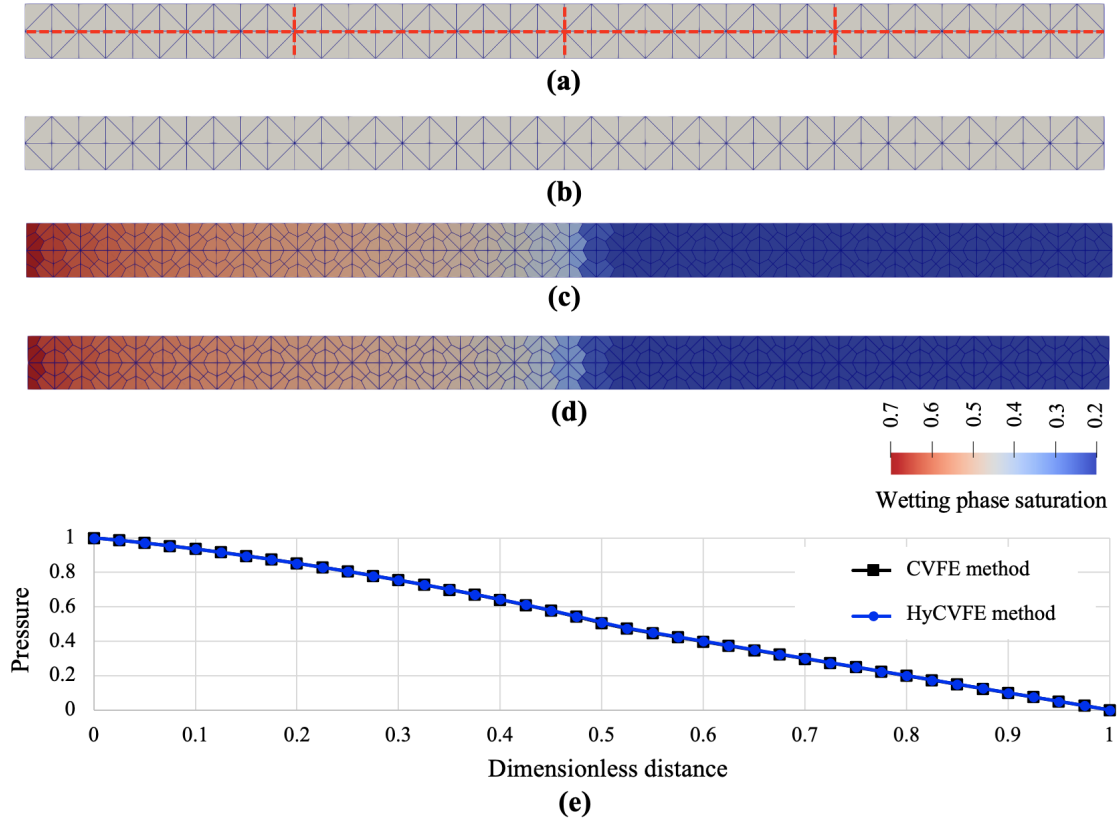


Figure 3.5: Pseudo one-dimensional numerical Buckley-Leverett experiment (3.3.2). (a) HyCVFE method element mesh with red dashed lines indicating discontinuous interfaces. (b) Reference CVFE method element mesh. The saturation solution after 0.2 PVI is displayed CV-wise for (c) the HyCVFE method and (d) the CVFE approach. (e) Comparison of the corresponding pressure solution for CVFE and HyCVFE methods.

We demonstrate the convergence of the proposed method to the semi-analytical solution of the Buckley-Leverett problem after 0.1 and 0.2 PVI in Fig. 3.6a. The saturation profile shows several numerical solutions obtained with different mesh resolutions ($n_x = 40, 80, 160, 320$) compared with the semi-analytical solution. We observe that refinement of the mesh results in a better agreement with the semi-analytical solution. In all cases, the area under the semi-analytical and numerical curves represents the same mass of wetting phase injected into the model. The flux continuity approach employed in the HyCVFE method guarantees local and global mass conservation. Fig. 3.6b, shows the L^1 -norm and

Table 3.4: Convergence of the numerical solution to semi-analytical B-L 3.3.2

	n_x	DoF	L^1 -norm	ROC
CVFE	40	566	1.61E-02	-
	80	1126	9.31E-03	0.79022176
	160	2246	5.96E-03	0.642958928
	320	4486	4.26E-03	0.486656226
HyCVFE	40	672	1.28E-02	-
	80	1312	8.81E-03	0.542941572
	160	2592	6.42E-03	0.456518867
	320	5152	4.22E-03	0.606270398

the rate of convergence of the numerical methods, compared to linear convergence trend. The additional nodes introduced at discontinuous interfaces in the HyCVFE approach introduce additional degrees of freedom that result in a slight shift of the curve for the HyCVFE method to the right when compared to the reference CVFE method. Table 3.4 compares the convergence rate of numerical solution for the CVFE and the HyCVFE methods against the semi-analytical B-L solution, convergence rates vary between 0.45 and 0.8.

3.3.3 Single fracture problem

We demonstrate the potential of the method to reduce numerical mass leakage with a two-dimensional example from Abushaikh et al. [2015] and Salinas et al. [2018]. A narrow conductive zone, representing a fracture, is enclosed in low permeability zones (Table 3.1). This case shows the performance of the HyCVFE method with multiple sub-domain interfaces with different material property contrasts and interface orientations with respect to the flow. The permeability field is shown in Fig. 3.7a. The fracture sub-domain consists of a thin layer of elements. The model features intermediate permeability zones to the right and left of the fracture sub-domain where pressure boundary conditions are applied. The

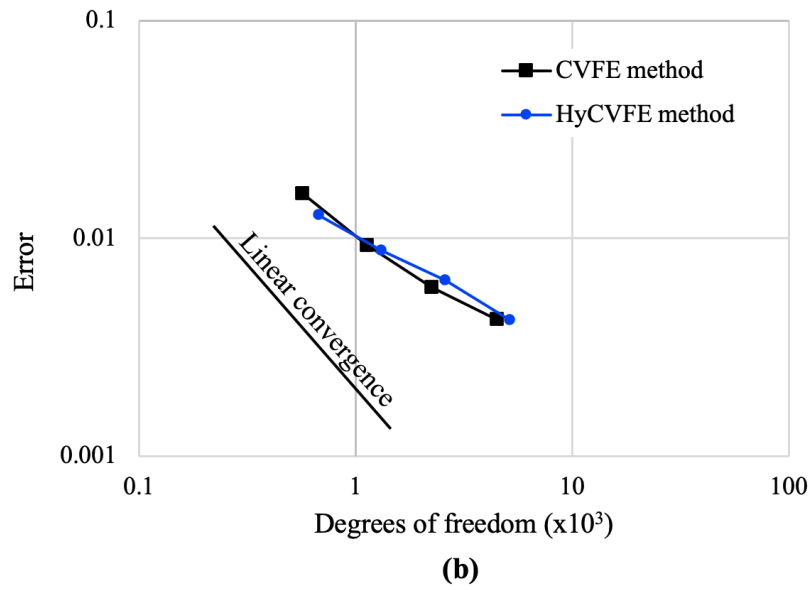
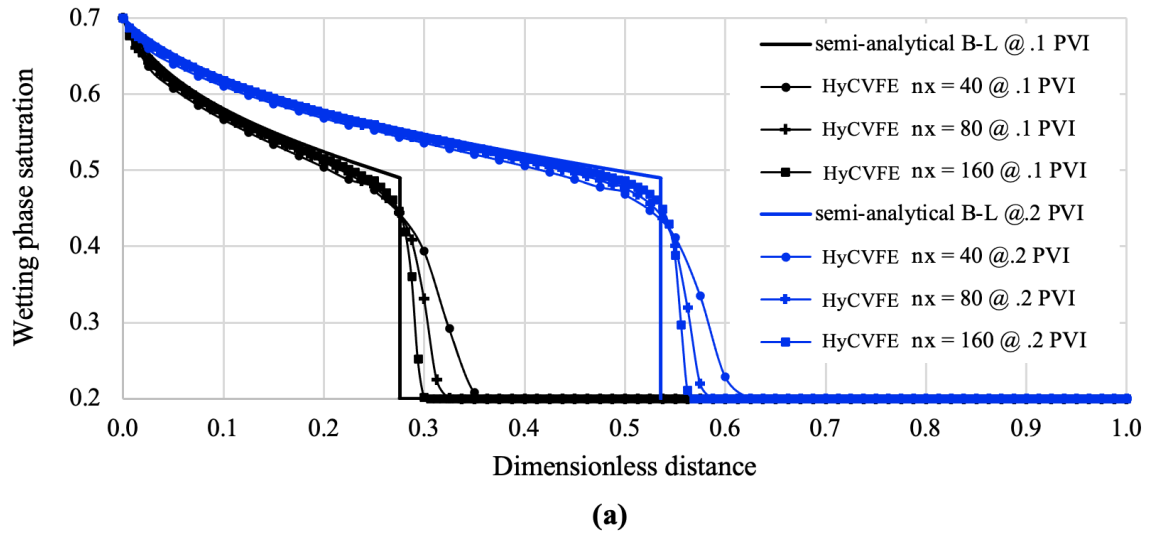


Figure 3.6: Convergence of the numerical solution to the semi-analytical Buckley-Leverett (B-L) experiment (3.3.2): (a) Comparison of the proposed, hybrid method to the semi-analytical B-L after 0.1 and 0.2 PVI. (b) L^1 -norm of the error for the HyCVFE and classical CVFE approximations.

model is initially saturated with the non-wetting phase, and the wetting phase is injected from the left boundary to displace the non-wetting phase through the right boundary. We compare the accuracy of the saturation solution at several timesteps in Fig. 3.7(b-e) for the HyCVFE approach and the reference CVFE method. The saturation profiles differ between the two methods because the CVFE approach suffers from numerical leakage from the fracture into the surrounding low permeability sub-domains via the control volumes that span the sub-domain boundaries. This leakage results in a delayed saturation front when compared to the HyCVFE solution. DoF_{CVFE} and DoF_{HyCVFE} used to model this problem are 2912 and 3060, respectively. Fig. 3.7e shows the wetting phase migrates into the low permeability zone towards the right-hand end of the fracture in the HyCVFE method only after the displacing phase reaches the intermediate permeability outlet zone.

We compare the normalized mass leakage of the proposed HyCVFE method (Fig. 3.8a) and the discontinuous approach of Salinas et al. [2018] (Fig. 3.8b) against the classical CVFE method; leakage using both methods is approximately two orders of magnitude lower than for the CVFE approach. The normalized mass leakage results from Salinas et al. [2018] were obtained using a 3D model but can be compared with our 2D results because the material properties of the model cross-section were simply extruded into the third dimension so the model was effectively 2D. We extract the number of degrees of freedom (Dof) required for the classical CVFE method on a given 2D mesh (DoF_{CVFE}), and use this as a reference against which to compare the number of DoF required by the new HyCVFE method (DoF_{HyCVFE}) and the discontinuous method ($N_{Salinas}$ et al. [2018]) for the same mesh. This allows us to cross-compare the DoF required for the different methods. Fig. 3.8c shows the resulting cross-plot of DoF_{HyCVFE} and $N_{Salinas}$ against DoF_{CVFE} . The unit slope on this plot corresponds to the case where the new hybrid or discontinuous method requires the same number of DoF as the classical CVFE method for a given mesh. The discontinuous method of Salinas et al. [2018] plots on a line which lies considerably above the unit slope, because the method requires 18 degrees of freedom per 2D element. In contrast, the new HyCVFE method plots almost exactly on the unit

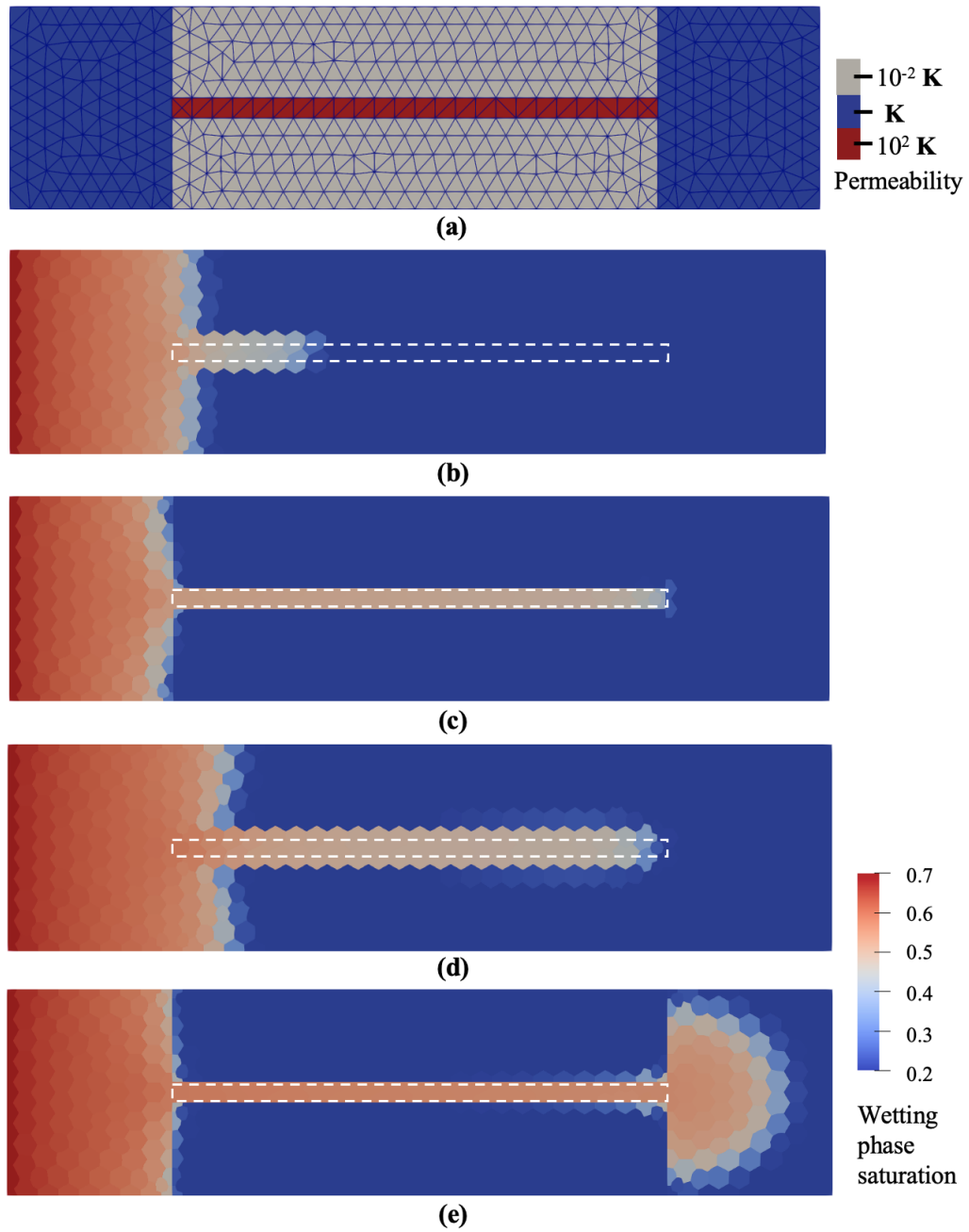


Figure 3.7: (a) The permeability field of the single fracture experiment (3.3.3). The fracture is enclosed in a low permeability zone above and below while the left and right boundaries include intermediate permeability zones. (b – e) Comparison of the saturation solution displayed using the control volume representation. (b) and (c) show the saturation solutions of the CVFE method and the HyCVFE method, respectively, after 0.1 PVI. (d) and (e) show the saturation solutions of the CVFE method and the HyCVFE method, respectively, after 0.14 PVI.

The dashed box in the plots outlines the fracture zone.

slope, showing that the number of additional DoF required by the method is insignificant compared to the classical CVFE approach on a given mesh. Thus, although both methods are effective in reducing mass leakage, the proposed HyCVFE approach requires far fewer additional DoF because the discontinuity between elements is applied locally, rather than globally as in Salinas et al. [2018].

3.3.4 Embedded box problem

We now consider the embedded box example from Abushaikh et al. [2015]. The two-dimensional model is comprised of a low permeability box embedded in a high permeability region via a sharp interface with permeability contrast of 4 orders of magnitude (Table 3.1). The permeability field is shown in Fig. 3.9a. Constant pressure boundary conditions are applied on the left and right boundaries, and the wetting phase is injected over the left boundary. The top and bottom boundaries are no-flow. Comparisons of the saturation solutions between the HyCVFE and CVFE methods are shown in Fig. 3.9(b-e) at two timesteps, after 0.12 and 0.25 PVI. The saturation solution in the outer region is in good agreement between the two methods after 0.12 PVI. However, after 0.25 PVI the CVFE method displays non-physical leakage of the saturation solution across the discontinuous material interface, due to the continuous control volumes that span the interface. In this numerical example, DoF_{CVFE} and DoF_{HyCVFE} are 966 and 1006, respectively.

Fig. 3.10a compares the normalized mass leakage for different mesh refinements. The HyCVFE approach shows several orders of magnitude less mass leakage in the saturation solution when compared with the reference CVFE method. Furthermore, we compare the computational requirements on the cross plot in Fig. 3.10b. Similar to the previous example, the slope of the DoF_{HyCVFE} method is very close to the unit slope, demonstrating that the additional DoF required for the HyCVFE approach are negligible when compared to the discontinuous method of Salinas et al. [2018].

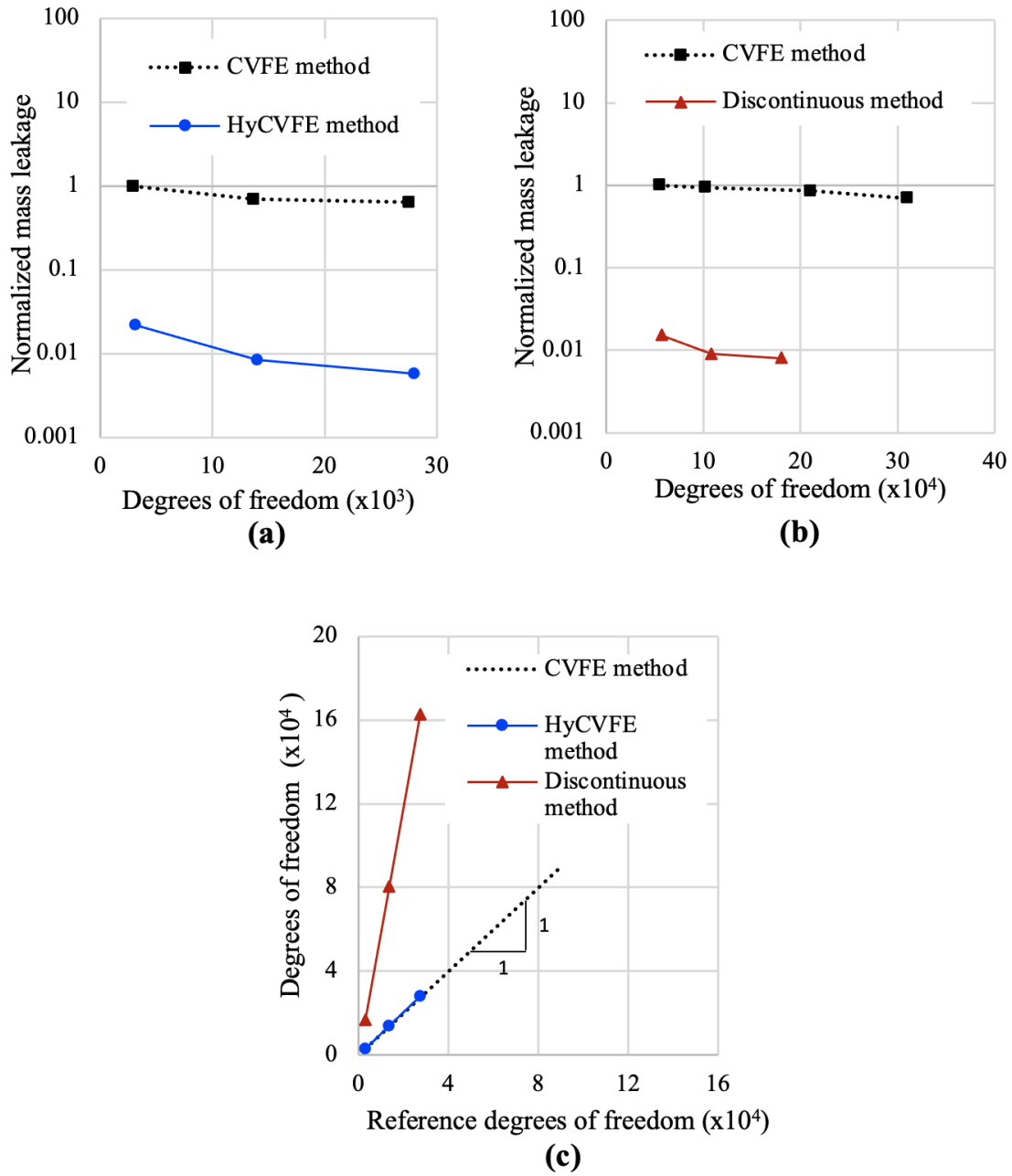


Figure 3.8: **(a-b)** Comparison of the normalized mass leakage as a function of the number of DoF for the single fracture experiment (3.3.3). **(a)** Two-dimensional model for HyCVFE and CVFE at 0.1 PVI. **(b)** Three-dimensional model using discontinuous and CVFE methods from Salinas et al. [2018]. **(c)** cross-plot of DoF_{HyCVFE} and $N_{Salinas}$ against DoF_{CVFE} for the 2D fracture model. The unit slope is the reference for the computational requirements of the classical CVFE method.

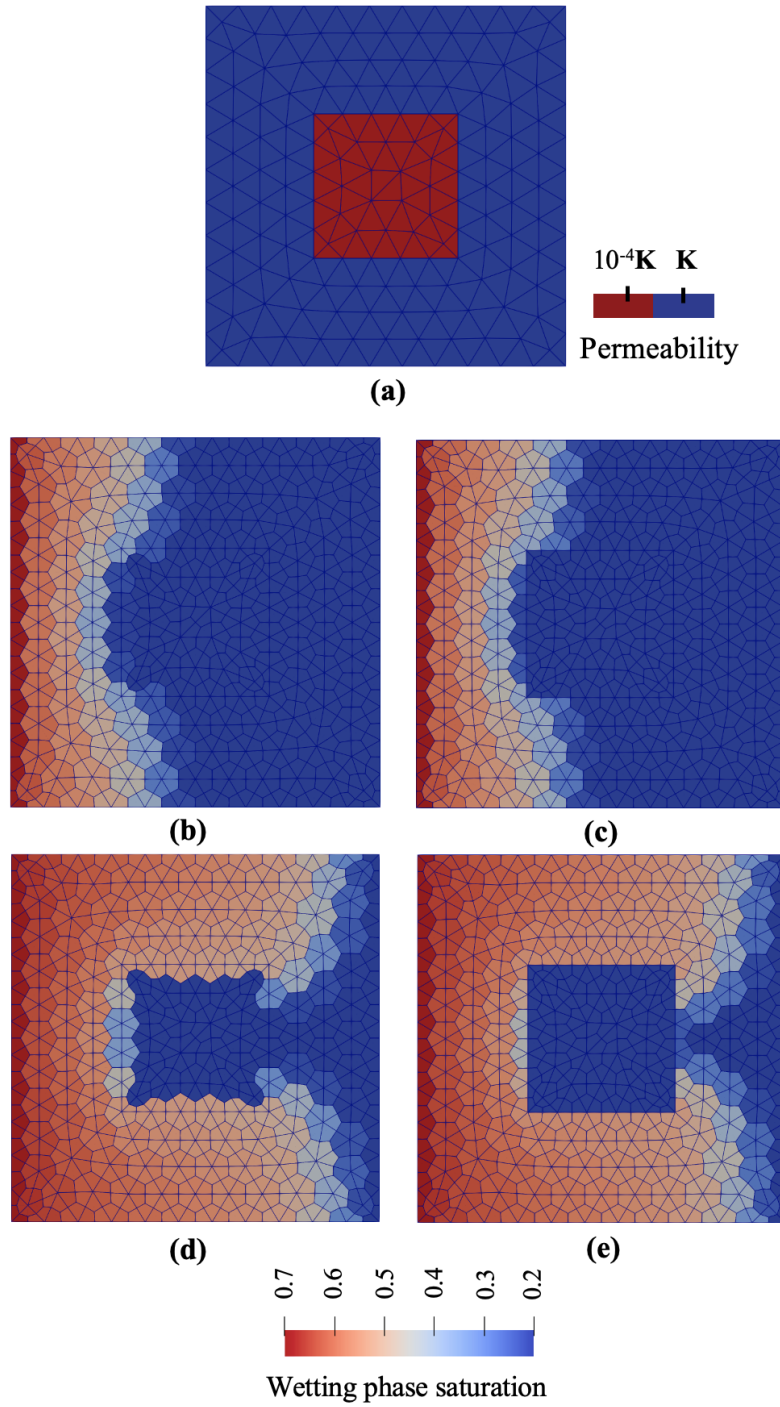


Figure 3.9: (a) The permeability field of the embedded box experiment (3.3.4). The contrast in the permeability is 4 orders of magnitude between the embedded box and the external region. (b – e) Comparison of the saturation solution displayed using the control volume representation. The middle column shows the CVFE method while the right column shows the HyCVFE method. (b) and (c) are the saturation solutions of the CVFE and the HyCVFE methods, respectively, after 0.12 PVI. (d) and (e) show the saturation solutions of the CVFE and the HyCVFE methods, respectively, after 0.25 PVI.

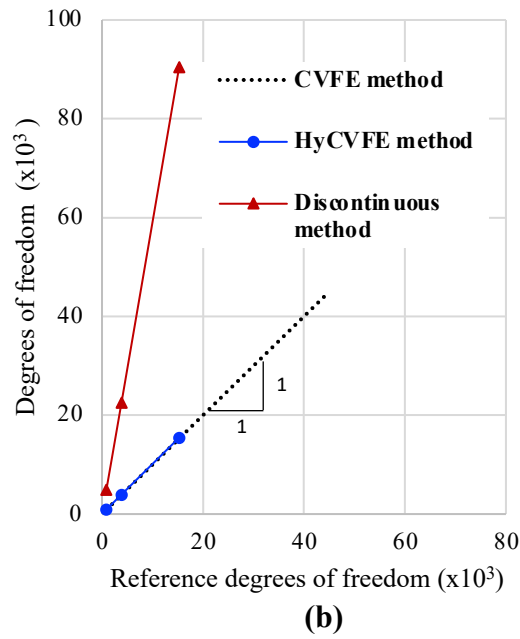
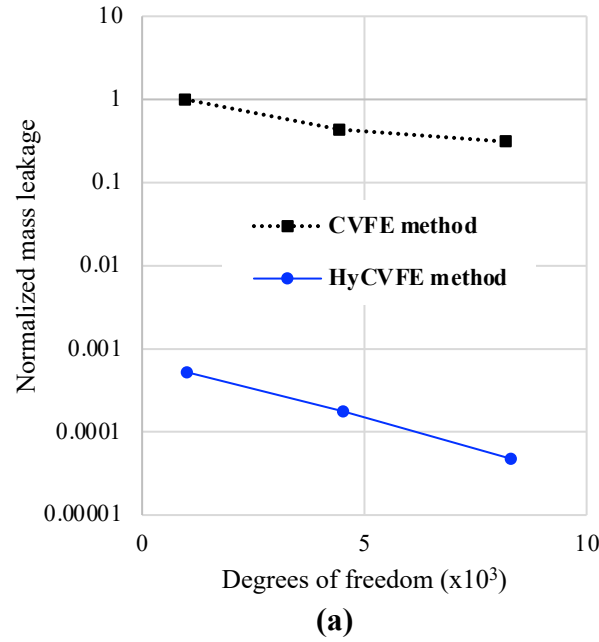


Figure 3.10: The embedded box experiment (3.3.4). **(a)** Comparison of the normalized mass leakage as a function of DoF for HyCVFE and CVFE methods at 0.2 PVI. **(b)** cross-plot of DoF_{HyCVFE} and $N_{Salinas}$ against DoF_{CVFE} for the embedded box model. The unit slope is the reference for the computational requirements of the classical CVFE method.

3.3.5 Wedge pinch out problem

This final case comprises of a high permeability wedge or fracture that pinches out. The tip of the wedge is made up of a few elements with large aspect ratio. The model represents the complex geometry of many geological systems and presents a challenge for accurate and efficient modeling [Jackson et al., 2015]. The permeability contrast between the sub-domains is 6 orders of magnitude (Fig. 3.11a and Table 3.1). We apply constant pressure boundary conditions on the left and right boundaries with no flow through the top and bottom boundaries and inject the wetting phase over the left boundary. The saturation distribution is displayed at two time steps in Fig. 3.11(b-e). After 0.014 PVI, the wetting phase reaches the tip of the wedge in the HyCVFE approach while the CVFE method displays a slower flow of the wetting phase through the wedge due to mass leakage into the surrounding low permeability domain via the control volumes that span the boundary. The wetting phase in the CVFE approach takes more than twice as long to reach the wedge tip at 0.034 PVI.

The (DoF_{CVFE}) and (DoF_{HyCVFE}) used to model this case are 874 and 920, respectively. The normalized mass leakage is approximately one order of magnitude lower for the HyCVFE method (Fig. 3.12a), yet the computational cost is similar and much smaller again than the discontinuous method of Salinas et al. [2018]. Fig. 3.12b shows the cross plot of the number of DoF_{HyCVFE} and $N_{Salinas}$ against DoF_{CVFE} . Unlike the HyCVFE approach that does not require many additional DoF, the Salinas et al. [2018] method again has a steep slope indicating the high computational cost for a given mesh with respect to the reference CVFE method. This case emphasizes the appropriate application of the HyCVFE method where the sub-domains are meshed according to the underlying material geometry without influencing the adjacent region or the need to apply mesh refinement to capture accurate multiphase flow behaviours.

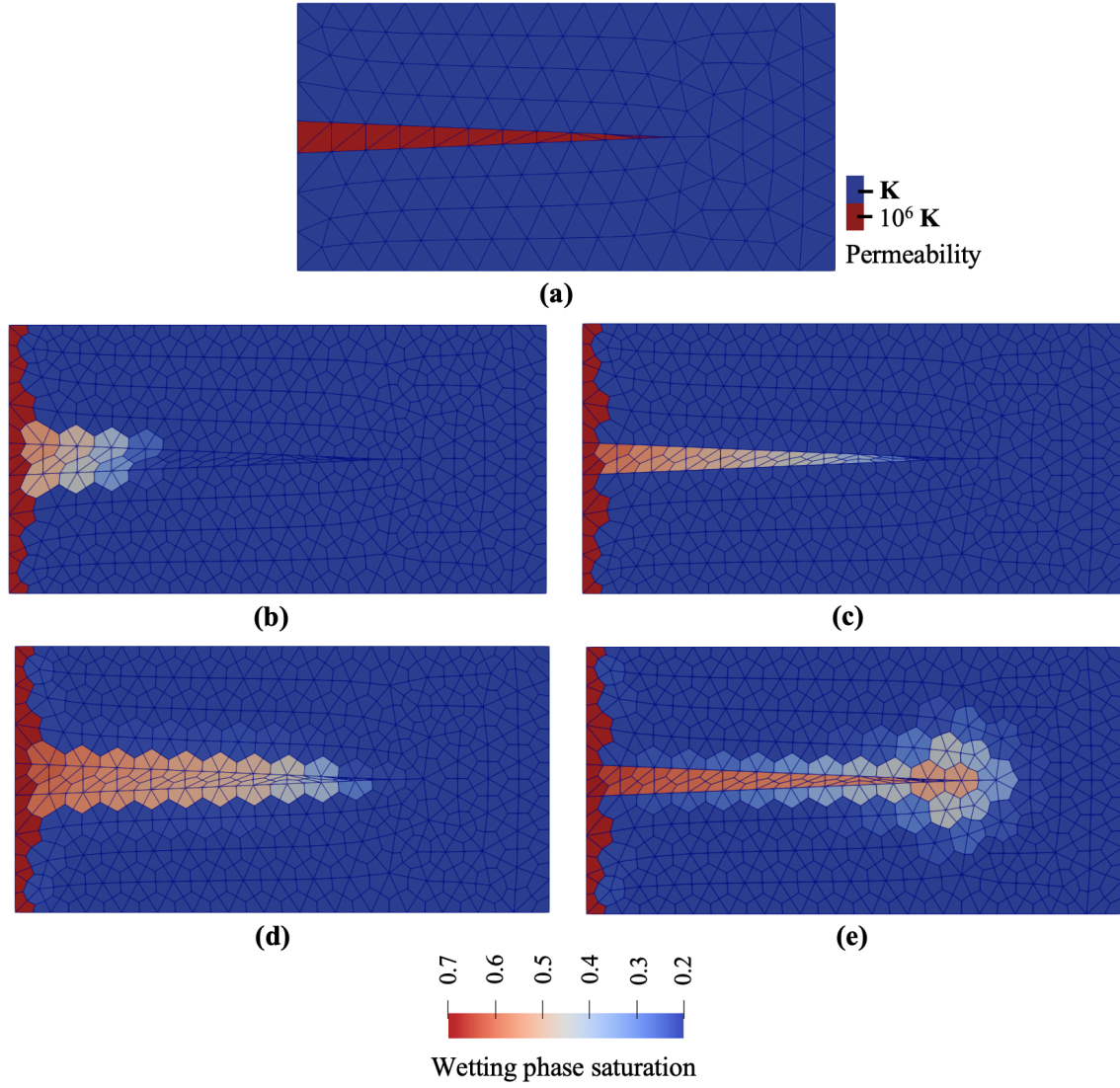
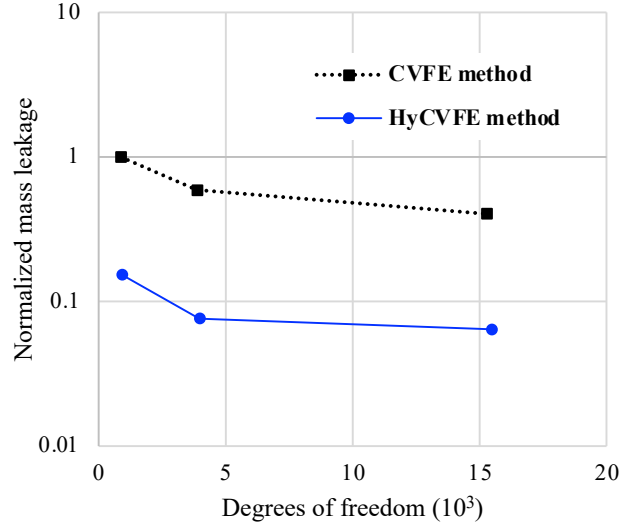
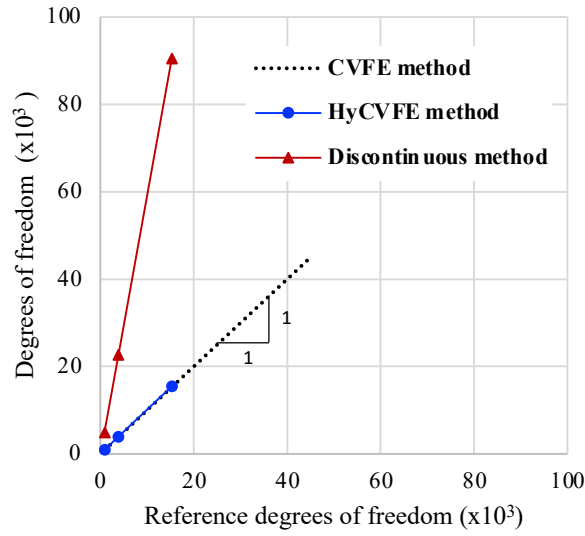


Figure 3.11: **(a)** The permeability field of the wedge experiment (3.3.5) with the contrast in permeability of 6 orders of magnitude. The tip of the wedge pinch out is made up of several elements with large aspect ratio. **(b-e)** Comparison of the saturation solution of the fracture problem displayed using the control volume representation. The left column shows the CVFE method while the right column shows HyCVFE method. **(b)** and **(c)**, **(d)** and **(e)** display the solution after 0.014 and 0.034 PVI, respectively.



(a)



(b)

Figure 3.12: (a) Comparison of the normalized mass leakage as a function of DoF for the HyCVFE and CVFE methods in the wedge experiment (3.3.5) at 0.014 PVI. (b) cross-plot of DoF_{HyCVFE} and $N_{Salinas}$ against DoF_{CVFE} for the wedge model. The unit slope is the reference for the computational requirements of the classical CVFE method.

3.4 Summary

The proposed HyCVFE formulation is a promising numerical method for simulating multiphase flow problems in highly heterogeneous porous media that require geometrically complex models discretized using unstructured meshes. The approach has the following advantages: 1) The element pair $P_{0,DG} - P_{1,H}$ provides stable numerical solutions for coupled flow and transport problems. 2) The discretization of the continuity equation in the HyCVFE approach yields locally and globally mass conservative solutions. 3) The formulation exploits the efficient continuous pressure approximation in sub-domains with uniform or smoothly varying material properties. The continuous control volumes constructed by spanning element boundaries within sub-domains are desirable for efficiency. 4) Along material property discontinuities that correspond to sub-domain boundaries, additional nodes are applied to preserve sharp saturation changes over the interface based on a discontinuous pressure approximation. These nodes prevent control volumes from spanning multiple sub-domains and thus reduce mass leakage. 5) The general approach of the HyCVFE formulation is well suited to incorporate additional physics such as gravitational and capillary forces and rock and fluid compressibility. Including these physics is the topic of future work. 6) The approach can be readily extended from 2D to 3D models by populating hybrid nodes on the vertices of the tetrahedral faces separating the sub-domains. In common with most investigations of new numerical methods, the HyCVFE approach is currently implemented in a 'proof of concept' 2D code; in future work, we will investigate the performance of the method in large 3D domains with parallel implementation. 7) The gains in accuracy far outweigh the overhead of additional computational cost to use this hybrid approach. The numerical examples show that only 4-5 % of additional degrees of freedom are introduced and provide significant improvements, up to several orders of magnitude, to the solution accuracy.

Chapter 4

A single mesh approximation

The work presented in this chapter has been submitted to the Journal of Computational Physics and is currently under review:

Al Kubaisy, J., Salinas, P., Jackson, M.D., A single mesh approximation for modeling multiphase flow in heterogeneous porous media

4.1 Introduction

In this chapter, we address the inherent inconsistency observed in control volume finite element (CVFE) methods employing a two-mesh approach. A new formulation is developed; essentially it eliminates the inconsistency of the two-mesh approach from the CVFE method. The approach is a generalization of the technique used for embedding the discontinuous Galerkin approximation in the HyCVFE approach presented in Chapter 3. Instead of capturing solution discontinuities only between model subdomains, we employ a new discontinuous element type that captures element to element variations in the material properties and the corresponding solution fields, accurately. As a result, the method addresses the general inconsistency described earlier of CVFE methods for modeling multiphase porous media flow. The main contributions of this work are three-fold:

1. The proposed new CVFE method employs a single mesh that ensures consistency of the flow and transport problems. Solutions are stable and mass-conservative.
2. A new element type is introduced for the discretization of velocity and pressure that allows application of the discontinuous Galerkin approximation globally in the domain. The derivation of the approach is non-trivial and is described accordingly.
3. Geo-statistical models with element-to-element variations in material properties can be modeled accurately using the proposed method.

In this chapter, we present the formulation of this new single-mesh control volume finite element (SM-CVFE) method. We introduce the new element, the discretization steps of the SM-CVFE approach, and the solution method implementation in section 4.2. Section 4.3 validates the approach for single and two phase flow, then tests a variety of challenging problems that include domains with complex geometries and geo-statistical models. Finally, sections 4.4 and 4.5 provide general discussion and summary, respectively.

4.2 Method

4.2.1 New element representation

The SM-CVFE approach introduces a new, fully discontinuous element pair $(P_{1,DG} - P_{0,DG})$ which represents a first order discontinuous Galerkin velocity approximation combined with an element-wise, discontinuous Galerkin pressure approximation, respectively, (Fig. 4.1). Unlike the classical CVFE method, in the SM-CVFE method the physical properties of the medium (permeability and porosity), the pressure, the saturation and the saturation dependent properties are represented constant element-wise for consistency. Despite the use of a discontinuous velocity approximation, the discretization described in the next section constructs globally continuous fluxes between elements.

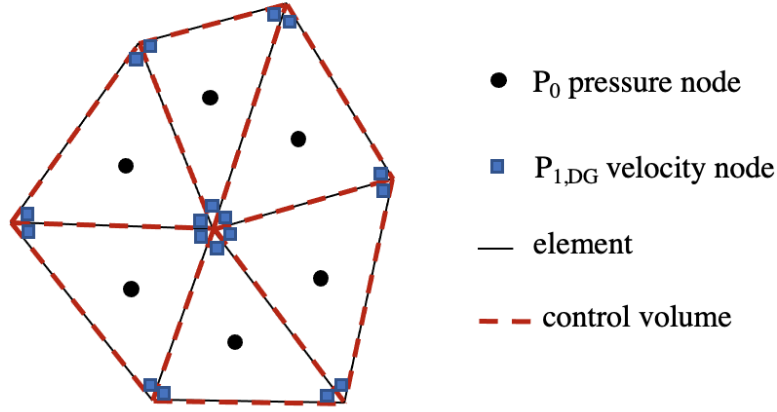


Figure 4.1: The new element pair used in the SM-CVFE method.

We employ the finite element method to resolve the flow problem following the CVFE approach [Durlafsky, 1994; Geiger et al., 2004; Jackson et al., 2015; Gomes et al., 2017; Salinas et al., 2018]. Consider the domain $(\Omega \in R^2)$ triangulated into N_e elements with a constrained conforming Delaunay triangulation [Shewchuk, 2002a]. The finite element approximation of the total Darcy velocity $(\mathbf{v}_t)$ is

$$\mathbf{v}_t(\mathbf{x}) = \sum_{j \in \Omega} \Phi_j(\mathbf{x}) v_{t,j}, \quad (4.1)$$

where $\Phi(\mathbf{x})$ denotes the linear basis function of the velocity and v_t is the velocity unknown coefficient. The pressure (p) is determined by

$$p = \sum_{j \in \Omega} \Psi_j p_j, \quad (4.2)$$

where Ψ_j is the pressure basis function that is 1 for element j and vanishes elsewhere and p_j is the pressure unknown coefficient. This approximation employs a discontinuous space for the pressure that varies element-wise.

It is worth remarking that the SM-CVFE element approximation described by this work differs from the MFE and the Salinas et al. [2018] approach. In the MFE method, the velocity is approximated using an RT-0 element. The Salinas et al. [2018] approach uses

two meshes; an element mesh and a control volume mesh as shown in Fig. 2.4c, and then requires higher order approximations for both flow variables, described by $P_{2,DG} - P_{1,DG}$.

4.2.2 Discretization of Darcy's equation

We capture the weak form of Darcy's equation by multiplying with Φ_i , a test function from the velocity basis function space. Then we integrate over the computational domain (Ω)

$$\int_{\Omega} \Phi_i \cdot \mathbf{v}_t \, d\Omega + \int_{\Omega} \Phi_i \cdot (\lambda_t \mathbf{K} \cdot \nabla p) \, d\Omega = 0. \quad (4.3)$$

The following steps are essential to incorporate the discontinuous Galerkin pressure approximation globally in the domain. We decompose the domain using the triangulation ($\mathcal{T} = \cup_{e=1}^{N_e} \Omega_e$) where N_e is the total count of elements and Ω_e is the element domain. To accommodate for the pressure discontinuity between elements, we apply integration by parts twice on the second term following Salinas et al. [2018] and the technique for embedding discontinuities in the HyCVFE approach (Section 3.2.1), which yields

$$\begin{aligned} \sum_{\Omega_e \in \Omega} \left[\int_{\Omega_e} \Phi_i \cdot \mathbf{v}_t \, d\Omega_e + \int_{\Omega_e} (\Phi_i \cdot \lambda_t \mathbf{K}) \cdot \nabla p \, d\Omega_e - \int_{\Gamma_e} (\Phi_i \cdot \lambda_t \mathbf{K} \tilde{p}) \cdot \mathbf{n} \, d\Gamma_e \right. \\ \left. + \int_{\Gamma_e} (\Phi_i \cdot \lambda_t \mathbf{K} p) \cdot \mathbf{n} \, d\Gamma_e \right] = 0, \end{aligned} \quad (4.4)$$

where Γ_e is the element boundary, $\mathbf{n}$ is the unit normal vector and $\tilde{p}$ corresponds to the pressure of the neighboring element that shares an interface with element Ω_e . We combine the third and fourth terms on the left hand side into a single term, jump term (see also Section 3.2.1). The finite element approximations, shown in Eqn. (4.1) and (4.2), for the velocity and pressure, respectively, are substituted in Eqn. (4.4), which gives

$$\begin{aligned} \sum_{\Omega_e \in \Omega} \sum_{j=1}^{N_v} \int_{\Omega_e} \Phi_i \cdot \Phi_j v_{t,j} \, d\Omega_e + \sum_{\Omega_e \in \Omega} \sum_{k=1}^{N_p} \int_{\Omega_e} (\Phi_i \cdot \lambda_t \mathbf{K}) \cdot \nabla \Psi_k p_k \, d\Omega_e \\ + \sum_{\Gamma_e \in \Omega} \sum_{k=1}^{N_p} \oint_{\Gamma_e} (\Phi_i \cdot \lambda_t \mathbf{K}_h \Psi_k (p_k - \tilde{p}_k)) \cdot \mathbf{n} \, d\Gamma_e = 0, \end{aligned} \quad (4.5)$$

N_v is the total count of velocity nodes, N_p is the total count of pressure nodes, and $\mathbf{K}_h$ denotes the harmonic permeability of the two neighboring elements that share the interface (Γ_e). The jump term described here differs from the one defined in the HyCVFE method (Chapter 3); by construction of the SM-CVFE method, the jump term contribution is nonzero between all neighboring elements (Fig. 4.2a), whereas the HyCVFE method incorporates a nonzero jump term only for elements at subdomain boundaries (Γ_d) (Fig. 4.2b). In the SM-CVFE approach, since the pressure is represented element-wise, the

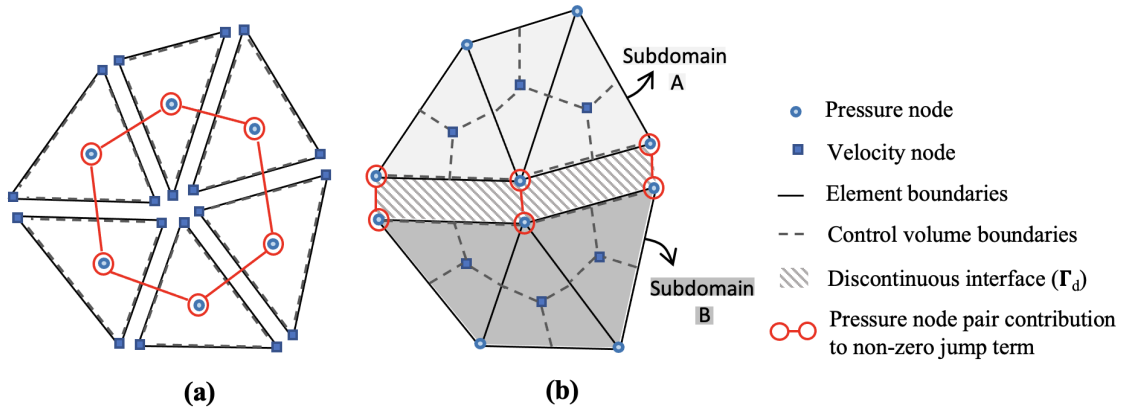


Figure 4.2: Snippet of a mesh comparison for the discretization of (a) the SM-CVFE method and (b) the HyCVFE method (Chapter 3) with 2 subdomains. The SM-CVFE discretization applies the jump term for all neighboring elements while the HyCVFE method incorporates the jump term solely along subdomain boundaries.

second term in Eqn. (4.5) vanishes because the derivative of the pressure basis function is zero. This approach for derivation of the new element pair ($P_{1,DG} - P_{0,DG}$) achieves the final discretized form of Darcy's equation as

$$\sum_{\Omega_e \in \Omega} \sum_{j=1}^{N_v} \int_{\Omega_e} \Phi_i \cdot \Phi_j v_{t,j} d\Omega_e + \sum_{\Gamma_e \in \Omega} \sum_{k=1}^{N_p} \oint_{\Gamma_e} \underbrace{\left(\Phi_i \cdot \lambda_t \mathbf{K}_h \Psi_k (p_k - \tilde{p}_k) \right)}_{\text{jump term}} \cdot \mathbf{n} d\Gamma_e = 0. \quad (4.6)$$

Contrary to the presented method, the HyCVFE applies a first order approximation for pressure, and thus the derivative of the pressure basis function does not vanish; the term analogous to the second term on the left hand side of Eqn. 4.5 is non-zero for the HyCVFE method.

4.2.3 Discretization of the continuity equation

In our SM-CVFE approach, the control volume mesh is the same as the element mesh. Consider Ω_e that denotes the element entity at which flux continuity is applied. In order to derive the weak form of the continuity equation, Eqn. (2.3), we multiply with Ψ_i , the pressure basis function, and integrate over the computational domain (Ω). We then substitute the finite element velocity approximation, Eqn (4.1) as follows

$$\sum_{\Omega_e \in \Omega} \sum_{j=1}^{N_v} \int_{\Omega_e} \Psi_i \nabla \cdot \Phi_j v_{t,j} d\Omega_e - \sum_{\Omega_e \in \Omega} \int_{\Omega_e} \Psi_i q_t d\Omega_e = 0. \quad (4.7)$$

Next, we use the divergence theorem for transforming the volume integral of the first term which yields

$$\sum_{\Gamma_e \in \Omega} \sum_{j=1}^{N_v} \int_{\Gamma_e} \Psi_i (\Phi_j \tilde{v}_{t,j}) \cdot \mathbf{n} d\Gamma_e - \sum_{\Omega_e \in \Omega} \int_{\Omega_e} \Psi_i q_t d\Omega_e = 0, \quad (4.8)$$

with $\tilde{v}_t$ indicating the velocity approximation over the control volume boundary (Γ_{cv}). We describe how to compute $\tilde{v}_t$ in section 4.2.6. The first term in Eqn. (4.8) accounts for fluxes between elements while the second term incorporates source terms.

4.2.4 Discretization of the transport equation

Consider the mass conservation equation, Eqn. 2.4 where we apply the spatial discretization over the elements (Ω_e) and an explicit time discretization. Here we employ the same linearization of the fractional flow term from Section 3.2.2. To determine the saturation of phase α (S_α), we use the integral-form of the equation, given by:

$$\begin{aligned} & \int_{\Omega_e} \frac{\phi(S_{\alpha,e}^{n+1} - S_{\alpha,e}^n)}{\Delta t} d\Omega_e = \\ & - \oint_{\Gamma_e} \left(f_{\alpha,e}^n \tilde{\mathbf{v}}_t^{n+1} + \frac{\partial f_{\alpha,e}}{\partial S_{\alpha,e}} \right)^n (S_{\alpha,e}^{n+1} - S_{\alpha,e}^n) \tilde{\mathbf{v}}_t^{n+1} \cdot \mathbf{n} d\Gamma_e \\ & + \int_{\Omega_e} q_\alpha d\Omega_e \end{aligned} \quad (4.9)$$

4.2.5 Coupled flow and transport

In the implementation of the SM-CVFE method presented here, we use an implicit-pressure explicit-saturation (IMPES) based approach to couple the flow and transport equations, see Section 3.2.3 from Chapter 3. The range of CFL numbers tested in the numerical experiments spans from 0.01 to 0.1. We recall from Section 3.2.3, the algebraic system of the flow model is setup by

$$\begin{bmatrix} \mathbf{A} & \mathbf{B} \\ \mathbf{C} & \mathbf{0} \end{bmatrix} \cdot \begin{bmatrix} \mathbf{v}_t^{n+1} \\ p^{n+1} \end{bmatrix} = \begin{bmatrix} b_1 \\ b_2 \end{bmatrix} \quad (4.10)$$

where $\mathbf{A}$ denotes the mass matrix, and $\mathbf{B}$ is the stiffness matrix that is assembled by the jump term connecting neighboring elements; see the first and third terms, respectively, in Eqn. (4.5). $\mathbf{C}$ is the divergence-free operator computed by the first term in Eqn. (4.8).

4.2.6 Interface approximations

We only consider one type of fluxes in this method, analogous to external fluxes spanning between subdomains from the HyCVFE approximation (Section 3.2.3). The velocity approximation at the interfaces between elements and, therefore, control volumes of the SM-CVFE is constructed by evaluating the effective contribution of the element velocity at the midpoint on either side of the interface, denoted by $\mathbf{v}_{t,e_A}$ and $\mathbf{v}_{t,e_B}$. These are combined using the harmonic average

$$\tilde{\mathbf{v}}_t(\mathbf{x}) = \frac{1}{2} \left(\mathbf{K}_h \mathbf{K}_{e_A}^{-1} \mathbf{v}_{t,e_A}(\mathbf{x}) + \mathbf{K}_h \mathbf{K}_{e_B}^{-1} \mathbf{v}_{t,e_B}(\mathbf{x}) \right), \quad (4.11)$$

where $\tilde{\mathbf{v}}_t$ is the velocity approximation on the interface shared by the two elements e_A and e_B , $\mathbf{K}^{-1}$ is the inverse of the element permeability, and $\mathbf{x}$ is the position vector of the interface midpoint (different from HyCVFE approach). The schematic of two neighboring

elements is shown in Fig. 4.3. By construction of the SM-CVFE approach, the velocity in each element is not uniform and differs based on the location of the midpoint, due to the first order Lagrangian approximation used for velocity. Therefore, the velocity on each interface of an element is not the same. The described velocity approximation is applied in the coefficients of the divergence-free operator ($\mathbf{C}$), Eqn. (4.8), and in the saturation equation, Eqn. (4.9). The remaining approximations of the interface terms applied here as the previous chapter (see Section 3.2.3); we adopted a first-order upwind scheme to approximate saturation dependent properties at the interface, including the total mobility (λ_t), the fractional flow term (f_α), and the derivative of the fractional flow term ($\frac{\partial f_\alpha}{\partial S_\alpha}$). In the next section, we show that the scheme is effective in producing stable, mass conservative, and monotonic solutions.

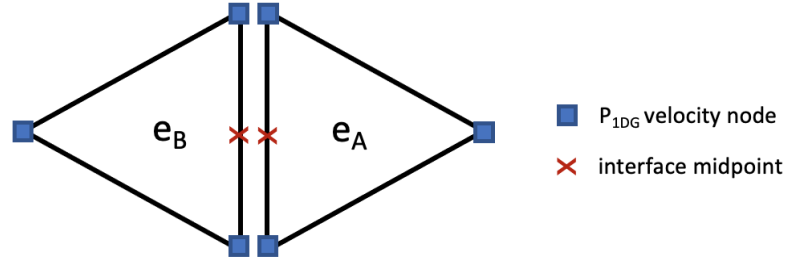


Figure 4.3: Diagram of two neighboring elements e_A and e_B to demonstrate the velocity approximation along an interface.

4.3 Numerical experiments

First, we validate the solution for single phase flow in experiment 4.3.1 and for two phase flow in experiment 4.3.2. We establish the convergence of the SM-CVFE approach for two phase flow with respect to the semi-analytical Buckley-Leverett solution [Buckley and Leverett, 1942]. Then we demonstrate the performance of the SM-CVFE in three additional experiments with geometrical complexities. In experiment 4.3.3 we test two fracture-barrier intersection scenarios. Next, geostatistical fields are generated for a single

Table 4.1: Model setup for the numerical experiments

	4.3.1	4.3.2	4.3.3	4.3.4	4.3.5
X-axis domain length (L_x)	1.	1.	1.	1.	1.
Y-axis domain length (L_y)	0.05	0.05	1.	0.5	1.
Porosity (ϕ)	0.1	0.1	variable	0.1	0.1
Corey exponent of wetting phase (n_w)	N/A	2.	1.	2.	2.
Corey exponent of non-wetting phase (n_{nw})	N/A	2.	1.	2.	2.
Residual wetting saturation ($S_{w,r}$)	N/A	0.2	0.	0.2	0.2
Residual non-wetting saturation ($S_{nw,r}$)	N/A	0.3	0.	0.3	0.3
Viscosity ratio (μ_{nw}/μ_n)	N/A	2.	2.	2.	2.

channel with meandering geometry and a challenging flow system of intersecting channels in experiments 4.3.4 and 4.3.5, respectively.

The parameters of the numerical experiments are provided in Table 4.1. The computational efficiency of the numerical experiments is compared using the Degrees of Freedom (DoF) or the total number of unknowns in a given time step. We use:

$$DoF_{SM-CVFE} = N_p + N_v + N_s, \quad (4.12)$$

to describe the computational requirements of the SM-CVFE approach similar to Eqn. (3.14) for the classical CVFE method. In Table 4.2, we highlight the DoF requirements used in the following numerical experiments.

4.3.1 Single phase flow

The validation for single phase flow is captured in two pseudo one-dimensional cases. In case I, a homogeneous medium is used with pressure boundary conditions applied on the left and right, with the top and the bottom boundaries set to no-flow. Case II has a similar setup except that the permeability is heterogeneous. The mesh used in the

Table 4.2: Comparison of the DoF requirements in the numerical experiments.

Numerical experiment	Number of elements	CVFE DoF	SM-CVFE DoF	Factor (increase)
4.3.1	160	443	1120	2.53
4.3.2 ($n_x = 40$)	160	566	1280	2.26
4.3.2 ($n_x = 80$)	320	1126	2560	2.27
4.3.2 ($n_x = 160$)	640	2246	5120	2.28
4.3.3 (case I)	1280	3934	10240	2.60
4.3.3 (case II)	1310	4024	10480	2.60
4.3.4 (case I, uniform mesh)	591	1844	4728	2.56
4.3.4 (case II, uniform mesh)	1428	4394	11424	2.60
4.3.4 (case III, uniform mesh)	2992	9132	23936	2.62
4.3.4 (non-uniform mesh)	3583	10834	N/A	N/A
4.3.5	3900	N/A	31200	N/A

model is shown in Fig. 4.4a where the number of elements along the x-axis (n_x) is 40, while the permeability of cases I and II are shown in Fig. 4.4b and 4.4c, respectively. The steady state solution of pressure (Fig. 4.4d) is a straight line for case I while the heterogeneity introduced in case II is reflected in the solution as a change of slope at position $x = 0.5$. In case II, the right region, shown between $[0.5, 1.0]$, has half the slope of the left region, between $[0., 0.5]$ which is correct with the change of property; the exact solution is the same as Eqn. (3.19). The continuous pressure solution obtained using the classical CVFE method on the same mesh is shown in Fig. 4.4d and corroborates the SM-CVFE results. Table 4.3 shows the convergence of the numerical solutions to the exact solution to cases I and II. In both cases, the SM-CVFE pressure solution converges linearly as we refine the mesh; this error is understood as a consequence of the simplified set of boundary condition (BC) implementations, discussed in Appendix A.3.1. Due to the lack of boundary nodes, the pressure is prescribed to the boundary element. This is an inherent feature of an element-wise approximation of pressure, which can be mitigated by refining the mesh, as shown in Table 4.3, or effectively incorporating ghost boundary

cells into the computational domain for the SM-CVFE approach [LeVeque, 2007]. In contrast, the CVFE method incorporates a first-order approximation of pressure and thus provides a direct approach for prescribing BCs to the boundary pressure nodes, yielding identical solution (case I) to the exact linear decline of the pressure in the domain. For comparison purposes with the HyCVFE, presented in Chapter 3, we incorporate the numerical experiments 3.3.1.

In both cases, the DoF_{CVFE} and $DoF_{SM-CVFE}$ are 443 and 1,120, respectively. Thus, the SM-CVFE method requires 2.5 times more degrees of freedom than the CVFE method, similar requirements to the MFE method [Durlafsky, 1994; Geiger et al., 2004]. The increase of the SM-CVFE method computational requirements is attributed to a higher resolution of the control volume mesh that is consistent with the element mesh and one higher order of the velocity approximation compared to the CVFE method.

4.3.2 Buckley-Leverett problem

For the two phase model validation, we simulate the Buckley-Leverett problem on a pseudo one-dimensional, homogeneous domain. The domain is discretized with 40 triangular elements along the x-axis ($n_x = 40$), see Fig. 4.4a. The model is initially saturated with the non-wetting phase ($S_{nw,i} = 0.8$), and the residual wetting phase saturation ($S_{wr} = 0.2$). We inject the wetting phase from the left to the right while the top and bottom boundaries are no-flow. The mesh is then refined along the x-axis for two additional cases ($n_x = 80, 160$). Fig. 4.5a provides a comparison of the SM-CVFE saturation solution to the semi-analytical Buckley-Leverett reference solution after 0.1 and 0.2 pore volume injected (PVI). We observe that the refinement of the mesh improves the agreement between the numerical and semi-analytical solution. We demonstrate that the system is locally and globally mass conservative from the representative area under the cluster of curves; for each time step, the area under the curve represents the same wetting phase mass injected into the system. Fig. 4.5b compares the L1-norm of the saturation solution

Table 4.3: Convergence of the pressure in numerical experiment 4.3.1

Case I				
	n_x	DoF	L^1 -norm	ROC
CVFE	40	443	4.42076E-17	-
	80	883	1.17271E-10	-
	160	1763	1.16610E-10	-
SM-CVFE	40	1120	0.008474578	-
	80	2240	0.004201656	1.012183389
	160	4480	0.002092022	1.00606004
Case II				
	n_x	DoF	L^1 -norm	ROC
CVFE	40	443	0.002094778	-
	80	883	0.001111908	0.918253463
	160	1763	0.000565433	0.978009389
SM-CVFE	40	1120	0.011539725	-
	80	2240	0.005736598	1.008341642
	160	4480	0.002859396	1.004484737
HyCVFE	40	446	2.12923E-10	-
	80	886	2.4283E-10	-
	160	1766	2.41503E-10	-

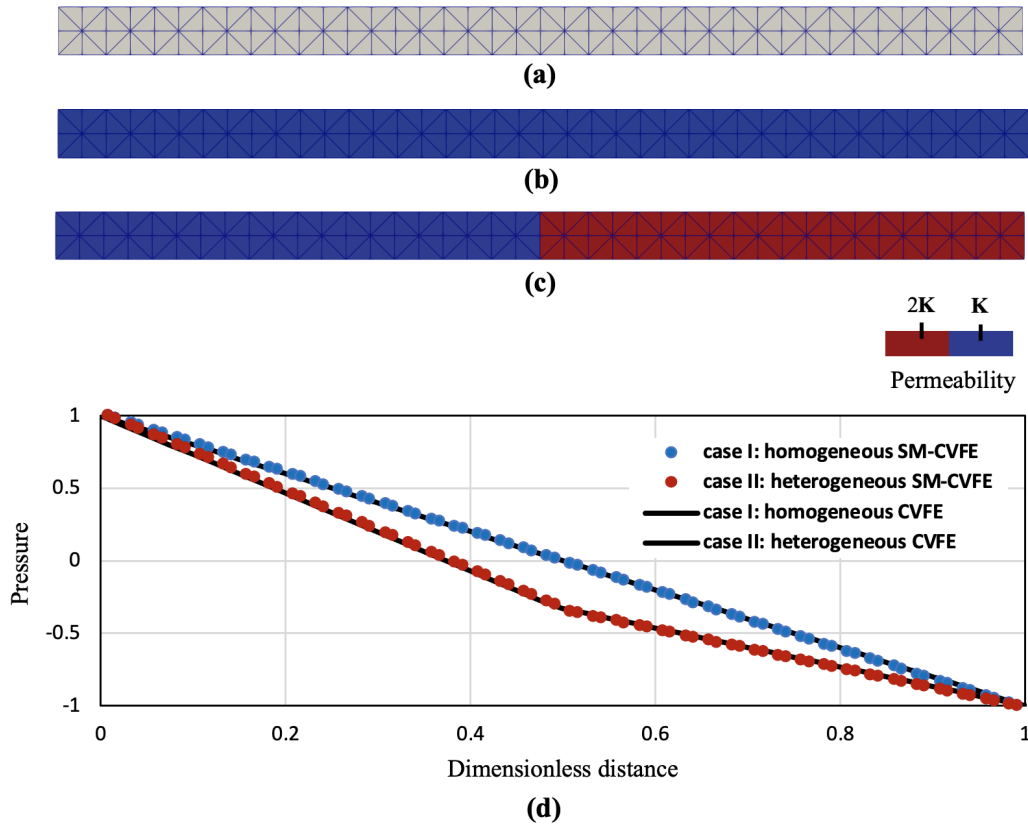


Figure 4.4: The single phase validation model experiment 4.3.1: (a) The mesh applied to the domain. (b) Case I permeability field. (c) Case II permeability field. (d) Comparison of pressure solution of both cases, I and II.

error of the SM-CVFE method and the classical CVFE with respect to the semi-analytical solution. The overlap of the two curves indicates that for a given number of degree of freedom, the error is essentially the same in both methods. Additionally, both curves follow the same convergence trend as we increase the mesh resolution and provide near linear convergence.

4.3.3 Fracture-barrier intersection

The experiment described here is adopted from Hoteit and Firoozabadi [2008]. We explore both of their cases I and II. In case I, a highly permeable fracture spans diagonally from the bottom left to the top right of the domain such that it reaches a barrier without

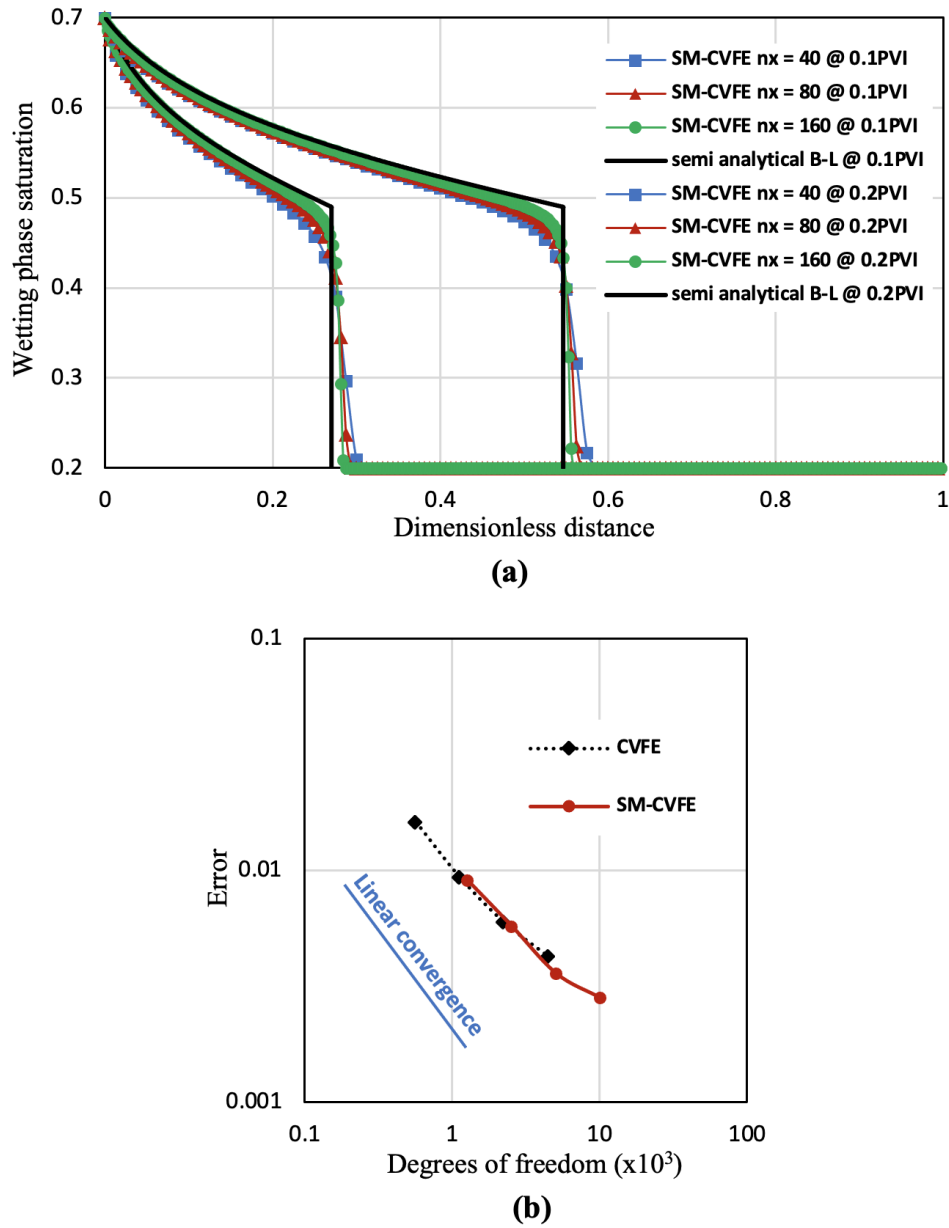


Figure 4.5: The two phase validation model in experiment 4.3.2 for the Buckley-Leverett problem. **(a)** The convergence of numerical SM-CVFE method to the semi-analytical solution as the mesh is refined. The two cluster of curves refer to 0.1 and 0.2 PVI. For the numerical comparison, we use several mesh resolutions along the x-axis including 40, 80, and 160 elements. **(b)** A comparison of the L1-norm of the error for the reference CVFE method and the SM-CVFE method.

crossing it (Fig. 4.6a and close up in Fig. 4.6c). Case II is similar except that the fracture penetrates the barrier (Fig. 4.6b and close up in Fig. 4.6d). Fracture and barrier petrophysical properties are provided in Table 4.4. We apply pressure boundary conditions from the bottom left corner to the top right corner and the wetting phase is injected at the bottom left corner. The remaining domain boundaries are set to no-flow. The number of elements in cases I and II are 1,280 and 1,310, respectively.

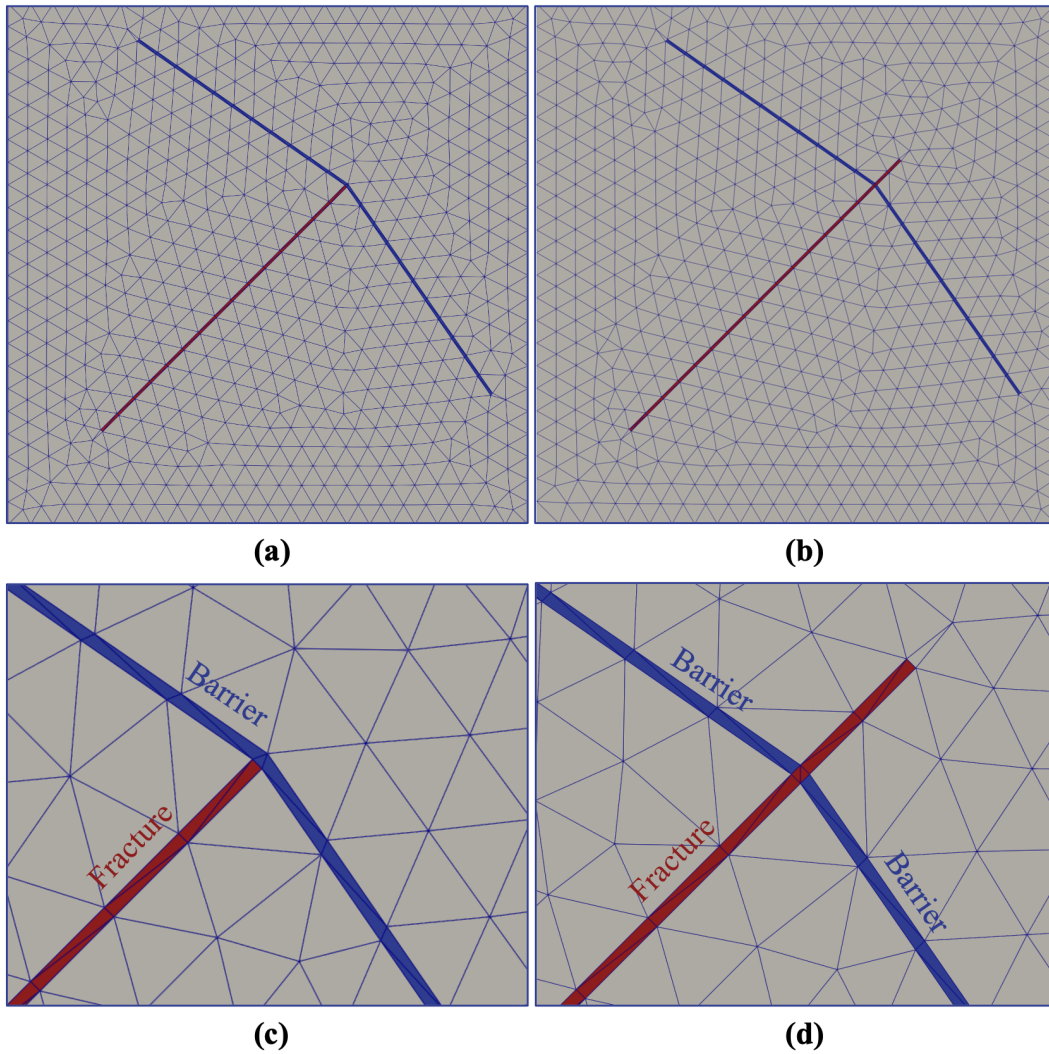


Figure 4.6: The mesh for experiment 4.3.3. The background, the fracture, and the barrier regions are denoted by grey, red, and blue colors, respectively. Case I: the fracture reaching the barrier without crossing through shown in (a) and the close up in (c). Case II: the fracture penetrating the barrier in (b) and the close up in (d).

We compare the saturation solutions obtained using the proposed SM-CVFE and the

Table 4.4: Geometry and petrophysical properties of different regions for experiment 4.3.3

	Fracture	Barrier	Background
Aperture	$0.005656L_x$	$0.005656L_x$	N/A
Porosity	1.	0.	0.1
Log permeability	6.	-6.	0.

L_x denotes the length of the domain with respect to the x-axis.

classical CVFE method for both cases (Fig. 4.7). For the early time step (Fig. 4.7a-b and Fig. 4.7e-f for case I and II, respectively), the saturation front of the proposed SM-CVFE method reaches the barrier whereas the CVFE solutions exhibit overall delay in the saturation fronts. At the later time step, we observe in both cases the injected fluid phase migration beyond the barrier in Fig. 4.7 c-d and Fig. 4.7 g-h with different flow behaviours in the fracture and barrier regions which in turn affect the flow in the matrix region. In both cases, the solutions of the classical CVFE method emphasize the inconsistency to preserve material properties due to the two mesh approach in comparison to the single mesh approach. The DoF_{CVFE} and $DoF_{SM-CVFE}$ for case I are 3,934 and 10,240, respectively, while case II required 4,024 and 10,480, respectively.

Next, we compare the saturation solutions of the classical CVFE, the proposed SM-CVFE, and the MFE-DG method [Hoteit and Firoozabadi, 2008] in Fig. 4.8. It is worth mentioning the differences in the approach and the employed mesh; the MFE-DG approach represented the fractures and barriers as lower dimensional entities and employed a mesh that is slightly different to the one used in the CVFE and the SM-CVFE results. Moreover, the MFE-DG method applied a slope limiter in the formulation to reduce the numerical dispersion of the saturation solution. Despite the aforementioned differences, after 0.5 PVI the flow patterns around the fracture and barrier in both cases I and II for the SM-CVFE and the MFE-DG are remarkably similar and are different to the solution obtained using the CVFE method. The reason is essentially due to the use of a single

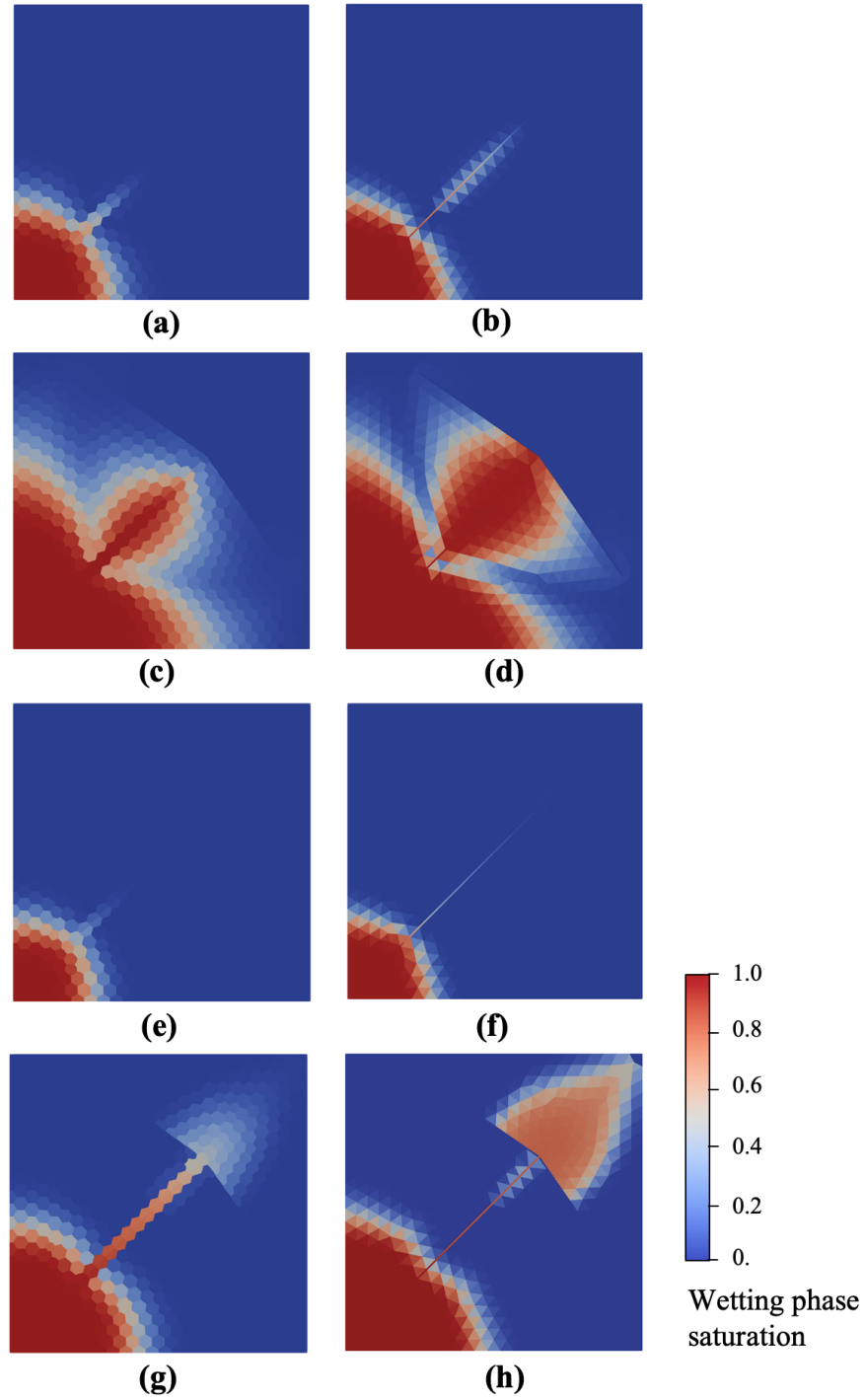


Figure 4.7: The wetting phase saturation solution for experiment 4.3.3. The top row refers to case I. The solution after 0.08 PVI is shown in (a) and (b) for the CVFE method and the SM-CVFE method, respectively. After 0.5 PVI, the solution is shown in (c) and (d) for the CVFE method and the SM-CVFE method, respectively. The bottom row features case II. After 0.05 PVI, the solution is shown in (e) and (f) for the CVFE method and the SM-CVFE method, respectively. After 0.5 PVI the solution is shown in (g) and (h) for the CVFE method and the SM-CVFE method, respectively.

mesh approach that is analogous to the MFE. The SM-CVFE solutions presented in this experiment are comparable to those obtained using specialized numerical methods that include, but are not limited to, discrete fracture networks (DFN) within the mixed finite element frameworks.

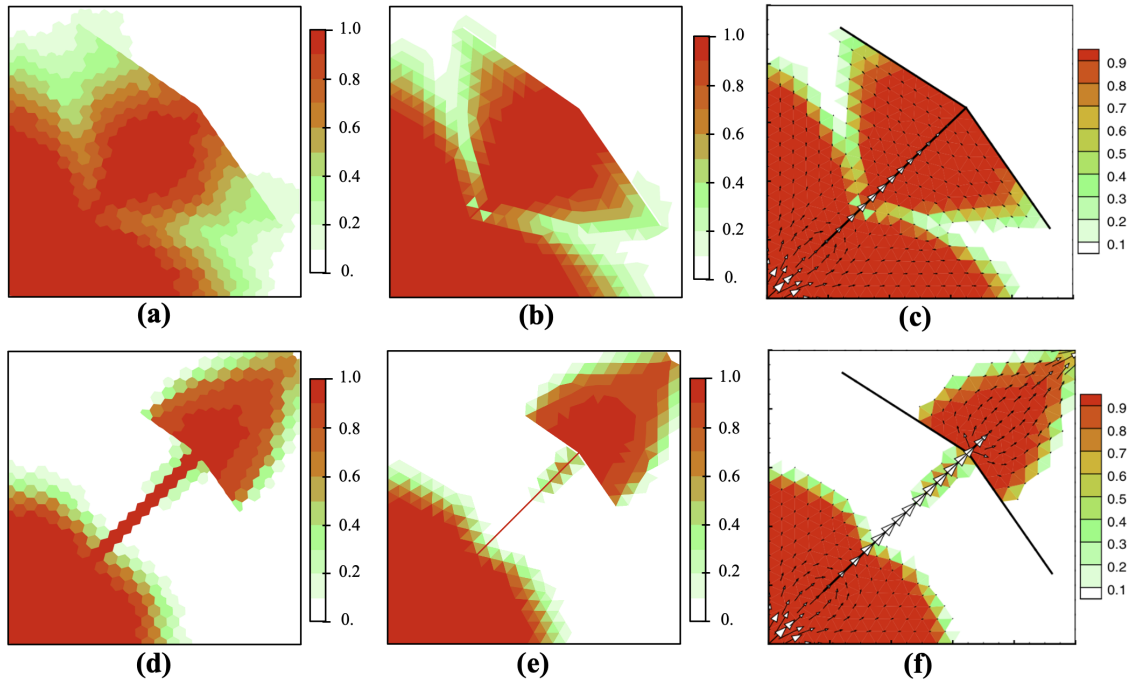


Figure 4.8: The saturation solution comparison including the results of MFE-DG method from Hoteit and Firoozabadi [2008] for experiment 4.3.3 at 0.5 PVI. For comparison purposes, the color map used here follows the one used by Hoteit and Firoozabadi [2008]. The top row shows case I results using the classical CVFE in (a), the SM-CVFE in (b), and the MFE-DG by Hoteit and Firoozabadi [2008] in (c). The bottom row shows case II using the classical CVFE in (d), the SM-CVFE in (e), and the MFE-DG by Hoteit and Firoozabadi [2008] in (f). The results shown in (c) and (f) were obtained from Fig. 12 in Hoteit and Firoozabadi [2008].

4.3.4 Meandering channel flow

The aim of the experiment is to highlight the effectiveness of the SM-CVFE formulation to capture accurate solutions of models with cell to cell variability in the underlying petrophysical properties while simultaneously eliminating the undesirable artificial mass leakage effects exhibited by the control volumes spanning different permeability regions in the classical CVFE method. We consider a channelized sand-shale system comprised

Table 4.5: The parameters used to generate the spatial permeability fields (GSTools package) for experiment 4.3.4

Region	Channel	Background
Variogram	exponential	exponential
Dimensions	2	2
Length scale	1.	0.4
Anisotropy ratio	1.	0.3
Seed	200000	100000
Nugget	0.	0.
Variance	1.	1.
increment [*]	6	0

^{*} parameter used as a post-processing step to combine the fields.

of a high permeability channelized sand body embedded in a low permeability, shale background. The permeability distribution is shown in Fig. 4.9 where two fields were generated then combined to create a bimodal permeability distribution. A geostatistical tool was used to generate those fields; GSTools python package used with the parameters provided in Table 4.5. We use several mesh resolutions in this model with the total elements of 591, 1428, and 2992 for cases I, II, and III, respectively. The average variance of the permeability distribution is preserved for all cases. The pressure boundary conditions are applied from the left to the right of the domain while the wetting phase is injected from the left boundary. The top and the bottom boundaries are set to no-flow.

We compare the saturation solution obtained using the classical CVFE method for cases I-III (see Fig. 4.10a-c) after 0.03 PVI. In case I, the left winding of the meander produces a non-physical connection in the channel, see Fig. 4.10a, as a result of the construction of the coarse control volume dual mesh. Case II uses relatively smaller control volumes which prevent the non-physical connection; however, the leakage exhibited around the channel is still considerable. Finally, case III utilizes a finer mesh which reduces the

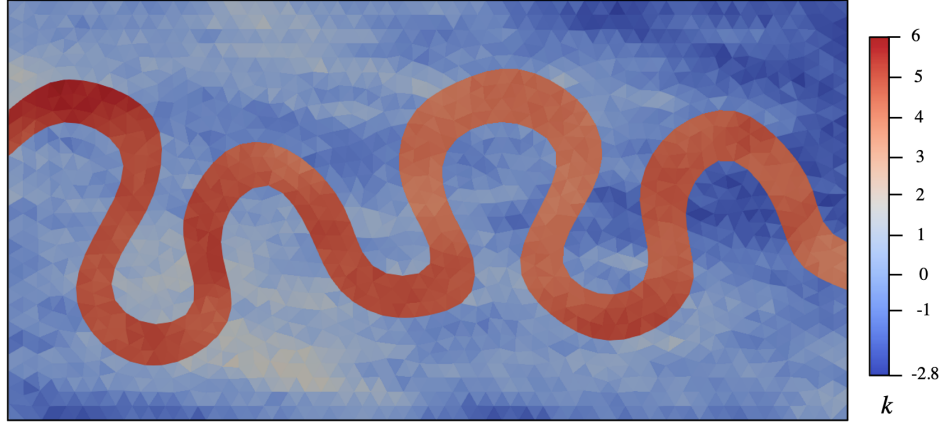


Figure 4.9: The log permeability distribution of experiment 4.3.4. The channel region is denoted with high permeability values. This permeability distribution refers to case III with 2992 elements.

leakage around the channel. From Fig. 4.10a-c we note that, at a given time step, the location of the wetting phase front differs considerably as the mesh is refined while using the CVFE method because a coarse mesh contributes to additional losses of injected fluid smeared across the large sand-shale interface, delaying the propagation of the saturation front in the channel region. Second, the meandering of the channel exaggerates the effect of the leakage when compared to a straight channel path. The meandering of the channel creates a larger interface with the background region and, therefore, increases the leakage effects. It is worth noting that the mesh employed in case III is referred to as a fine mesh, however, it is not equivalent to $\Omega_{cv} \rightarrow 0$. This experiment shows that the use of CVFE method is inadequate to capture the flow and transport dynamics without exploiting a very fine mesh. Now consider the saturation solutions provided in Fig. 4.10d-f which show the corresponding SM-CVFE solution for cases I-III, respectively. We observe excellent agreement of the saturation front for the SM-CVFE solution at a given time step irrespective of the mesh size, due to the use of single mesh that eliminates the non-physical mass leakage in the transport solution. We note that the effect of numerical dispersion of the saturation front is reduced as we refine the mesh (Fig. 4.10d compared to Fig. 4.10e and Fig. 4.10f) that is consistent with convergence analysis demonstrated in numerical experiment 4.3.2.

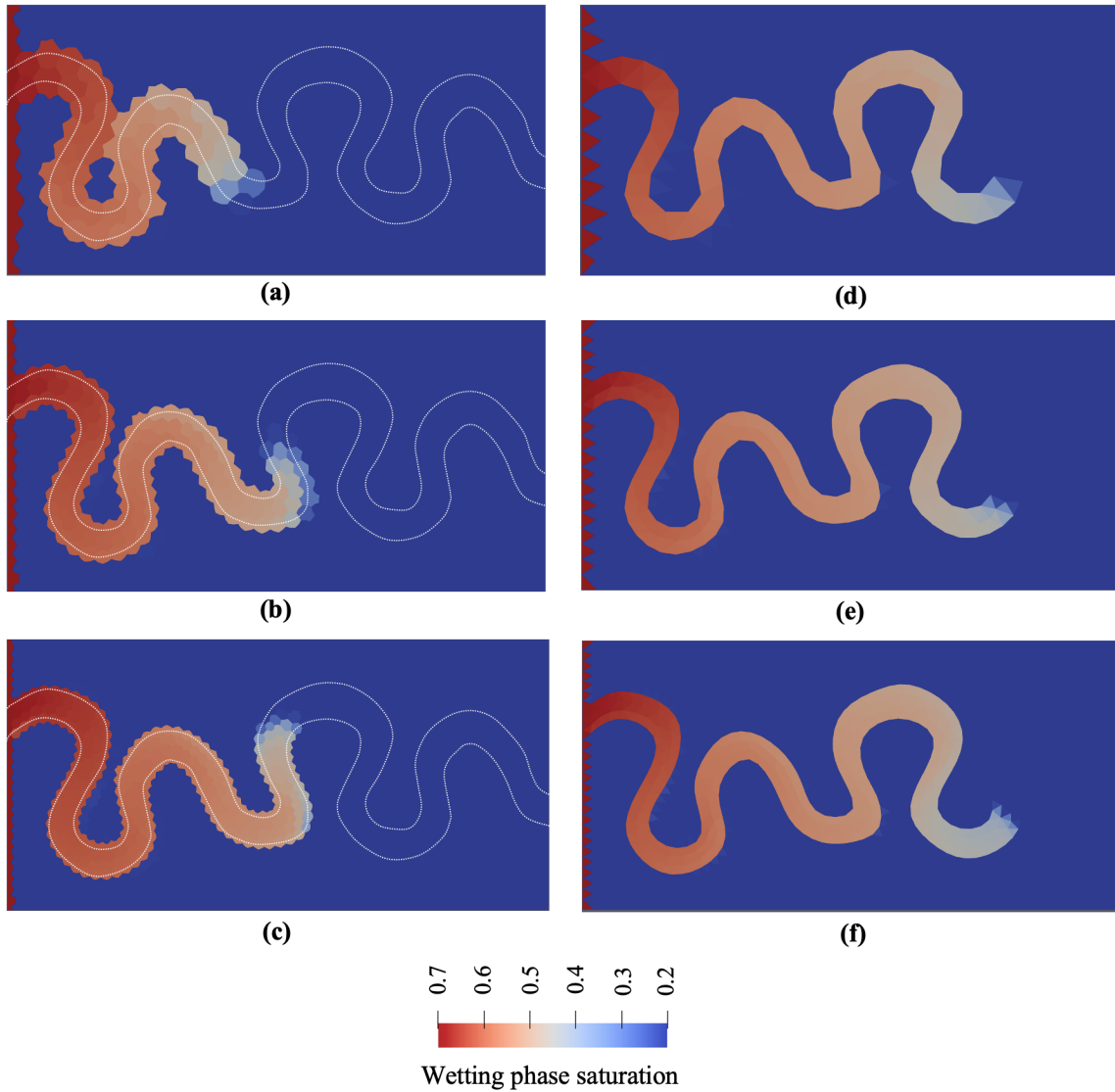


Figure 4.10: The wetting phase saturation of experiment 4.3.4 after 0.03 PVI. The saturation distribution of the classical CVFE method solution is displayed on the left column and the SM-CVFE method is displayed to the right. Case I: the coarse mesh in (a) and (d). Case II: medium refinement in (b) and (e). Case III: the fine mesh in (c) and (f). Note that the left boundary's inlet saturation that does not coincide with the channel is not accounted for in the PVI approximation in order to eliminate the irrelevant mesh effects from our study. We include an outline of the channel boundaries on the left column to emphasize the leakage along the boundaries as we refine the mesh in cases I, II, and III.

Next, we extend this experiment with an additional case for the classical CVFE method to accommodate non-uniform meshes. As shown in Fig. 4.11a, the mesh refinement is applied near the interface between the channel and background region. The saturation solution in Fig. 4.11b, captured after 0.03 PVI, shows the saturation front has advanced further into the channel compared to previous cases (I-III). However, we note that the position accuracy of this saturation front is not comparable with that achieved by the SM-CVFE method. This case highlights the necessity of minimizing control volumes that span different regions when employing the CVFE method. Ideally, the control volume size need to approach zero to yield solutions comparable to those obtained with the SM-CVFE approach.

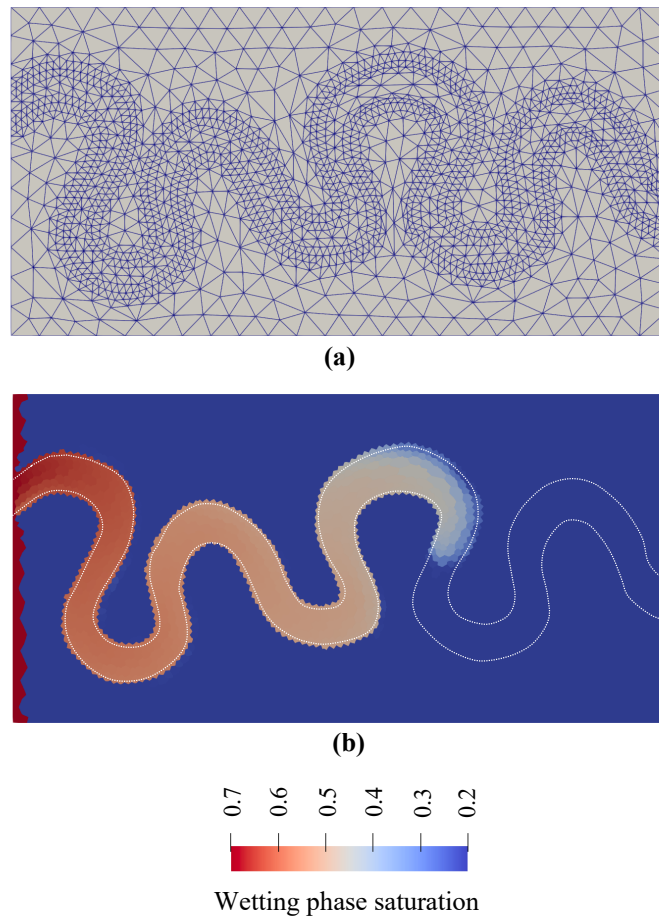


Figure 4.11: The non-uniform mesh for experiment 4.3.4. **(a)** Refinement is applied near the channel boundaries in the non-uniform mesh. **(b)** The wetting phase saturation of the CVFE method after 0.03 PVI.

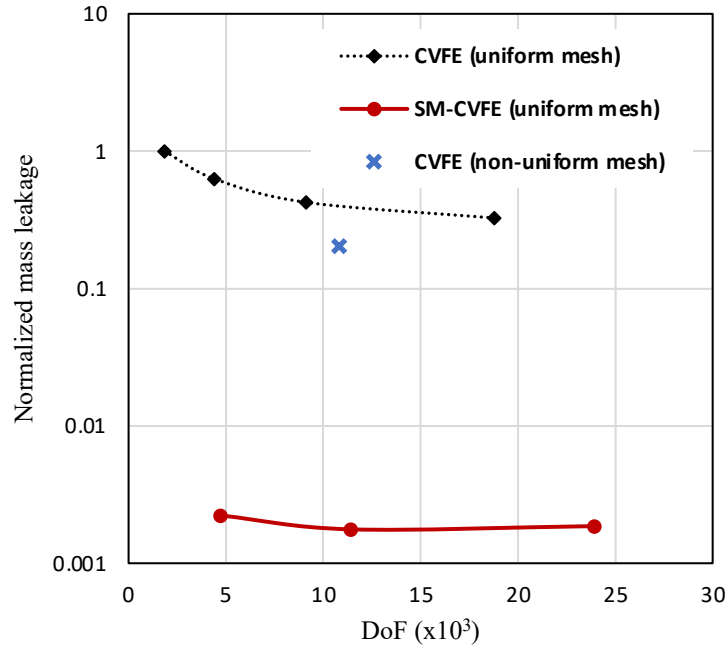
We demonstrate each method's mesh sensitivity with respect to the non-physical leakage. We compute the non-physical leakage to the low permeability, background region (Ω_{low}) using Eqn. (3.18). This follows the work of Salinas et al. [2018] and the approach presented in Chapter 3 in order to quantify the undesirable leakage effects in the saturation solution. Fig. 4.12a compares the non-physical leakage (ϵ_{max}) in the SM-CVFE and the CVFE methods. We observe a consistent improvement in the saturation solution of the SM-CVFE such that the leakage is reduced by more than 2 orders of magnitude compared to the CVFE approach. Additional refinement of the mesh in the CVFE does not close the 2 order of magnitude gap with the SM-CVFE. The blue cross shown in Fig. 4.12a refers to the non-uniform mesh employed for the CVFE method. Despite the marginal improvement in leakage reduction, a comparison at equivalent DOF between the SM-CVFE (uniform mesh) and CVFE (non-uniform mesh) methods reveals that the SM-CVFE method still exhibits a two order of magnitude improvement in accuracy compared to the classical CVFE method.

Finally, we compare the DoF of the reference CVFE with the SM-CVFE and the Salinas et al. [2018] approximations in Fig. 4.12b. The cross-plot enables us to compare the computational requirements of the different methods for a given mesh. The CVFE reference unit slope is a benchmark. The SM-CVFE method computational requirements are slightly less than half that of the Salinas et al. [2018] method despite both approximations relying on discontinuous discretization techniques. The SM-CVFE is more effective since it is based on a lower order approximation while employing a single, consistent mesh; it requires about 2.5 times the DoF of the reference CVFE method for the same mesh. In this experiment we show that the saturation solution obtained from the SM-CVFE exhibits significant reduction in the undesirable leakage compared to the reference CVFE independent of the mesh resolution. When modeling flow through complex geometry, this approximation outperforms conventional methods due to the elimination of the secondary mesh that introduces inaccurate solutions along subdomain interfaces. In the SM-CVFE method, the ability to capture accurate flow model in complex geometrical domains stems

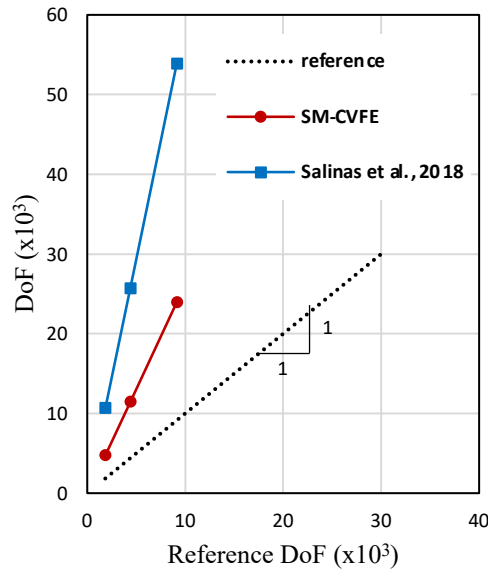
from the use of unstructured, flexible elements rather than mesh refinement.

4.3.5 Intersecting channels

In this experiment, we introduce a complex 2D domain of intersecting channels with the permeability distribution shown in Fig. 4.13. Similar to the previous experiment, we generate several geostatistical fields then combine them to create the final permeability distribution. We note that the high permeability regions are concentrated in the channels (1-5 in Fig. 4.13) where it is nonuniform and spans over a wide range of values. The setup parameters needed to generate the geostatistical permeability fields are provided in Table 4.6. In the table, the irregular channel settings are used for channels 2 and 4, while the sinusoidal channel refers to channels 1, 3, and 5. A single mesh resolution is demonstrated in this experiment where the domain is discretized into 3,900 triangular elements and the corresponding $DoF_{SM-CVFE}$ required for modeling the coupled flow and transport is 31,200. Pressure boundary conditions are applied from the left to the right boundary while injection of the non-wetting phase is taking place from the left boundary. The top and bottom boundaries are set to no-flow. We provide the saturation solution at several time steps in Fig. 4.14. After 0.035 PVI (Fig. 4.14a) the saturation solution shows the migration of injected fluid phase from channels 4 to 3, as well as the inter-connectivity between channels 1 and 2 as a result of intersections near the inlet. The next time step shown in Fig. 4.14b refers to the saturation solution after 0.07 PVI with the injected fluid advanced over half way through channel 3 which provides the shortest flow path to the outlet. After breakthrough, both Fig. 4.14c and 4.14d show that the overall sweep through the bottom region is more efficient when compared to the top region. In this example, we demonstrate that the general SM-CVFE approach is applicable to model flow and transport through complex intersecting domains, including highly heterogeneous and nonuniform permeability fields.



(a)



(b)

Figure 4.12: Comparison of different methods in experiment 4.3.4. **(a)** The mass leakage plot for the reference CVFE method and the proposed SM-CVFE method as we refine the mesh. We observe over two orders of magnitude improvement in the solution of the SM-CVFE compared to the reference. **(b)** Comparison of the DoF requirements as the mesh is refined showing the reference CVFE, the proposed (SM-CVFE) method, and Salinas et al. [2018] method. The dotted line has a slope of one and is used as a reference to the CVFE method's computational requirements.

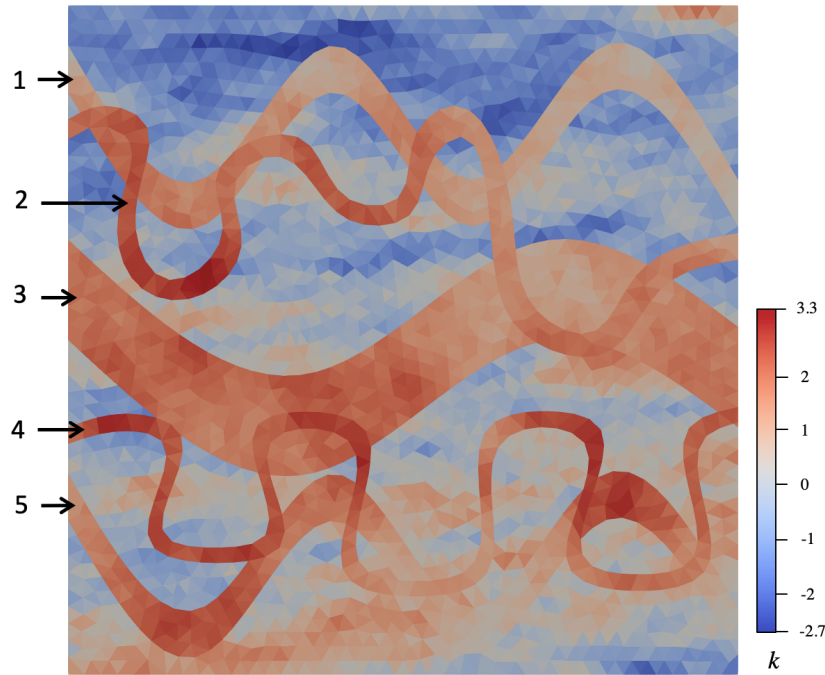


Figure 4.13: The log permeability distribution of experiment 4.3.5. The numbers to the left aid to identify individual channels in the text.

4.4 Discussion

In this chapter, we have described the original formulation of the single-mesh CVFE (SM-CVFE) method and demonstrated the versatility of the approach using several numerical experiments featuring domains with complex geometries. In the last two numerical experiments, 4.3.4 and 4.3.5, we constructed highly heterogeneous, geostatistical permeability fields. Those are challenging to resolve accurately without resorting to a very fine mesh when using the classical CVFE approach especially along boundaries between subdomains. Now consider a slight modification to the last two experiments where we assign distinct permeability values and apply them uniformly to each region [Osman et al., 2021; Jackson et al., 2015]. The use of HyCVFE method (Chapter 3) will outperform the proposed SM-CVFE, the MFE, the classical CVFE, and the Salinas et al. [2018] methods. In such a model, the uniform permeability regions are accurately and efficiently resolved using the subdomain approach where we combine the continuous pressure approximation in homogeneous subdomains while exclusively assigning hybrid nodes that account for jumps in

Table 4.6: The parameters used to generate the spatial permeability fields (GSTools package) for experiment 4.3.5

Region	irregular channel	sinusoidal channel	Background
Variogram	exponential	exponential	exponential
Dimensions	2	2	2
Length scale	1.	1.	0.4
Anisotropy ratio	1.	1.	0.3
Seed	208	208	62534
Nugget	0.	0.	0.
Variance	1.	1.	1.
increment*	1.5	1.	0

* parameter used as a post-processing step to combine the fields.

the solution along material boundaries, by preventing the control volumes from spanning subdomain boundaries. The approach is very efficient since it has similar DoF count to the CVFE and only introduces a small overhead to the computational requirements. The computational overhead associated with using the HyCVFE method in comparison to the classical CVFE for numerical experiment 4.3.4 is 5% ,7%,and 11% for cases I, II, and III, respectively, while for numerical experiment 4.3.5 the HyCVFE method introduces about 11%.

We note that the benefits offered by the SM-CVFE approximation can extend beyond porous media flow problems. For example, the study of Hu et al. [2018] applied the CVFE method to approximate the shallow water equations for an urban flooding model. Despite using a refined mesh where accuracy is needed, the model exhibited non-physical leakage along the boundaries separating the buildings from the surrounding region. The potential advantages offered by the SM-CVFE approach to model shallow water equations while eliminating the inconsistency of using the two-mesh approach is promising.

4.5 Summary

In this chapter, we presented a new discretization approach: the single mesh control volume finite element (SM-CVFE) method. The approach overcomes a well known challenge facing the family of CVFE methods by employing the element pair $P_{1,DG} - P_{0,DG}$ that requires a single, consistent mesh for the discretization of flow and transport variables. The computational requirements are comparable to the MFE methods; the SM-CVFE approach requires about 2.5 times the degrees of freedom (DoF) when compared to the CVFE method. The SM-CVFE approach establishes stable solutions that are mass conservative. We validated the approximation of the single phase pressure solution and the two phase Buckley-Leverett model. Additionally, we presented several numerical experiments with challenging aspects including complex geometries and incorporated geostatistical models with strong heterogeneities. The presented SM-CVFE method offers a powerful framework that applies a consistent discretization and achieves accurate solutions while requiring a simple implementation that, in retrospect, seems quite natural. We believe that the SM-CVFE techniques put forth in this work provide interesting avenues for generalization and extension within and beyond the scope of porous media flow problems.

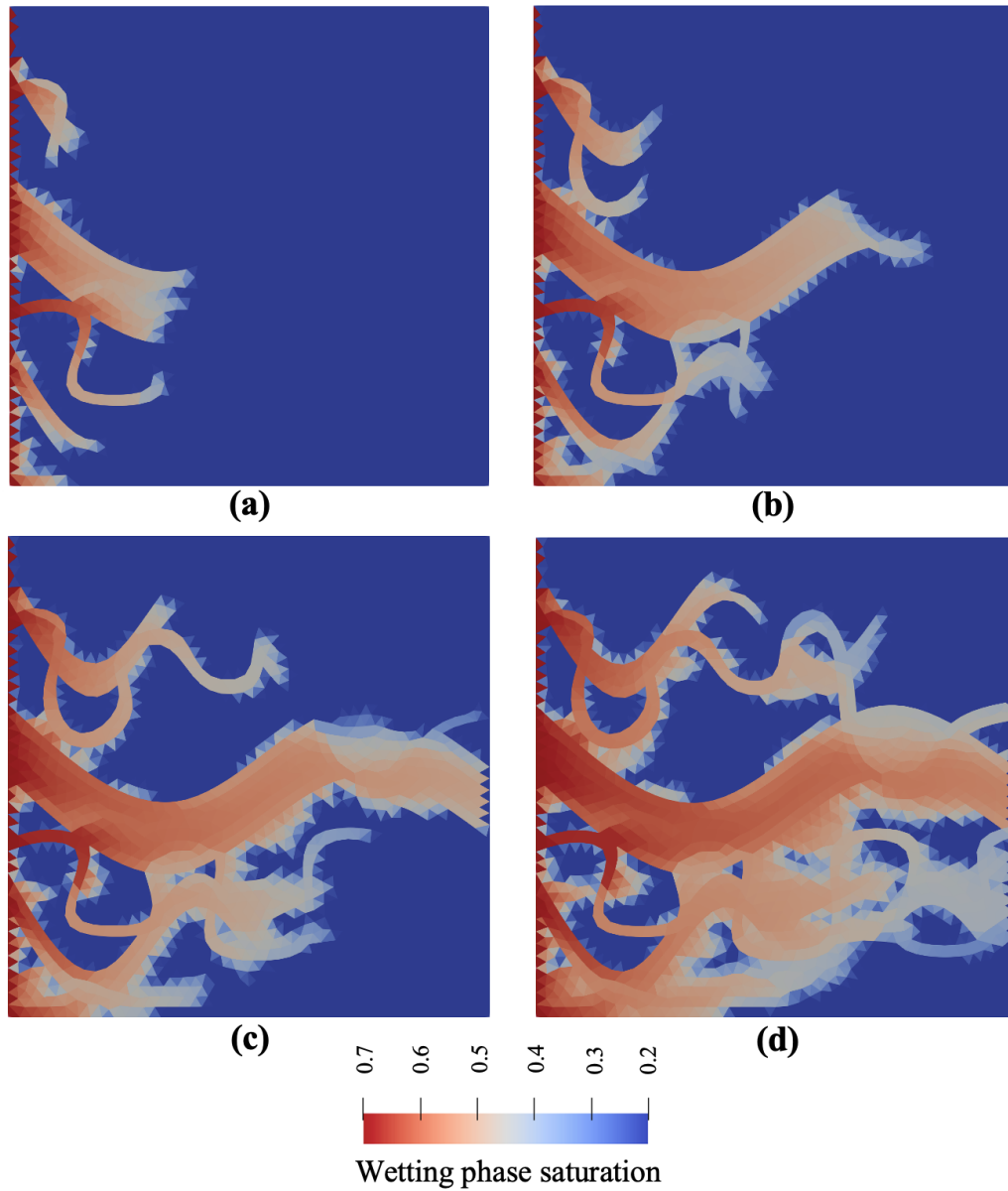


Figure 4.14: The wetting phase saturation profile for experiment 4.3.5. The saturation solution before breakthrough in (a) and (b) with 0.035 and 0.07 PVI, respectively. The saturation solution after breakthrough in (c) and (d) with 0.13 and 0.25 PVI, respectively.

Chapter 5

Extensions of the single mesh approximation

5.1 Introduction

Many realistic applications that require capturing multiphase flow patterns in complex porous media structures involve modeling three dimensional, accurate representation of the physical systems. So far in this work, we have presented two methodologies implemented for two dimensional models, the HyCVFE (Chapter 3) and the SM-CVFE (Chapter 4) methods. Each has a distinct approach for capturing discontinuities of the material properties as well as the transport solution. The HyCVFE approach effectively captures solution discontinuities through a subdomain-based approach using an efficient formulation with minimal introduction of additional degrees of freedom. On the other hand, the SM-CVFE method is versatile given that: 1) it is inherently capable of capturing element to element variability in material properties which can be advantageous to a variety of applications, 2) it provides a fully flexible, discontinuous approximation that require one, consistent mesh. Given the benefits offered by the SM-CVFE and its numerous potentials, in the remaining chapters of this thesis, we shift gear and focus

primarily on the SM-CVFE as the preferred approach.

In this chapter, we extend the SM-CVFE formulation presented in Chapter 4 to handle three dimensional models. We describe the components needed to generalize the implementation in section 5.2. Then we validate the developed approach and apply it to a numerical experiment using a realistic fractured 3D model in section 5.3.

5.2 Method

5.2.1 Flow variable discretization with tetrahedral element

A tetrahedron is used in 3D models to represent each element. It is the simplest type employed in unstructured 3D meshes and capable of adapting to complex geometries found in the subsurface [Muron, 2005]. For the discretization of the flow variables, used here, on a tetrahedral element [Zienkiewicz et al., 2005], four nodes are used for the discretization of the velocity field, while the pressure is approximated with a single node, representing a scalar field as described in chapter 4. Fig 5.1 shows the element type employed in 3D models. The element has 4 triangular interfaces with adjacent elements.

For the $P_{1,DG} - P_{0,DG}$ element pair discretization on a tetrahedron, the velocity and pressure basis functions, similar to the triangular element, we recall employing a Lagrangian first-order approximation for the velocity basis function [Zienkiewicz et al., 2005], Eqn. (3.1), and a discontinuous low order approximation for the pressure basis function that evaluates to 1 in the element and vanishes elsewhere, described in Eqn. (3.2).

5.2.2 Flux approximation

Fig. 5.2 shows how fluxes are approximated across triangular interfaces connecting neighboring elements. This represents a generalization from flux approximation across element

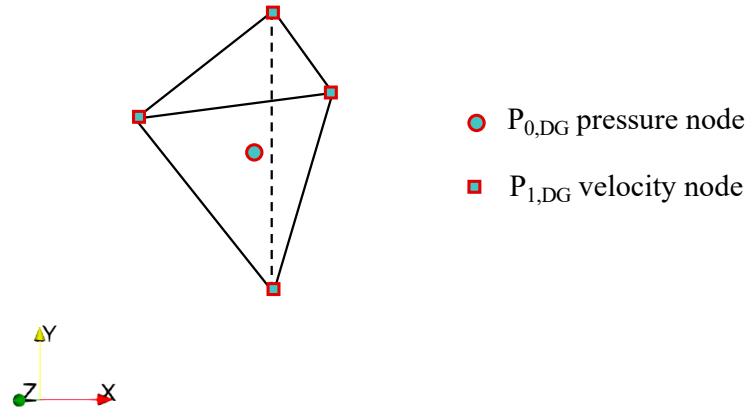


Figure 5.1: Discretization of flow variables on a tetrahedral element

edges in 2D models. For the interface between e_A and e_B shown in Fig. 5.3, the velocity components, $\mathbf{v}_{t,e_A}$ and $\mathbf{v}_{t,e_B}$, are determined at the barycenter of the common interface of each element, denoted by the X (the quadrature point) in Fig. 5.3. Here we use a single quadrature point to satisfy the exact numerical integration. Next, the velocity approximation between the two elements is computed using the harmonic average, Eqn. (3.13).

5.3 Numerical experiment

We first validate the extended SM-CVFE approximation with the Buckley-Leverett (B-L) problem where we assess the convergence rate of the numerical solution against the semi-analytical solution [Buckley and Leverett, 1942]. Then we test a 3D fracture intersections experiment with a realistic geometry that describes fracture orientations with varying angles and exhibits large discrepancies in element sizes between the fractures and the surrounding region. The parameters used in the setup of the experiments are shared in Table 5.1.

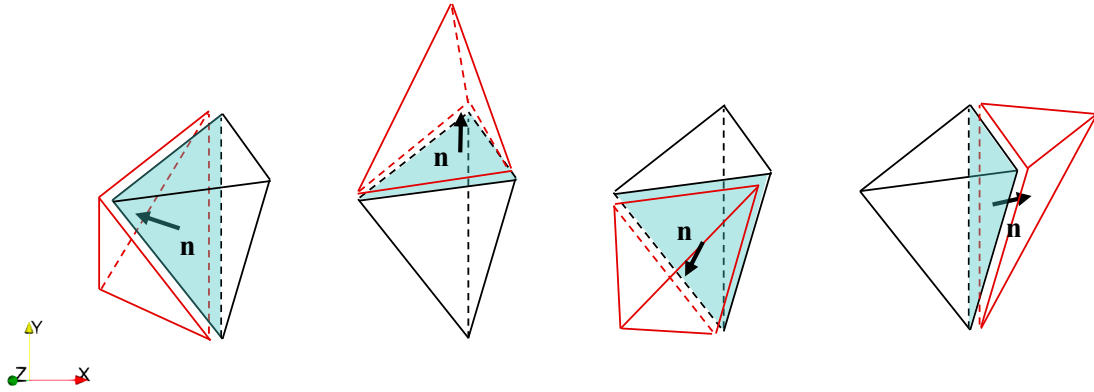


Figure 5.2: A tetrahedral element outline (black) and the adjacent neighbors (red). The direction of fluxes between adjacent elements are normal to the triangular interface.

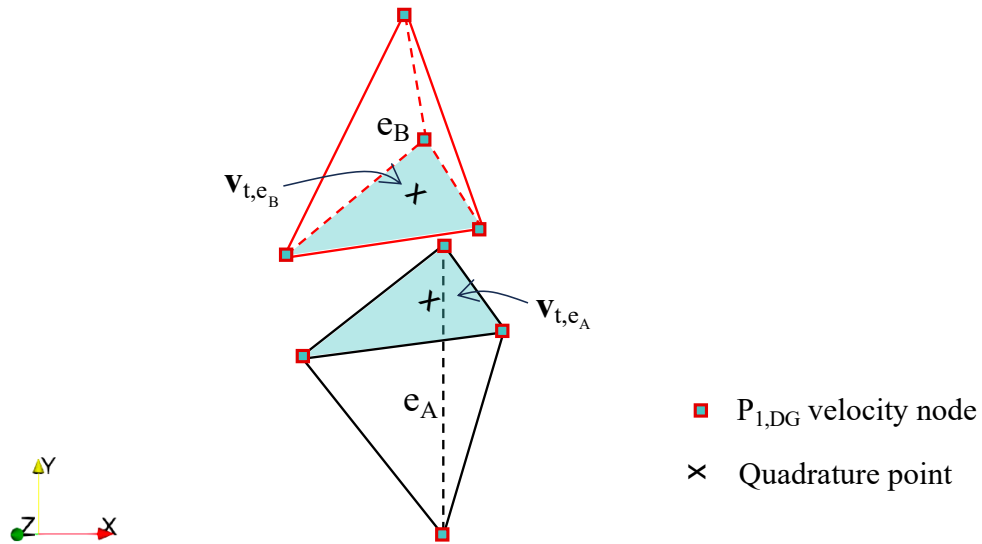


Figure 5.3: A sketch showing the position of velocity approximation computed over an interface shared by two tetrahedral elements.

Table 5.1: Model setup for the numerical experiments

	5.3.1	5.3.2
X-axis domain length (L_x)	1.	1.
Y-axis domain length (L_y)	0.05, 0.025, 0.0125	1.
Z-axis domain length (L_z)	0.05, 0.025, 0.0125	0.05
Corey exponent of wetting phase (n_w)	2.	1.
Corey exponent of non-wetting phase (n_{nw})	2.	1.
Residual wetting saturation ($S_{w,r}$)	0.2	0.2
Residual non-wetting saturation ($S_{nw,r}$)	0.3	0.3
Viscosity ratio (μ_{nw}/μ_n)	2.	2.

5.3.1 Buckley-Leverett problem

In this experiment, we validate the numerical solution of the SM-CVFE extension by applying it to the pseudo one-dimensional Buckley-Leverett problem and comparing it with the classical CVFE method. For the numerical experiment, we employ various mesh resolutions along the x-axis: the mesh is discretized into 40, 80, and 160 elements for cases I, II, and III, respectively. The mesh used for case I is illustrated in Fig. 5.4; the structured mesh has the advantage of even element spacing, aiding in processing and comparison with the semi-analytical solution.

A comparison of the pressure for the initial time step obtained from both approximations is presented in Fig. 5.4b-d. The element-wise pressure approximation (SM-CVFE) demonstrates excellent agreement with the continuous CVFE, exhibiting a linear decline between the inlet and the outlet. In Table 5.2, we compare the L^1 -norm values of pressure solutions obtained from the classical CVFE method and the SM-CVFE method with the exact solution. The L^1 -norm of the SM-CVFE pressure solution decreases linearly as we refine the mesh; we understand that this error contribution results from the simplified set of boundary condition (BC) implementations, discussed in Section 4.3.1 and further described in Appendix A.3.1.

Table 5.2: L^1 -norm of the pressure solution for numerical experiment 5.3.1

	Case	n_x	DoF (10^3)	L^1 -norm	ROC
CVFE	I	40	3.618	8.42564E-17	-
	II	80	7.218	1.13692E-16	-
	III	160	14.418	9.95186E-16	-
SM-CVFE	I	40	13.44	0.02329104	-
	II	80	26.88	0.011689233	0.994594833
	III	160	53.76	0.005855404	0.997339656

The saturation distribution for cases I-III are plotted at two time steps, 0.1 PVI and 0.2 PVI, in Fig. 5.5a. The solution shows that as we refine the mesh, both the rarefaction wave and the shock front are captured with improved accuracy. Moreover, the saturation solution is monotone and mass conservative. This numerical experiment shows that as the dimensionality of the problem increases, the convergence rate varies, as evident from Fig. 5.5a, where the saturation front in the 3D model is considerably more diffused than in the 2D BL model results shown in Fig. 4.5. It is worth noting that the developed SM-CVFE approach for 3D models is exploiting an explicit time stepping scheme, described in Section 4.2.5. Here we recall here that the stability is achieved by restricting the CFL number to unity [Aziz and Settari, 1979]. We compare the convergence of the numerical solutions of SM-CVFE and CVFE with two CFL numbers, $CFL \leq 0.01$ and $CFL \leq 0.1$, where we observed that the convergence rate varies for different CFL. In Fig. 5.5b, we show that both approximations, CVFE and SM-CVFE, exhibit near-linear convergence to the semi-analytical Buckley-Leverett solution with $CFL \leq 0.01$. The rate of convergence (ROC) is reduced as the CFL number is increased one order of magnitude ($CFL \leq 0.1$), see Table 5.3.

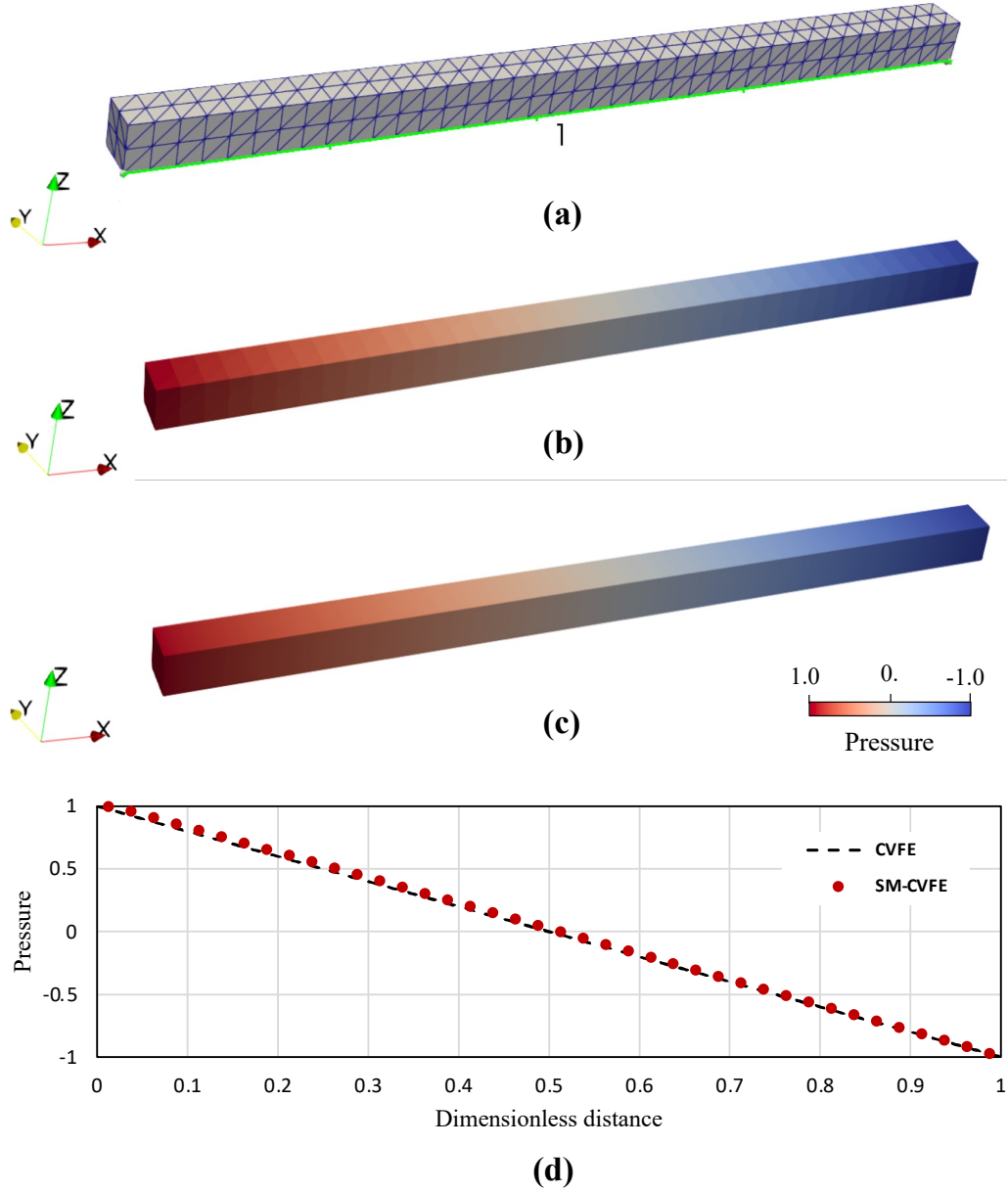
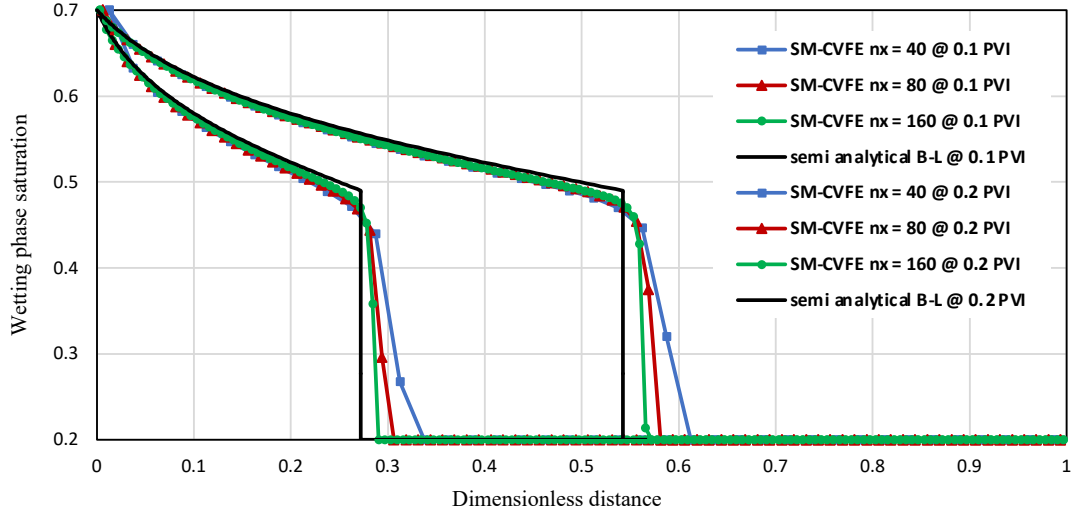
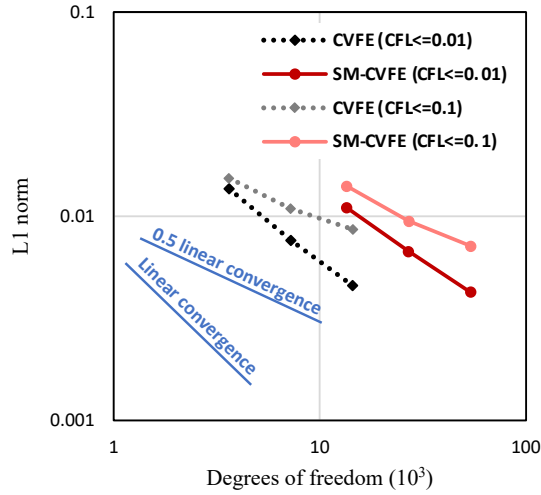


Figure 5.4: The Buckley-Leverett problem in numerical experiment 5.3.1: The mesh used in case I with 40 elements along the x-axis is shown in (a). The initial pressure solution for the SM-CVFE method in (b) and the CVFE method in (c). 1D comparison of the initial pressure in (d).



(a)



(b)

Figure 5.5: The Buckley-Leverett problem in numerical experiment 5.3.1: **(a)** Comparison of the numerical solution obtained using the SM-CVFE method and compared with the semi-analytical Buckley-Leverett solution after 0.1 and 0.2 PVI for $CFL \leq 0.01$. **(b)** The convergence rate for both approximations, the SM-CVFE and the CVFE methods follows the same convergence trend. For $CFL \leq 0.01$, the convergence is near linear, and for $CFL \leq 0.1$, the convergence is halved.

Table 5.3: Convergence analysis for BL saturation in numerical experiment 5.3.1

$CFL \leq 0.01$					
	Case	n_x	DOF ($\times 10^3$)	L1 norm	ROC
CVFE	I	40	3.618	0.013680554	-
	II	80	7.218	0.007646082	0.842360901
	III	160	14.418	0.004574172	0.742546573
SM-CVFE	I	40	13.44	0.011048585	-
	II	80	26.88	0.006715222	0.718354594
	III	160	53.76	0.004244141	0.661962684
$CFL \leq 0.1$					
	Case	n_x	DOF ($\times 10^3$)	L1 norm	ROC
CVFE	I	40	3.618	0.0153957	-
	II	80	7.218	0.010894178	0.500769524
	III	160	14.418	0.008631632	0.33645763
SM-CVFE	I	40	13.44	0.01409366	-
	II	80	26.88	0.009476235	0.572660494
	III	160	53.76	0.007157609	0.404836118

5.3.2 3D fracture intersections

The fracture geometry used in this numerical experiment is based on the fractured rock pattern identified in Kilve, Somerset, United Kingdom [Belayneh et al., 2006]. The petrophysical properties are described in Table 5.4. The fracture geometry and the employed mesh, discretized with 25,031 tetrahedral elements, are shown in Fig. 5.6. We note that the number of elements utilized in this experiment is significantly fewer than what is often demanded by alternative numerical 3D approximations, such as CVFE and FV methods. The domain is initially saturated with the non-wetting phase ($S_{nw,initial} = 0.7$, $S_{w,r} = 0.3$). We apply pressure boundary conditions from the left boundary (at $x = 0$) to the right boundary (at $x = 1$) with the injection of the wetting phase applied from the left boundary (at $x = 0$). We show the SM-CVFE pressure profile in the system in Fig. 5.7 (a) along with a line spanning from the left boundary to the right boundary at which pressure solution is compared with the classical CVFE method. In Fig. 5.7 (b), the 1d comparison shows the pressure profile along the marked line. Despite the SM-CVFE method having a one-order lower approximation for pressure ($P_{0,DG}$) compared to the CVFE method (P_1), the pressure solutions exhibit good agreement. Starting from the inlet, the pressure gradually decreases until it reaches fracture 1 (box 1) in Fig. 5.7 (b), after which it levels off in the isolated region between fracture 1 and fracture 2 (spanning box 1 to box 2). Subsequently, the pressure profile undergoes a sudden increase upon crossing fracture 3 near the outlet (box 3).

It is worth noting that the stair-stepping effect observed in the SM-CVFE pressure solution (Fig. 5.7b) arises from the element-wise approximation. The width of each step indicates the extent to which the line intersects an element, with short widths resulting from either small elements or minimal element intersection with the line, close to the vertex.

Fig. 5.8 compares the saturation solution of the classical CVFE method and the SM-CVFE method after 0.03, 0.09, and 0.14 PVI. In Fig. 5.8b, the SM-CVFE wetting phase saturation reaches the right boundaries once it occupies the narrow fracture corridors after

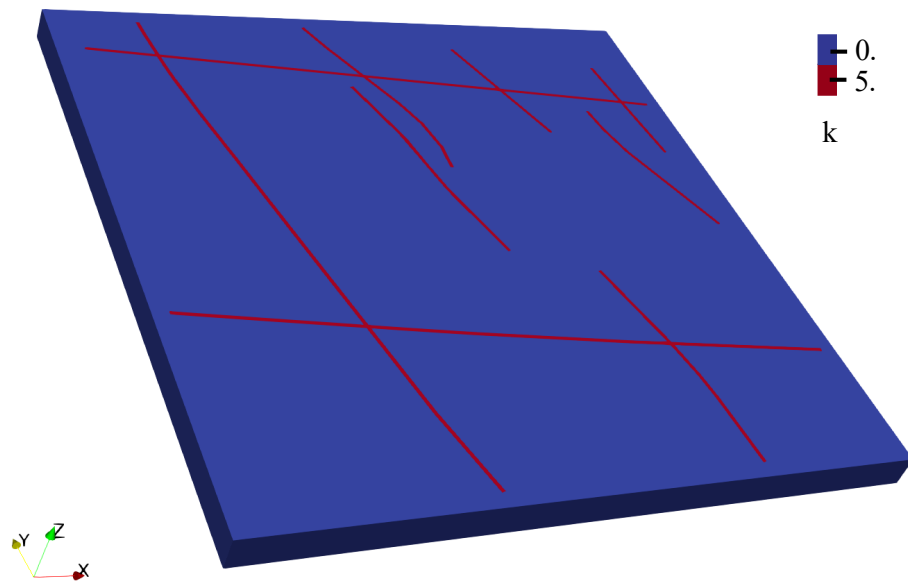
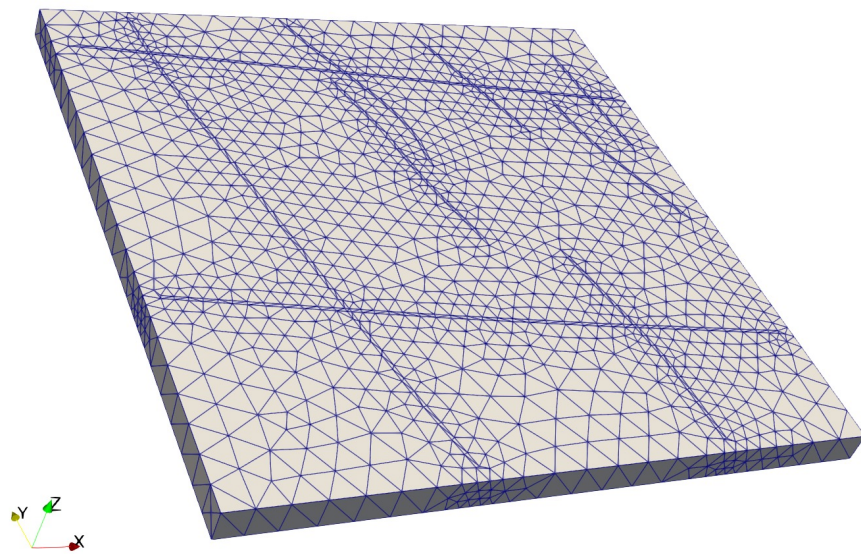
**(a)****(b)**

Figure 5.6: The 3D geometry of numerical experiment 5.3.2: **(a)** The log permeability in the 3D fracture domain. **(b)** The mesh employed in the simulation.

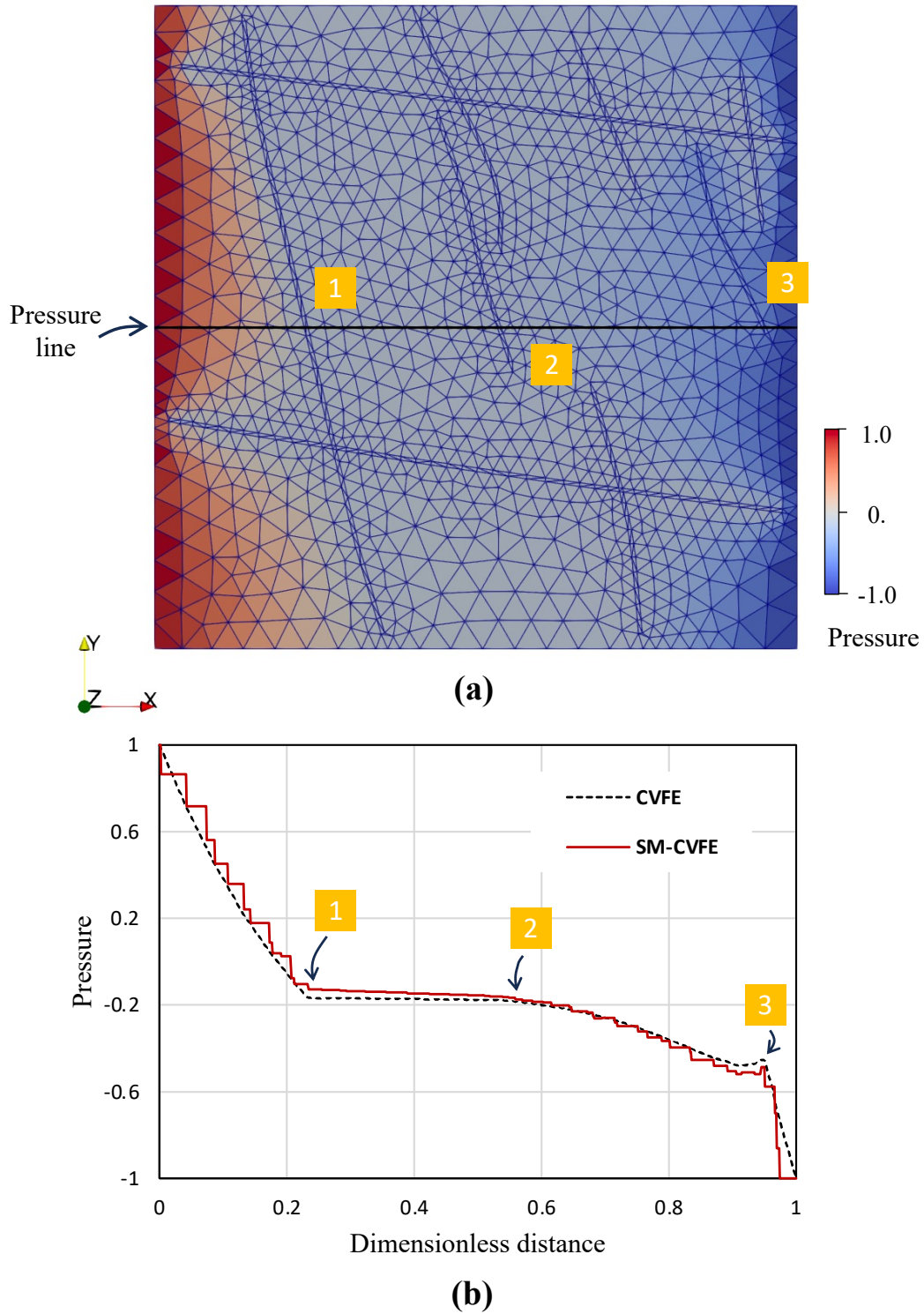


Figure 5.7: The pressure profile of numerical experiment 5.3.2: **(a)** the pressure solution of the SM-CVFE method at the initial time step for the z-normal surface (at $z = 0.05$). **(b)** A comparison of the pressure solution for the SM-CVFE and the classical CVFE methods. The pressure solution is measured over the labelled line in **(a)** with the yellow boxes, 1-3, indicating fracture intersections with the line.

Table 5.4: The geometry and petrophysical properties of different regions for experiment 5.3.2

	Fracture	Background
Fracture aperture	$0.00585L_x$	N/A
Fracture depth	L_z	N/A
Porosity	1.	0.1
Log permeability	5.	0.

L_x , L_z denote the length of the domain with respect to the x-axis and z-axis, respectively.

0.03 PVI whereas the classical CVFE saturation solution (Fig. 5.8a) is leaked into the control volumes spanning the fracture and the surrounding region and, therefore, resulting in a severely delayed saturation front. The remaining time steps, after 0.09 (Fig. 5.8d) and 0.14 PVI (Fig. 5.8f), show the dominating transport mechanism is facilitated by flow through the fracture in the SM-CVFE with minimal transfer into the low permeability region located in the middle of the domain. We find similar flow profiles when employing the classical CVFE shown in the later time steps (Fig. 5.8c and 5.8e).

While employing the same mesh resolution, the SM-CVFE method requires approximately four times the number of degrees of freedom compared to the classical CVFE method for 3D models. However, the computational requirements for an adequately refined mesh employing the CVFE method are considerably higher than the mesh used in this numerical experiment, demonstrated in Chapter 4 for 2D models (numerical experiment 4.3.4).

It is worth mentioning that the increase in computational requirements for the SM-CVFE, from a factor of 2.5 in 2D models to 4 in 3D models compared to the CVFE is attributed to additional unknowns, along the third dimension, for velocity vector introduced by the tetrahedral element.

The leakage of saturation solutions for both the SM-CVFE and classical CVFE methods

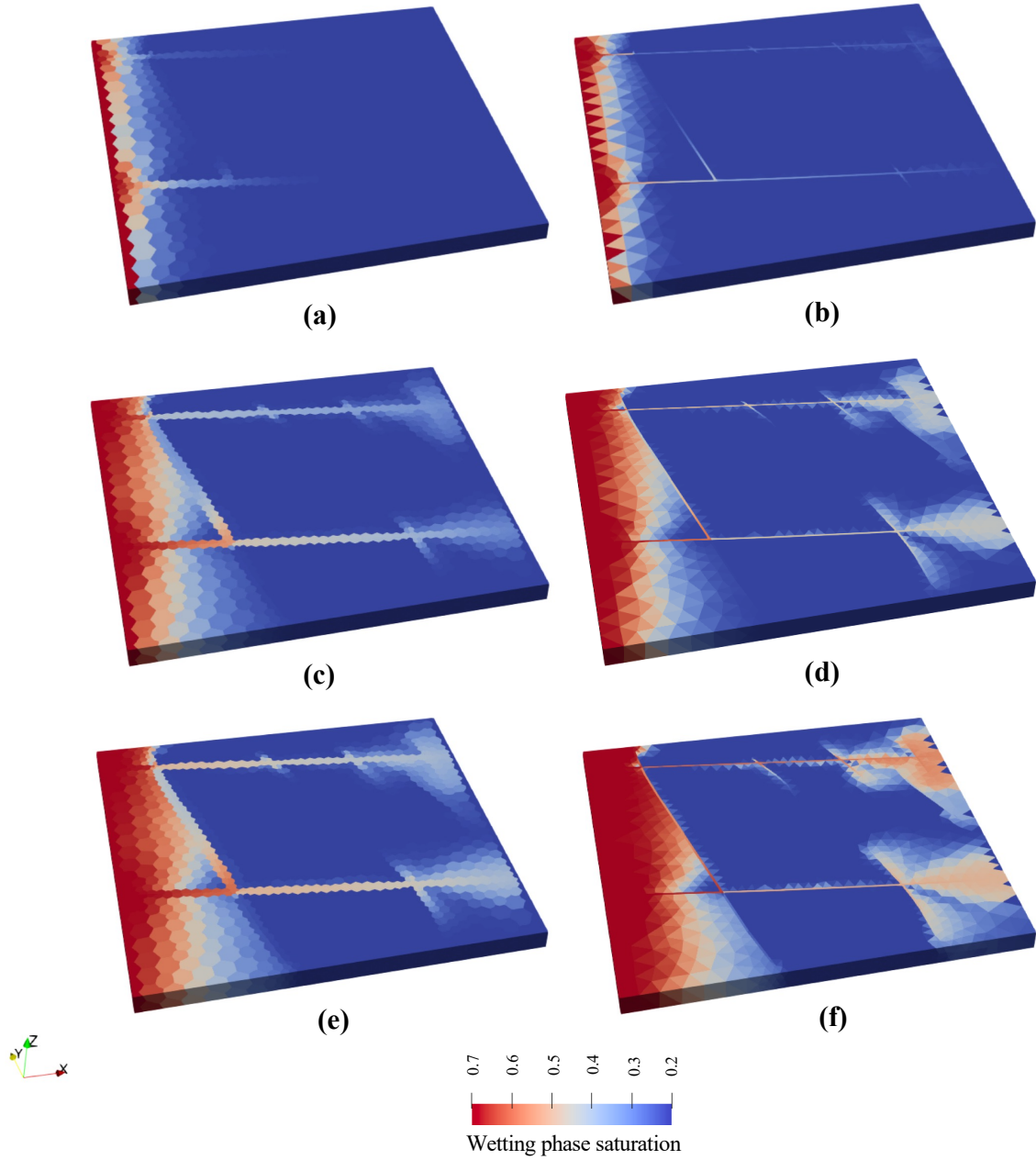


Figure 5.8: Comparison of the saturation solution for the 3D fractures model 5.3.2. The left column shows the classical CVFE solution and the right column shows the SM-CVFE solution. The top row (a) and (b) correspond to 0.03 PVI, the middle row (c) and (d) correspond to 0.09 PVI, and the bottom row (e) and (f) correspond to 0.14 PVI. Note that the saturation values are not displayed for elements coinciding on the outlet.

is compared in Fig. 5.9. The region of interest for this comparison is the isolated region between the fractures in the middle of the domain, outlined by the red box in Fig. 5.9a. The saturation solution leakage while employing the classical CVFE is shown in Fig. 5.9b, where the leakage is primarily concentrated in the control volumes spanning the fractures. In contrast, the SM-CVFE solution (5.9c) emphasizes the effectiveness of the developed approach, demonstrating a significant reduction achieved with the same mesh resolution. The SM-CVFE approach captures accurate solutions by eliminating the leakage effects even with coarser meshes, a feature not attainable with the CVFE method.

5.4 Summary

In this chapter, we extended the formulation of the single mesh CVFE approach to three-dimensional models. The method is versatile and provides a general framework for modeling multiphase flow through a variety of complex porous media systems. The 3D implementation of the SM-CVFE method requires about four times the degrees of freedom as the classical CVFE approach for the same mesh. Nonetheless, the SM-CVFE method is capable of capturing accurate saturation solutions without necessarily demanding fine meshes in the presence of complex geometries and material heterogeneities. In the next chapter we explore the potential of further simplification of the numerical implementation of the SM-CVFE method.

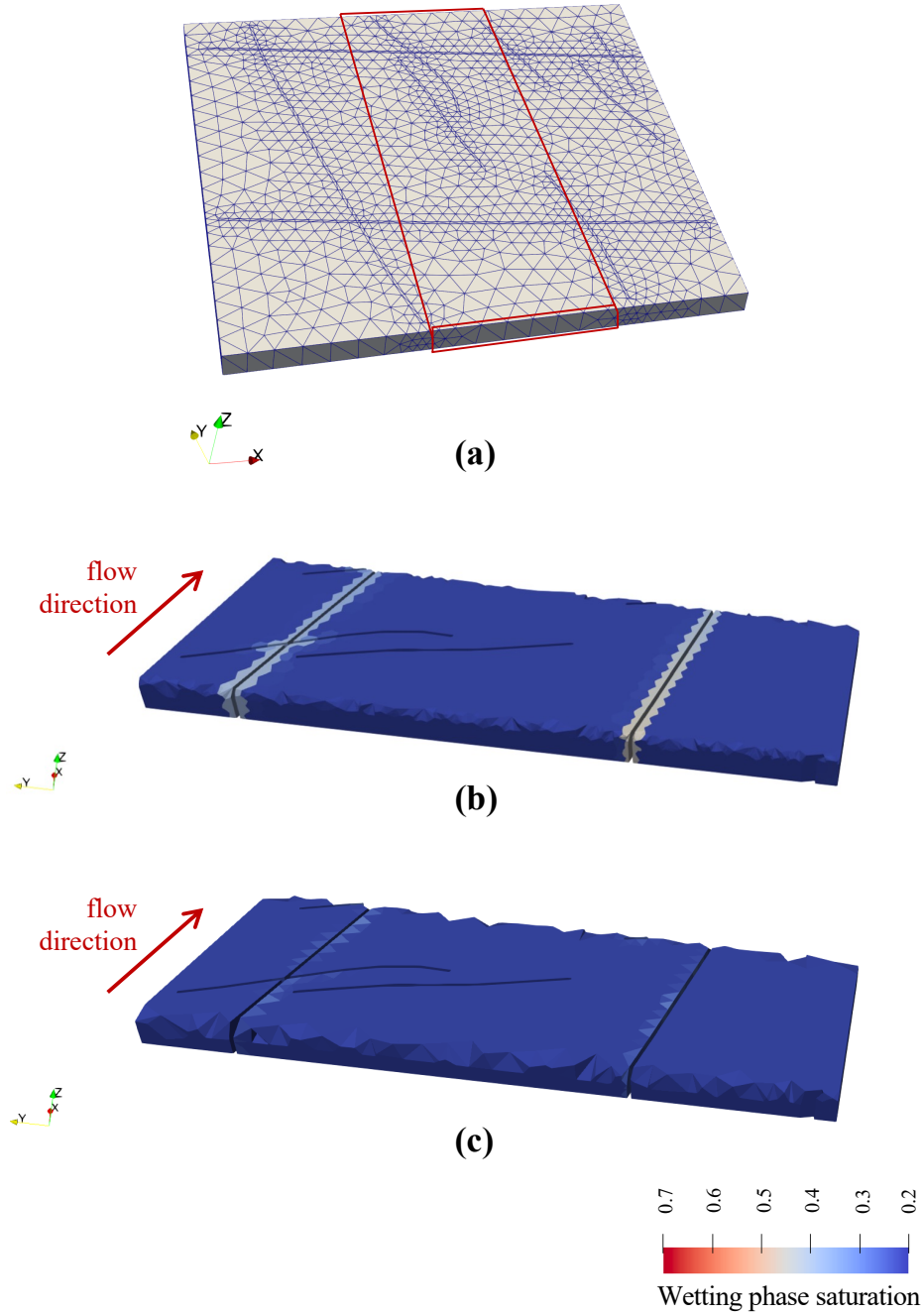


Figure 5.9: Comparison of the solution leakage in the 3D fractures model 5.3.2 in the low permeability region in the middle of the domain after 0.09 PVI: (a) The red box marking the selected region to examine the leakage at $x = [0.35, 0.7]$. (b) The wetting phase saturation in the classical CVFE solution in the background region showing the leakage of the saturation solution. (c) The wetting phase saturation in the SM-CVFE solution in the background region showing minimal leakage effects.

Chapter 6

A new framework for flux approximation

6.1 Introduction

The numerical approximation of pressure using the finite element method entails constructing basis functions defined across the elements. The extent to which these basis functions are shared between elements, or lack thereof, influences either an increase or constraint on the local stencil necessary to establish and solve the numerical problem. In the classical control volume finite element method, the approximation relies on a nodal Lagrangian approach. This approximation exhibit continuity between elements. As shown in Fig. 6.1b, the local stencil for the pressure solution within the element involves numerous neighboring connections (red arrows) around the highlighted (blue) element vertices.

In contrast, the pressure approximation in SM-CVFE, employing an element-wise approach, establishes a smaller stencil confined to the element boundaries (Fig. 6.1a). These element boundaries serve as the foundation for the flux approximation stencil in the SM-CVFE method. We recall the similarity in the TPFA stencil used in the implementation of the finite volume method on structured, K-orthogonal grids, as described

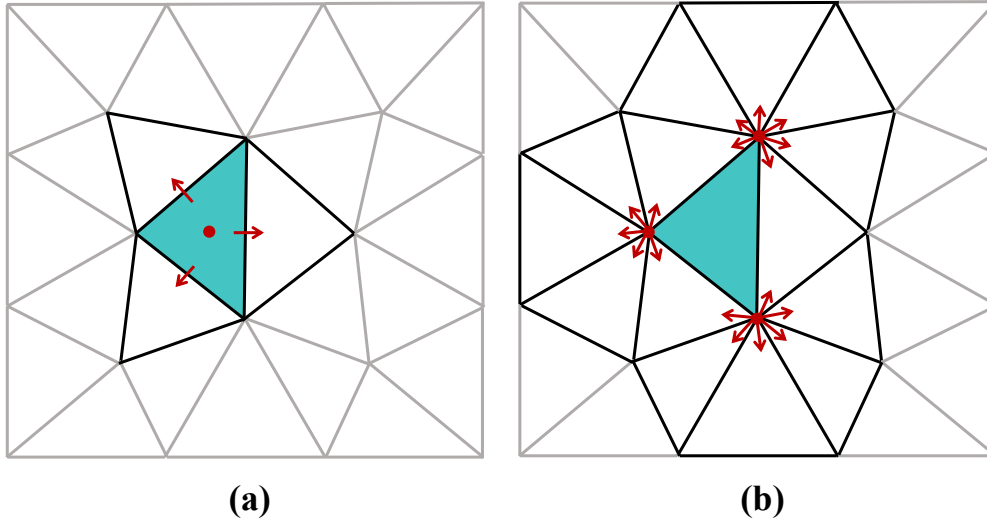


Figure 6.1: Comparison of the local element stencils in 2D required to solve the pressure for the SM-CVFE approach in **(a)** and the classical CVFE approach in **(b)**. The black outlined elements constitute the local stencil of the blue highlighted element while the faded elements are not considered.

in section 2.3.1. Essentially, the TPFA and the SM-CVFE approaches construct fluxes with neighboring elements sharing common interfaces. The novel aspect of the SM-CVFE formulation is the elimination of inconsistency errors and geometrical flexibility over the TPFA.

The objective of this chapter is to investigate an alternative implementation describing the Single Mesh Control Volume Finite Element (SM-CVFE) method, the topic discussed in Chapter 4 and further extended in Chapter 5. Our focus is on providing a practical implementation of the SM-CVFE method, which simplifies to a local problem, allowing for an alternative local implementation approach. In this context, we present a formulation based on a local element stencil for assembly, emphasizing minimal stencil connectivity with neighboring elements.

We setup the system to solve the pressure directly, while the velocity unknowns embedded and recovered in a sequential step to compute the fluxes. Detailed insights into solving the coupled flow and transport model are provided in section 3.2.3, but our emphasis here lies on the foundational components of the flow model, specifically matrix assembly from

the element stencil.

We briefly revisit the system of equations constituting the flow model in section 6.2, followed by a description of the inter-connectivity matrix that extracts the element stencil from essentially any mesh (section 6.2.1). The complete assembly of the element mass matrix and an explicit inverse formulation are presented in section 6.2.2. Subsequent sections, 6.2.3 and 6.2.4, briefly describe the stiffness matrix and the divergence-free matrix with additional work required to achieve an explicit stencil formula.

In this chapter, we delve into the foundations of an alternative implementation for the SM-CVFE approach. While the current findings mostly shed light on mass matrix assembly (section 6.2.2), it is necessary to note that this work marks the beginning of a broader investigation. Sections 6.2.3 and 6.2.4 outline the groundwork laid in this study and point towards future development for the SM-CVFE approach.

6.2 Method

To solve the the flow model, we recall the algebraic system of equations given by

$$\begin{bmatrix} \mathbf{A} & \mathbf{B} \\ \mathbf{C} & \mathbf{0} \end{bmatrix} \cdot \begin{bmatrix} \mathbf{v}^{n+1} \\ p^{n+1} \end{bmatrix} = \begin{bmatrix} b_1 \\ b_2 \end{bmatrix} \quad (6.1)$$

Here, the top row is Darcy's law, Eqn. (2.1), and the bottom row is the continuity equation, Eqn. (2.3). The block matrix on the left hand side shows the components we study in the subsequent sections where $\mathbf{A}$ is the mass matrix, $\mathbf{B}$ is the stiffness matrix, and $\mathbf{C}$ is the divergence-free matrix. Before describing and assembling those matrices, we first establish the necessary inter-connectivity matrix in the next section.

6.2.1 Inter-connectivity matrix

The inter-connectivity matrix, or the element adjacency matrix, is a square symmetric matrix used to identify element connectivity in an undirected graph that represents the mesh. In this matrix, both rows and columns correspond to elements. The matrix has zero entries on the diagonal, while a value of 1 represents a connection with a neighboring element. In $\mathbb{R}^2$ meshes, a triangular element has at most 3 adjacent elements, while in $\mathbb{R}^3$, a tetrahedral element has at most 4 adjacent elements.

The inter-connectivity matrix is essential in the algorithmic implementation presented here for determining the element local stencil, especially as the method is designed for general, unstructured meshes. We utilize the sparsity pattern of the matrix to establish the local stencil. This is in contrast to structured meshes, where element connectivity is known. For example, the internal cell of a 3D model with a structured mesh identified by its i, j, k position, connectivity can be determined with neighbors $N = \{i - 1, i + 1, j - 1, j + 1, k - 1, k + 1\}$.

To illustrate the presented methodology throughout this chapter, we consider a small 2D triangular mesh (Fig. 6.2a), the graph network representation of element connectivity (Fig. 6.2b), and its inter-connectivity matrix (Fig. 6.3). In the inter-connectivity matrix, the red-shaded row indicates element 9 and its connectivity to neighboring elements.

6.2.2 Mass matrix ($\mathbf{A}$)

The mass matrix represents how the mass of the dynamical system is distributed across discrete nodes in the computational domain [Zienkiewicz et al., 2005]. In general, the matrix is symmetric. For discontinuous Galerkin (DG) methods, the mass matrix ($\mathbf{A}$ in Eqn. (6.1)) forms a block diagonal structure where each block is formed by the nodes of the element. Block diagonal matrices offer desirable features for modeling due to their computational and storage efficiency which will be exploited further in our local approach.

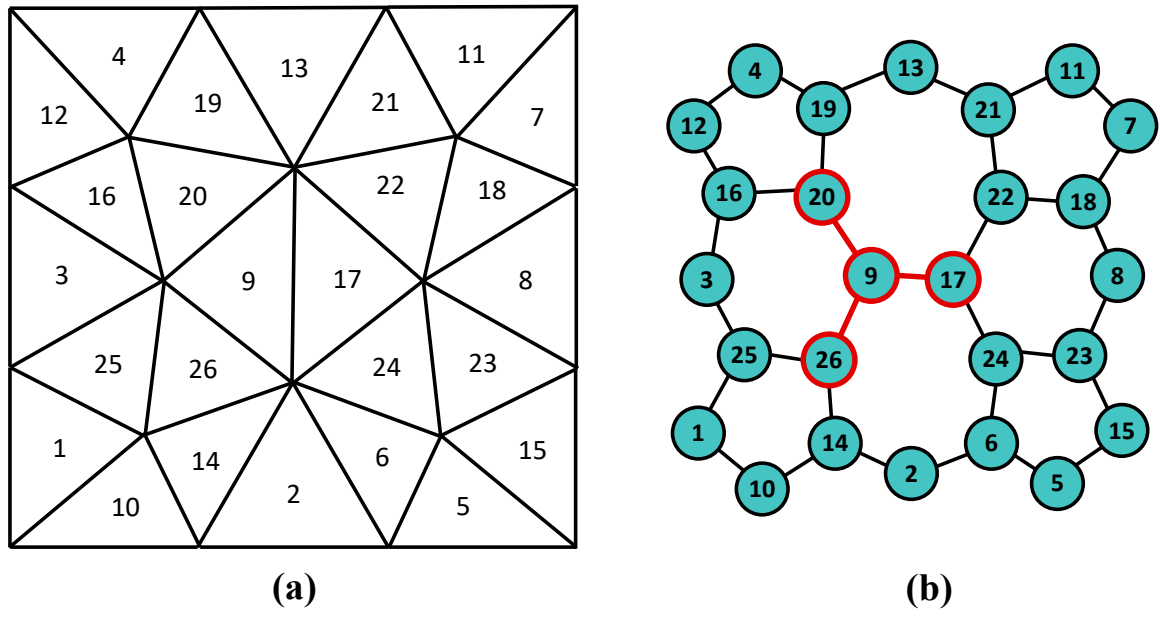


Figure 6.2: (a) Simple 2D triangular mesh. (b) The graph representation of element connectivity in the mesh.

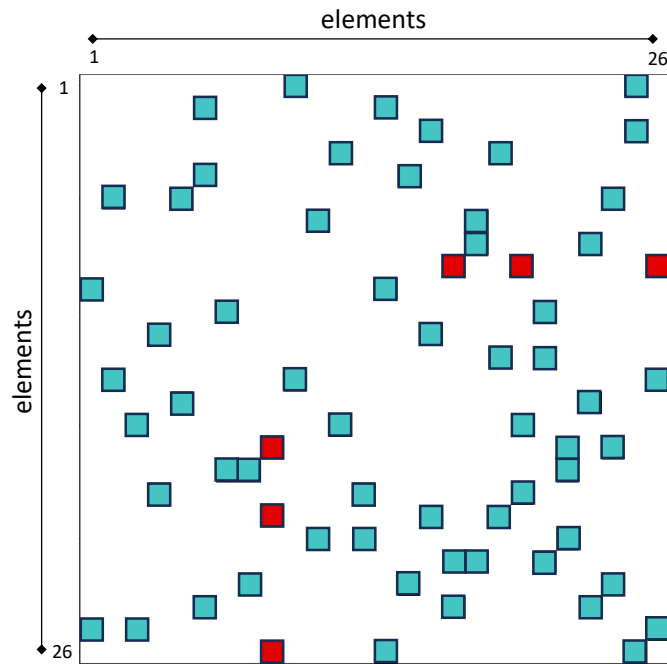


Figure 6.3: The non-zeros of the inter-connectivity matrix constructed for the graph representation of the unstructured mesh. The red highlighted non-zeros are the adjacency of element 9.

In this section, we emphasize the robust approach to obtain the mass matrix inverse, as the setup of the flow model using Darcy's law and the continuity equation involves matrix manipulation and, eventually inverting the mass matrix to obtain the pressure field.

First, to form the mass matrix, we consider the velocity nodes in each element. For example, Fig. 6.4 shows element 9 with the mass matrix structure. We have considered several ordering of the degrees of freedom in the system. One notable ordering scheme within each element block that yields smaller block diagonal structure for each axis; in 2D meshes with triangular elements, an element block (6x6) can be simplified to 2 (3x3) blocks representing the x-axis and y-axis velocity components. The 2D triangular element unknown vector $\mathbf{v}^{(e)}$ is

$$\mathbf{v}_{(x,y)}^{(e)} = \{v_{1,x} \quad v_{2,x} \quad v_{3,x} \quad v_{1,y} \quad v_{2,y} \quad v_{3,y}\}^T \quad (6.2)$$

The coefficients of the mass matrix are described by

$$A_{ij} = \rho_e \int_{\Omega_e} \Phi_i \cdot \Phi_j \, d\Omega_e \quad (6.3)$$

After carrying out the integration of the basis function, we obtain for each block diagonal

$$A_{e,d} = \frac{V_e \rho_e}{6} \begin{bmatrix} 1. & 0.5 & 0.5 \\ 0.5 & 1. & 0.5 \\ 0.5 & 0.5 & 1. \end{bmatrix}, \quad (6.4)$$

where the subscript d refers to x-axis or y-axis velocity components, V_e is the element volume, ρ_e is the fluid density in the element. While modeling problems of interest in this work, the element mass matrix is the same for both components along the different axes. This equivalence reduces the number of matrix inversion operations required for computation by 50% in 2D and 67% in 3D. Moreover, The inverse of the presented block

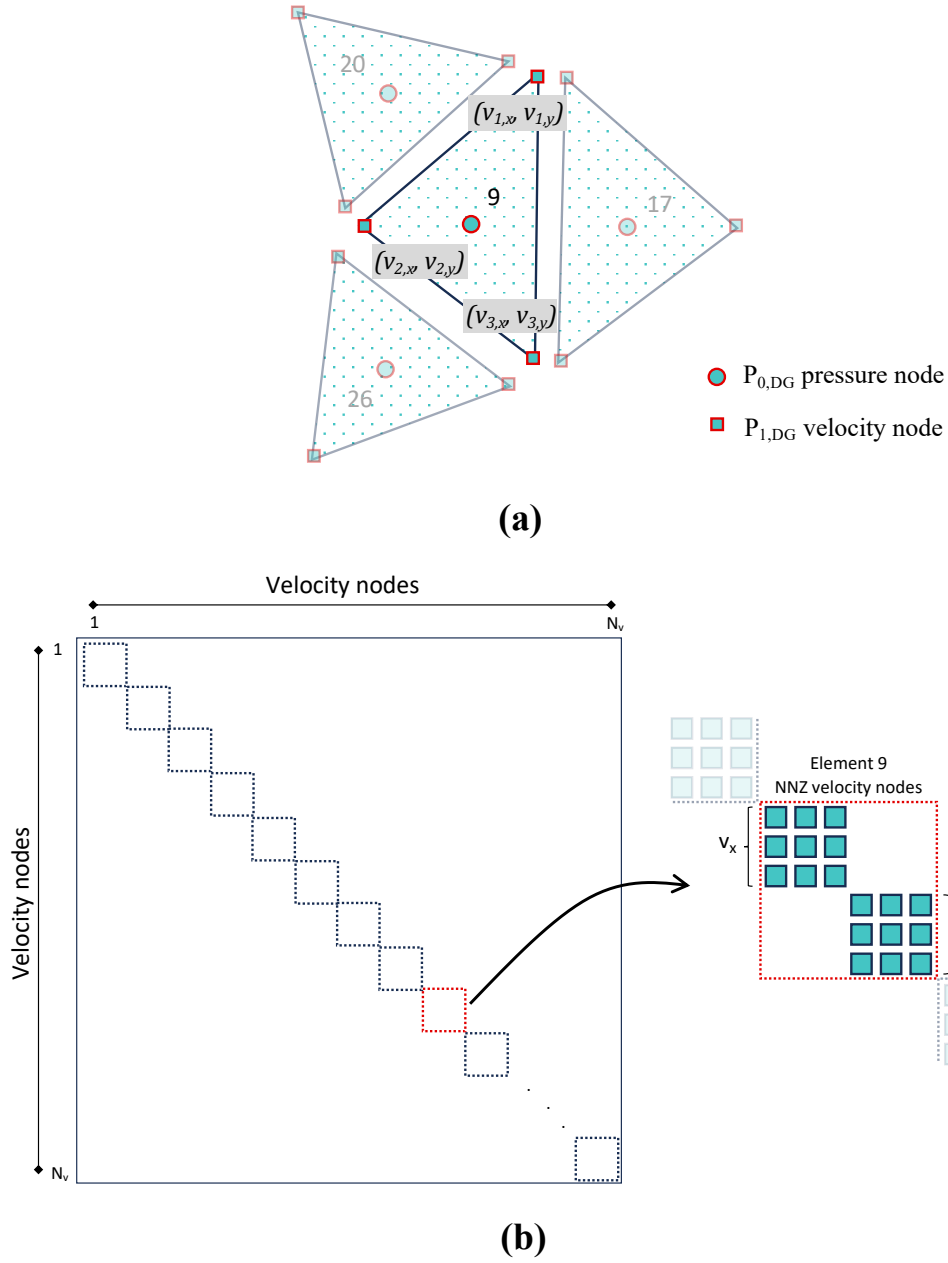


Figure 6.4: (a) Snippet of the 2D mesh highlighting element 9 with its velocity degrees of freedom using a local numbering scheme. (b) The non-zero (NNZ) structure of the mass matrix with the block diagonals constructed for the velocity nodes of each element.

diagonal 2D matrix is given by

$$A_{e,d}^{-1} = \frac{3}{V_e \rho_e} \begin{bmatrix} 3. & -1. & -1. \\ -1. & 3. & -1. \\ -1. & -1. & 3. \end{bmatrix}. \quad (6.5)$$

This a priori formulation of the inverse for the block diagonal matrix effectively provides the inverse of the mass matrix by addressing each element independently. Consequently, it eliminates the computationally demanding task of mass matrix inversion, essentially mitigating the computational complexity associated with inverse operations, which is $O(n^3)$ with n denoting the size of the matrix.

For 3D models, the same ordering scheme can be extended to tetrahedral elements with each element block (12x12) simplified to 3 (4x4) blocks for the x-axis, y-axis and z-axis. The tetrahedron unknown velocity vector ($\mathbf{v}^{(e)}$) of the (3D) element is

$$\mathbf{v}_{(x,y,z)}^{(e)} = \{v_{1,x} \quad v_{2,x} \quad v_{3,x} \quad v_{4,x} \quad v_{1,y} \quad v_{2,y} \quad v_{3,y} \quad v_{4,y} \quad v_{1,z} \quad v_{2,z} \quad v_{3,z} \quad v_{4,z}\}^T \quad (6.6)$$

The tetrahedral element mass matrix is determined with

$$A_{e,d} = \frac{V_e \rho_e}{10} \begin{bmatrix} 1. & 0.5 & 0.5 & 0.5 \\ 0.5 & 1. & 0.5 & 0.5 \\ 0.5 & 0.5 & 1. & 0.5 \\ 0.5 & 0.5 & 0.5 & 1. \end{bmatrix}. \quad (6.7)$$

And the inverse of the tetrahedral element mass matrix

$$A_{e,d}^{-1} = \frac{4}{V_e \rho_e} \begin{bmatrix} 4. & -1. & -1. & -1. \\ -1. & 4. & -1. & -1. \\ -1. & 1. & 4. & -1. \\ -1. & -1. & -1. & 4. \end{bmatrix}. \quad (6.8)$$

As mentioned previously, the mass matrix in this discontinuous approximation is, therefore, fully decoupled from adjacent elements and can be assembled and inverted robustly in parallel. Throughout this section we have presented the mass matrix using a consistent form. We basically avoided mass lumping since our analysis showed that mass lumping that is used conventionally to simplify inverting the mass matrix results in fill-in observed in the final pressure matrix. By employing a consistent mass matrix, the resultant left hand side matrix of the pressure system has a similar structure to that of the inter-connectivity matrix and additional non-zeros only present in the diagonal. Additional details are provided in section 6.2.5.

6.2.3 Stiffness matrix (**B**)

The stiffness matrix characterizes the system behaviour in response of pressure changes. The entries in the matrix (**B** in Eqn. (6.1)) are the coefficients of the pressure gradient term in Darcy's equation. As shown in Fig. 6.5, the rows and columns of the matrix are the velocity and pressure nodes, respectively. The discretization of the element described by the SM-CVFE method result in non-zero jump terms that connects the element to the local stencil such that the entries of the matrix are populated using

$$\mathbf{B}_{ik} = \sum_{\forall \Gamma_{e_{int}}} \int_{\Gamma_e} \left(\Phi_i \cdot \lambda_t \mathbf{K}_h \Psi_k \right) \cdot \mathbf{n} \, d\Gamma_e - \sum_{\forall \Gamma_{e_{ext}}} \int_{\Gamma_e} \left(\Phi_i \cdot \lambda_t \mathbf{K}_h \Psi_k \right) \cdot \mathbf{n} \, d\Gamma_e \quad (6.9)$$

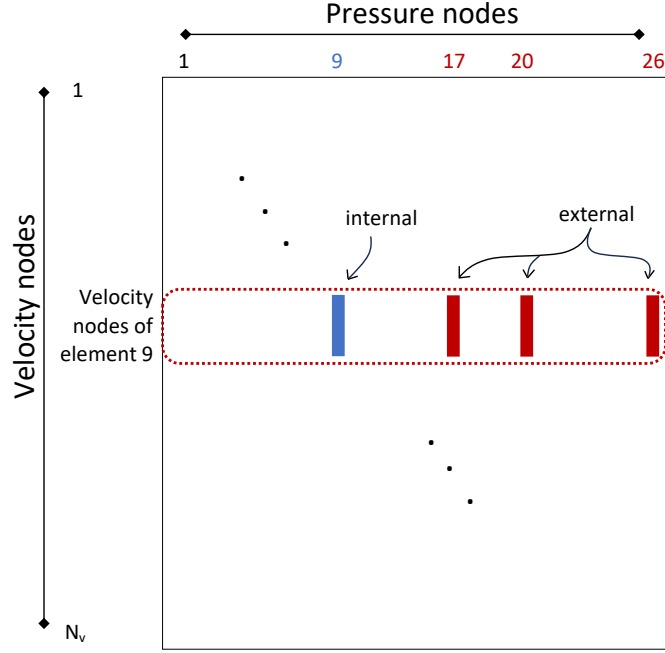


Figure 6.5: The stiffness matrix for the velocity nodes of element 9, the block of rows, are populated with the jump term on the element stencil. The first term in Eqn. (6.9) is highlighted by the blue column while the second term contributions are highlighted in red columns.

where the first positive term is internal to the element and the second negative term is driven by external, elements from the local stencil. Fig. 6.5 demonstrate the contribution of element 9 velocity nodes and the associated entries from the element stencil.

6.2.4 Divergence-free operator matrix ($\mathbf{C}$)

The matrix is constructed by applying the continuity equation which represents the conservation of mass in the system; it symbolizes the divergence of the velocity vector field in the computational domain ($\mathbf{C}$ in Eqn. (6.1)). As shown in Fig. 6.6, the rows and columns are the pressure and velocity nodes, respectively. We use

$$\mathbf{C}_{ij} = \sum_{\forall \Gamma_{e_{int}}} \int_{\Gamma_e} \frac{1}{2} \Psi_i \left(\Phi_j \cdot \mathbf{K}_h \mathbf{K}_e^{-1} \right) \cdot \mathbf{n} d\Gamma_e + \sum_{\forall \Gamma_{e_{ext}}} \int_{\Gamma_e} \frac{1}{2} \Psi_i \left(\Phi_j \cdot \mathbf{K}_h \mathbf{K}_{e_{ext}}^{-1} \right) \cdot \mathbf{n} d\Gamma_e \quad (6.10)$$

to construct the matrix. Consider Fig. 6.6a that shows element 9 with a single quadrature point marked on each internal and external interface. The first term in Eqn. (6.10) correspond to velocities over internal element interfaces (Γ_{int}) which result in non-zero entries populated in the red highlighted portion of row 9 in Fig. 6.6b. The second term contributes to velocities over adjacent element interfaces (Γ_{ext}) which result in non-zero entries populated in the blue highlighted portions of row 9 in Fig. 6.6b. The harmonic permeability weighting of velocity components is key in this approximation as described in 4.2.6.

6.2.5 Pressure Solution

The pressure solution is first obtained by eliminating the velocity unknowns from the system of equations (Eqn. (6.1)), such that the following equation

$$\underbrace{(\mathbf{CA}^{-1}\mathbf{B})}_{\text{LHS}} p^{n+1} = (\mathbf{CA}^{-1}b_1) - b_2, \quad (6.11)$$

is setup to resolve the pressure unknowns. Two cases were tested to construct the left hand side (LHS) matrix. Case I corresponds to $\mathbf{A}^{-1}$ derived from a consistent mass matrix (CMM) while case II includes $\mathbf{A}^{-1}$ derived from a lumped mass matrix (LMM); lumping is achieved by using a the row-sum method [Zienkiewicz et al., 2005]. Fundamentally, CMM and LMM are based on exact integration and inexact integration approaches, respectively [Giraldo, 2020, 1998].

We investigate the sparsity pattern of the LHS matrix obtained using each method. Case I yields a matrix structure consistent with the inter-connectivity matrix with added non-zero contributions to the diagonal elements (Fig. 6.7a). This implies that the relevant entries of the LHS matrix in our proposed approach depend solely on the element stencil. As discussed in earlier section 6.2.2, the inverse of the mass matrix can be assembled directly and, therefore, eliminate the computationally demanding task of computing ma-

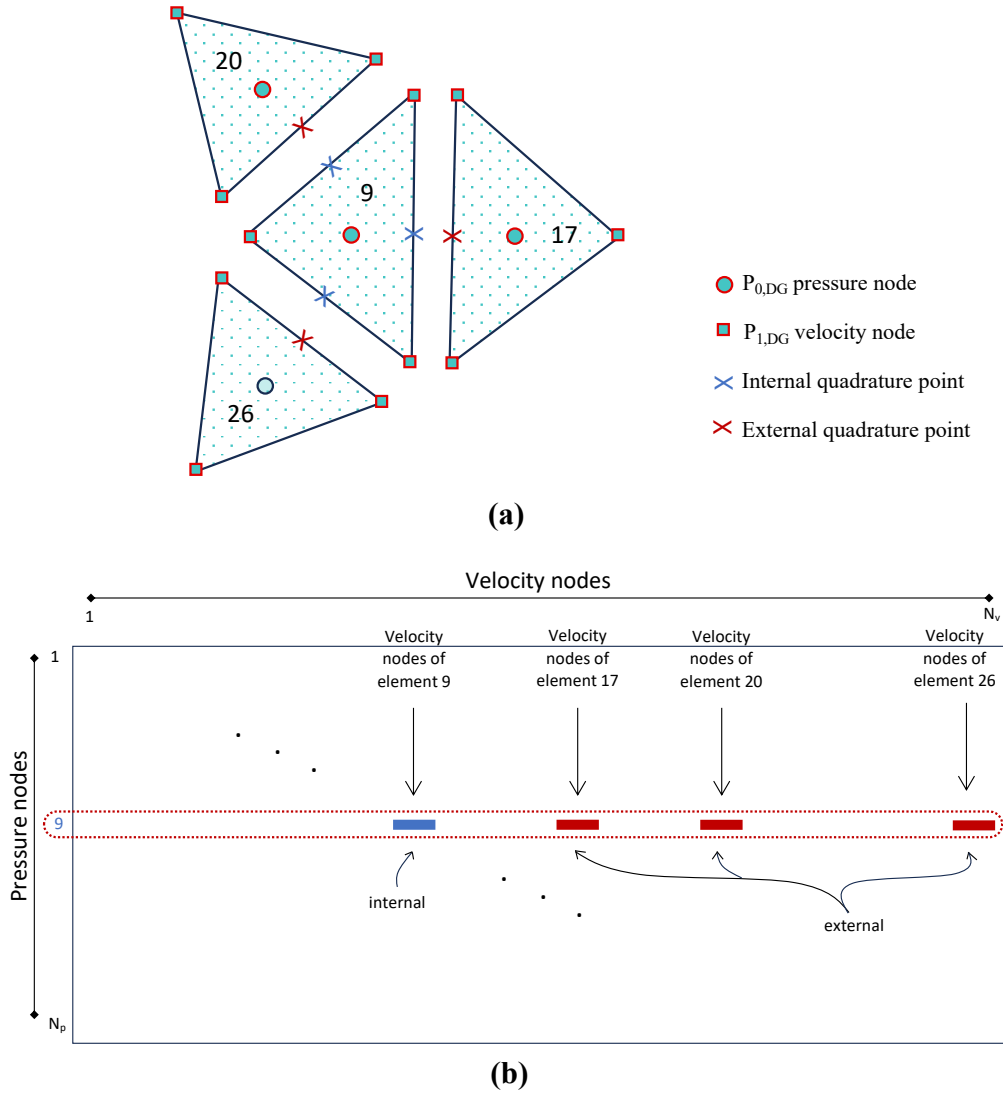


Figure 6.6: The stencil of element 9 demonstrating construction of divergence-free operator in (a). (b) The row representing pressure node 9 (dotted red box) in the divergence free operator ($\mathbf{C}_{9,:}$) which is constructed by evaluating the integral with the quadrature points internal to the element (blue crosses in (a)) and external to the element (red crosses in (a)) for the first and second terms, respectively, in Eqn. (6.10). The internal quadrature points populate the velocity nodes of element 9 (blue highlighted section of row 9), while the external quadrature points populate the velocity nodes elements 17, 20, and 26 (red highlighted sections of row 9).

trix inverse. Conversely, Case II, which incorporates LMM into the system, introduces numerous fill-ins (more than 50%, as demonstrated in Fig. 6.7b). Despite the popularity of LMM for efficiently inverting the mass matrix, we observe many additional entries that need to be populated beyond the local element stencil, not aligning with the motivation of this work. Next, we compared the LHS matrix conditioning for both cases, CMM and LMM, and found the transition from CMM to LMM has no impact on the conditioning of the system.

6.2.6 Velocity update

Once the pressure is determined in the domain, we compute the velocity unknowns (v^{n+1}) by substituting p^{n+1} into Darcy's equation given by

$$\mathbf{A}v^{n+1} = b_1 - \mathbf{B}p^{n+1}, \quad (6.12)$$

where the velocity approximation ($\tilde{\mathbf{v}}$) on interfaces between adjacent elements can then be reconstructed by using Eqn. (3.13).

6.3 Summary

The presented work in this chapter lays the foundation for the new flux approximation with a special emphasis placed on understanding individual components needed to construct matrices from the element stencil for the flow model. Further work is required to finalize explicit formulations of the pressure matrix components and deliver compact terms for implementation, analogous to the classical finite volume approximation.

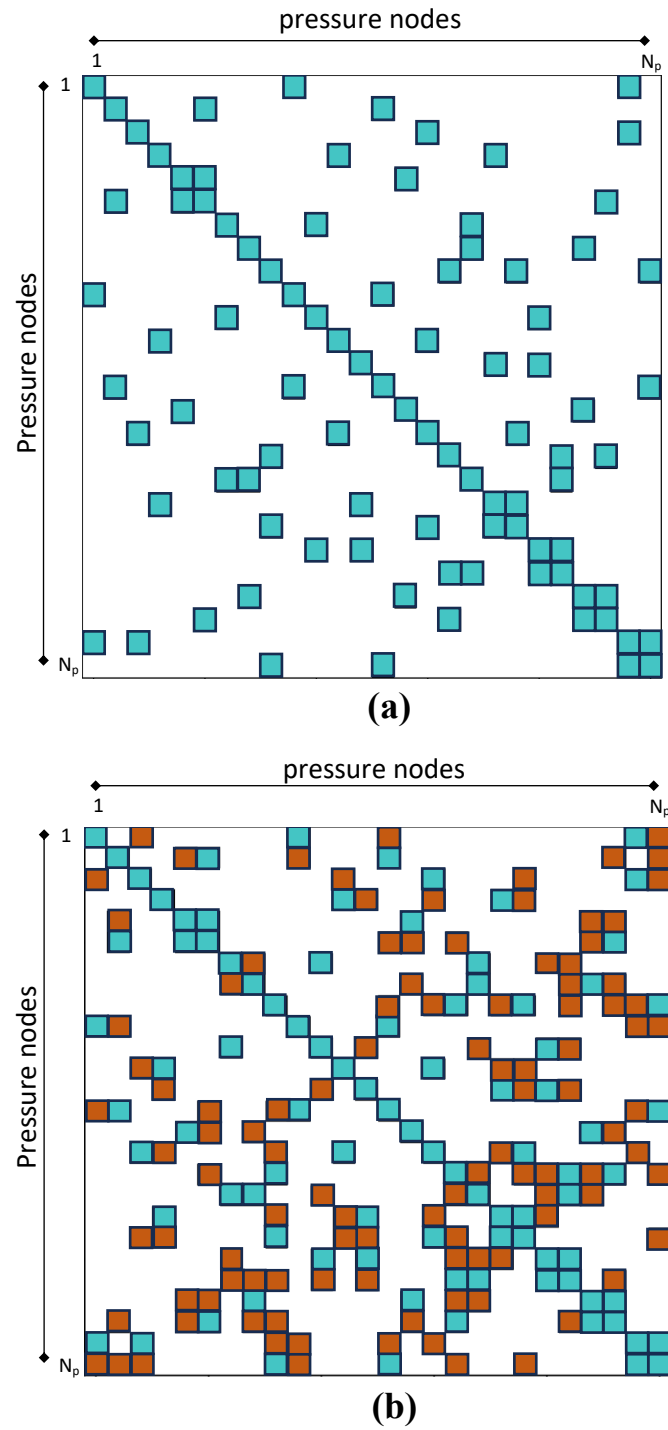


Figure 6.7: The LHS matrix assembled to resolve the pressure in the domain for the two cases: **(a)** Case I that represent the system assembled using a consistent mass matrix (CMM). **(b)** Case II for the system assembled using the lumped mass matrix (LMM). The fill-ins are highlighted in brown.

Chapter 7

Conclusions

Modeling multiphase flow in porous media provides insights into understanding the complex dynamics that govern fluid flow and migration in the subsurface. The continuous research and development of more advanced numerical methods are closely linked to and facilitated by the progress of computer hardware and software. This evolution not only addresses current computational challenges but also positions us to tackle new complexities related to designing systems that mitigate negative environmental impacts of subsurface activities and developing effective technologies to leverage the complexity of the subsurface to our advantage. Throughout this work, two methodologies were proposed for capturing accurate and efficient numerical solutions to multiphase flow problems.

In Chapter 3, we developed a new method based on a hybrid approach for modeling multiphase flow in porous media structures characterized by highly heterogeneous properties. The hybrid control volume finite element (HyCVFE) method combines the strengths of both continuous and discontinuous approximations within a single framework. By employing continuous approximations within subdomains, the HyCVFE method achieves computational efficiency typically associated with continuous methods. Simultaneously, the discontinuous approach is applied along subdomain interfaces, ensuring global continuity and accuracy of transport solutions in the presence of abrupt changes in material

properties.

The HyCVFE method, discussed in Chapter 3, offers a robust solution for models with well-defined subdomain boundaries. In cases where this separation is less distinct but variations from element to element are necessary, a discontinuous discretization emerges as a flexible method. In the subsequent chapters (4-6), the focus shifted towards developing a generalized approach for modeling multiphase flow in complex porous media domains.

In Chapter 4, we tackled the general inconsistency in CVFE methods that employs two meshes for coupling the physical processes. We introduced a flexible approach that allows the utilization of a single, consistent mesh. The SM-CVFE method introduces a new element type for discretizing flow variables, ensuring global incorporation of discontinuity in the discretization process. This enables element-to-element flexibility, ensuring accuracy while resolving geo-statistical models with complex domains. The extension of the SM-CVFE approach to accommodate 3D models, discussed in Chapter 5, demonstrated superior performance compared to classical methods. The SM-CVFE method achieved several orders of magnitude improvement in accuracy compared to traditional approaches, while requiring fewer degrees of freedom than nuanced methods (e.g., Salinas et al. [2018]).

Chapter 6 presents an alternative implementation approach for the SM-CVFE method. This approach employs small, local stencils defined along 2D triangular or 3D tetrahedral element boundaries, similar to finite volume's TPFA implementation. It provides an alternative to conventional finite element frameworks. The element mass matrix is decoupled when employing the element pair discretization utilized by the SM-CVFE method. This decoupling ensures the robust determination of the inverse of the mass matrix.

7.1 Recommendations for future work

Chapter 3 established the groundwork for a hybrid pressure approximation approach, showcasing its efficiency through 2D models. An immediate extension involves validating

the 3D formulation of HyCVFE to broaden its application to subdomains featuring abrupt material properties.

Chapters 4 to 6 introduced and expanded the single mesh CVFE method. Chapter 4 employed an IMPES-based approach to couple the flow and transport model. Ultimately, a fully implicit (FI) or a sequential fully implicit (SFI) [e.g., Jenny et al., 2006b; Lee et al., 2008] approximations are appropriate to overcome the CFL number limitation associated with explicit time stepping. With the current implementation of the SM-CVFE approximation for 3D models, additional work is necessary to run large field models with many more elements. Like many other simulation tools, a robust implementation of parallel framework will provide significant improvement to speedup the computation.

Both the HyCVFE method (Chapter 3) and the SM-CVFE method (Chapter 4) formulations are promising for extensions to include additional physical effects. Incorporating capillarity effects would enable applications in modeling underground CO_2 storage and robustly capturing capillary trapping effects in complex geological porous formations.

The numerical experiments developed throughout this work incorporated isotropic material properties (e.g., the permeability tensor $\mathbf{K}$) despite the general implementation of the HyCVFE and SM-CVFE formulations for both isotropic and anisotropic materials. Further testing is recommended for experiments involving anisotropic material properties to validate for the solution monotonicity. We also recommend additional testing for both formulations, HyCVFE and SM-CVFE, using meshes with high aspect ratio to ensure the methods suitability for large realistic 3D models.

In Chapter 6, further work is needed to provide explicit terms for the stiffness matrix and the divergence-free operator matrix. The new implementation approach shows potential for handling large-scale systems, particularly when integrated with a matrix-free implementation for efficient memory storage. Another recommendation includes comparison of the pressure matrix assembled from the SM-CVFE method with the corresponding transmissibility matrix of TPFA scheme for the same mesh.

To advance this work, the incorporation of the HyCVFE and SM-CVFE methods into an open-source, accessible code is essential. The Imperial College Finite Element Reservoir Simulator (IC-FERST) provides an ideal platform for ensuring the longevity of this implementation and fostering a wider impact.

Appendix A

Code Development

The presented numerical methods involve the development of two new approaches, which are described in the following sections. First, we provide an overview of the classical CVFE method, the reference solution, described in Section A.1. Then, the HyCVFE approach (Chapter 3) is a framework based on combining subdomains and is described in Section A.2. Finally, Section A.3 describes the single mesh method from Chapter 4. The development of this code was performed using Python with several third-party tools, most notably FEniCS [Logg et al., 2012; Alnaes et al., 2015].

A.1 The classical CVFE method

We provide an overview of the time loop employed in the classical CVFE method in Algorithm 1. The coupled flow and transport models are solved sequentially using the IMPES-based method.

Algorithm 1: Time Loop for solving coupled flow and transport using IMPES-based CVFE method.

```

1: Read model parameters, initial conditions and boundary conditions
2: Read mesh file
3: Setup flow fields on the element mesh
4: Setup transport fields on the control volume mesh
5: Setup mass matrix ( $\mathbf{A}$ )
6: Invert mass matrix ( $\mathbf{A}^{-1}$ )
7: Setup divergence-free operator matrix ( $\mathbf{C}$ )
8: Setup RHS vectors ( $b_1$  and  $b_2$ )
9: //Initialize saturation
10:  $S \leftarrow S_{initial}$ 
11: for  $t = t_{start}$  to  $t_{end}$  with time step  $\Delta t$  do
12:   Setup or update stiffness matrix ( $\mathbf{B}$ ) using saturation ( $S$ )
13:   // Solve flow model
14:   Solve pressure field ( $p$ ):  $(\mathbf{CA}^{-1}\mathbf{B})p = (\mathbf{CA}^{-1}b_1) - b_2$ 
15:   Solve velocity field ( $v$ ):  $\mathbf{A}v = b_1 - \mathbf{B}p$ 
16:   // Solve transport on the control volume mesh
17:   Approximate fluxes from velocity
18:   Update saturation explicitly ( $S_{new}$ ) using fluxes and current saturation ( $S$ )
19:   // Store new saturation
20:    $S \leftarrow S_{new}$ 
21:   // Update time step
22:    $t \leftarrow t + \Delta t$ 
23: end for

```

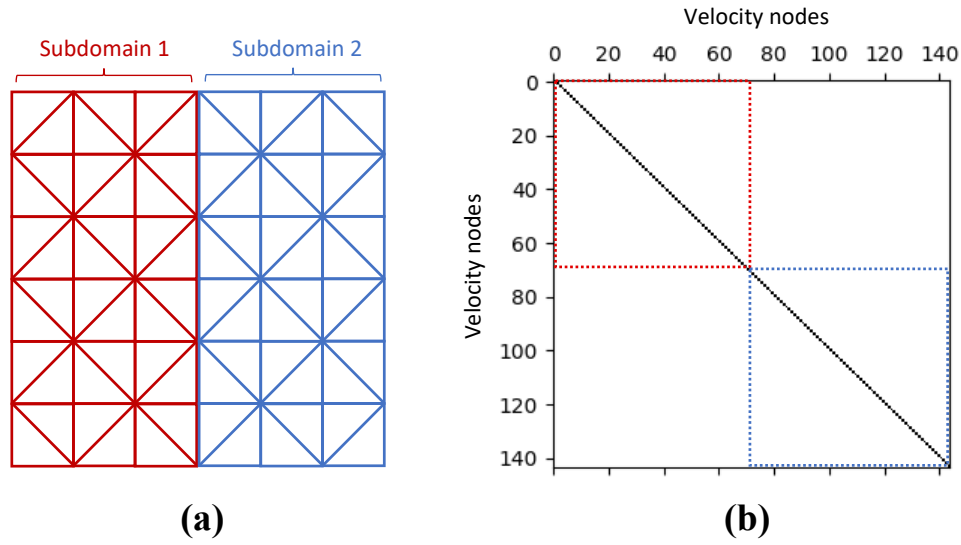


Figure A.1: (a) A mesh constitutes of 2 subdomains. (b) The sparsity pattern of the diagonal mass matrix with the two subdomain contributions highlighted in corresponding colors.

A.2 The hybrid CVFE method

The hybrid approach involves a framework that combines multiple subdomains. We follow a similar solution method to the CVFE approach described by Algorithm 1. However, we incorporate three essential components into this work, including:

- Embedding multiple subdomains while assembling matrices (Section A.2.1).
- Applying the jump term in the global stiffness matrix (Section A.2.2).
- Applying external fluxes between subdomains in the global divergence-free matrix (Section A.2.3).

For demonstration purposes, consider the mesh composed of two subdomains shown in Fig. A.1a.

A.2.1 A subdomain approach

The CVFE method's Algorithm 1 can be modified to establish the HyCVFE framework by incorporating subdomain assembly of the three matrices ($\mathbf{A}$, $\mathbf{B}$, and $\mathbf{C}$). The mass matrix ($\mathbf{A}$), by construction, is completely decoupled for each element, and hence for each subdomain. We highlight the sparsity pattern in Fig. A.1b and the subdomain approach for constructing the matrix in Algorithm 2 for the mesh in Fig. A.1a. We note that the inverse of the mass matrix ($\mathbf{A}^{-1}$) can be robustly computed for the diagonal matrix.

Algorithm 2: Subdomain approach for constructing mass matrix.

```

1: Initialize global mass matrix ( $\mathbf{A}$ )
2: for  $i = 1$  to  $n_d$  do
3:   Setup local mass matrix ( $\mathbf{A}_i$ )
4:   // Update global mass matrix
5:    $\mathbf{A} \leftarrow \mathbf{A} + \mathbf{A}_i$ 
6: end for
```

A.2.2 The jump term

The second component involves populating the stiffness matrix ($\mathbf{B}$) for each subdomain, as well as incorporating the contribution of the jump term along the discontinuous interfaces, as shown in Fig. A.2a. Algorithm 3 outlines the methodology used. Following the execution of the first for loop, the resulting global stiffness matrix ($\mathbf{B}$) is shown in Fig. A.2b. The second for loop in the algorithm addresses the jump term associated with pressure nodes located on the interface, thus populating the off-block diagonal entries in the final stiffness matrix of the global system.

A.2.3 Applying global continuity

In this section, we outline the approach for constructing the divergence-free operator matrix, incorporating the external fluxes necessary for ensuring continuity between subdomains. In Fig. A.3, we provide a schematic representation of two elements lying

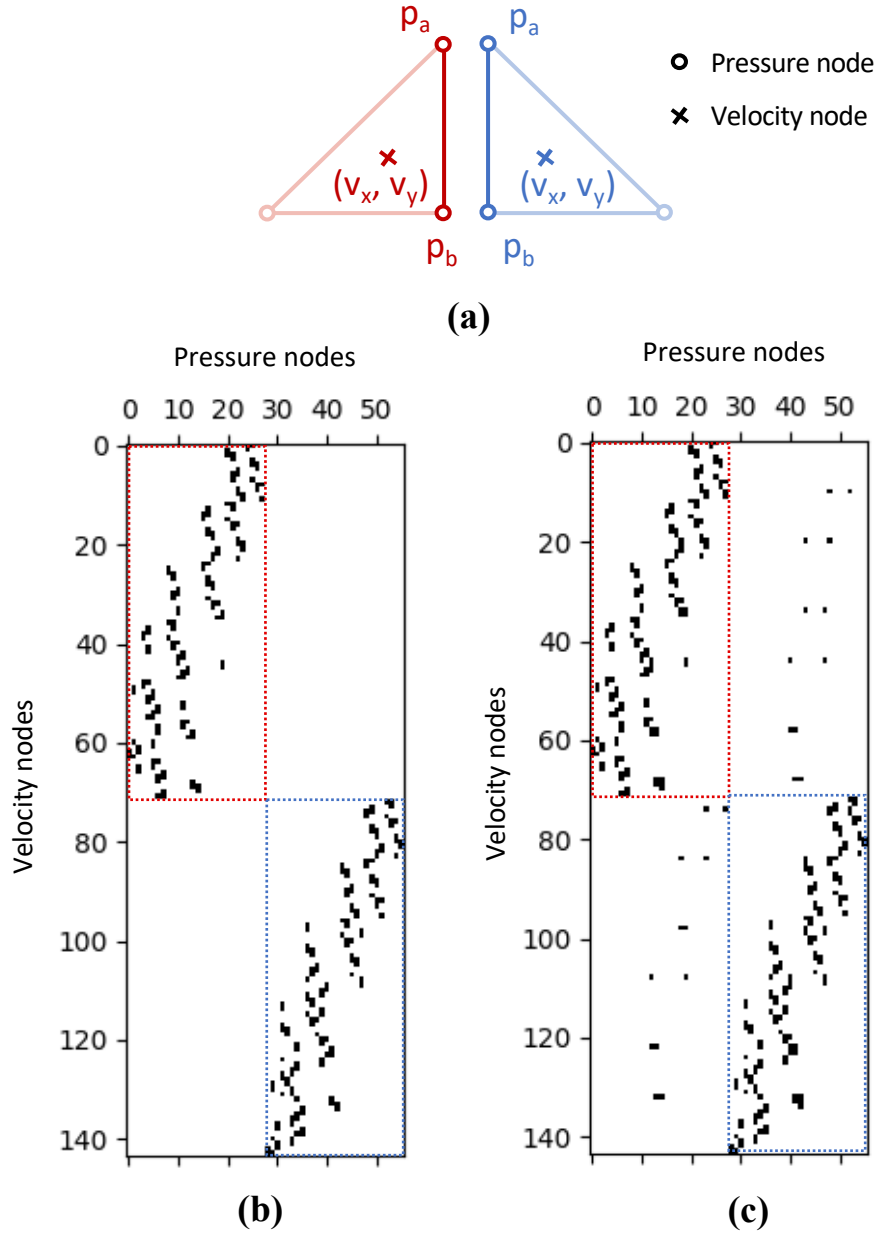


Figure A.2: (a) A schematic of a discontinuous interface with pressure nodes lying on the interface. (b) The sparsity pattern of the stiffness matrix with the two subdomain contributions highlighted in corresponding colors. This pattern is captured at an intermediate step. (c) The final sparsity pattern including the jump contribution in the off-block diagonal entries.

Algorithm 3: Subdomain approach for creating stiffness matrix and populating the jump term.

```

1: Initialize global stiffness matrix ( $\mathbf{B}$ )
2: for  $i = 1$  to number of subdomains ( $n_d$ ) do
3:   Setup local stiffness matrix ( $\mathbf{B}_i$ )
4:   // Update global stiffness matrix
5:    $\mathbf{B} \leftarrow \mathbf{B} + \mathbf{B}_i$ 
6: end for
7: for  $i = 1$  to number of discontinuous interfaces do
8:   for  $j = 1$  to number of pressure nodes on interface  $i$  do
9:     Add jump term to stiffness matrix ( $\mathbf{B}$ )
10:  end for
11: end for

```

on the interface. Algorithm 4 highlights the subdomain approach for constructing each divergence-free local matrix, which yields the sparsity pattern at the intermediate step following the first for loop, as shown in Fig. A.3b. The contribution of external fluxes results in the sparsity pattern shown in Fig. A.3c.

Algorithm 4: Subdomain approach for creating divergence-free matrix and capturing fluxes between subdomains.

```

1: Initialize global divergence-free matrix ( $\mathbf{C}$ )
2: for  $i = 1$  to number of subdomains ( $n_d$ ) do
3:   Setup local divergence-free matrix ( $\mathbf{C}_i$ )
4:   // Update global divergence-free matrix
5:    $\mathbf{C} \leftarrow \mathbf{C} + \mathbf{C}_i$ 
6: end for
7: for  $i = 1$  to number of discontinuous interfaces do
8:   Add the interface external flux component to ( $\mathbf{C}$ )
9: end for

```

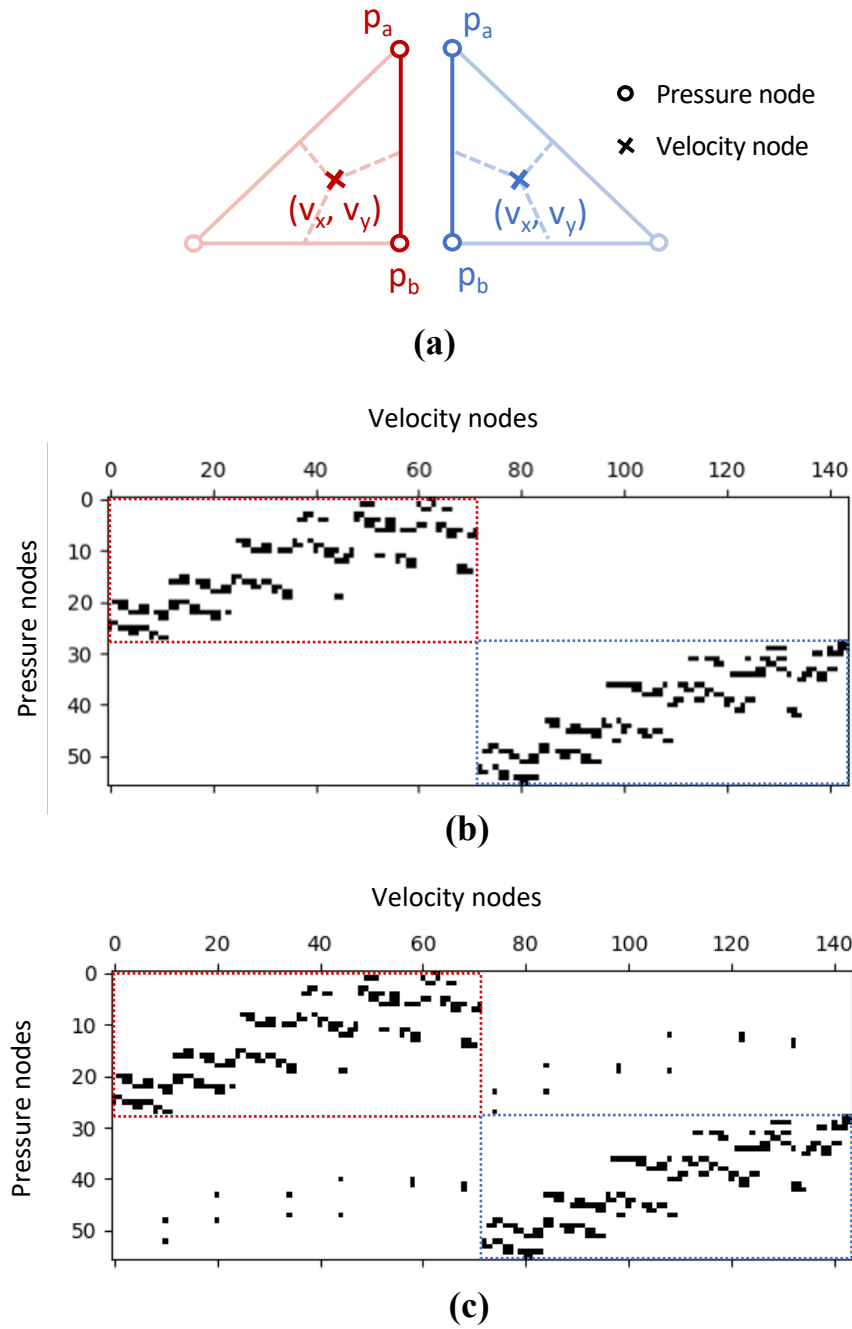


Figure A.3: (a) A schematic of a discontinuous interface with the dashed line representing the control volume mesh. (b) The sparsity pattern of the divergence-free matrix with the two subdomain contributions highlighted in corresponding colors at an intermediate step. (c) The final sparsity pattern including the external fluxes contribution in the off-block diagonal entries.

A.3 The single Mesh CVFE method

The second methodology developed in this work is the Single Mesh CVFE approach, which is the topic of Chapters 4, 5, and 6. The time loop, described in the pseudo code as Algorithm 1, is applied here for the single mesh implementation, ensuring that the control volume mesh aligns with the element mesh. For demonstration purposes, we employ the same mesh shown in Fig. A.1a to highlight the sparsity pattern of different matrices.

Another distinction from the previous approaches is the utilization of a fully discontinuous element pair $(P_{1,DG} - P_{0,DG})$ globally in the domain for the discretization of the flow model, as detailed in Section 4.2.1. Unlike the CVFE and HyCVFE methods, the mass matrix assembled for the SM-CVFE is block diagonal (Fig. A.4a), with each block representing an element's contribution. Refer to Algorithm 5 and Section 6.2.2 for further details.

Algorithm 5: Mass matrix for the SM-CVFE method

```

1: Initialize global mass matrix ( $\mathbf{A}$ )
2: for  $e = 1$  to number of elements  $e_n$  do
3:   Setup block diagonal element mass matrix ( $\mathbf{A}_e$ )
4:   // Update global mass matrix
5:    $\mathbf{A} \leftarrow \mathbf{A} + \mathbf{A}_e$ 
6: end for

```

The stiffness matrix for the SM-CVFE approach is described in Algorithm 6, see Section 6.2.3 for additional details, and the corresponding sparsity pattern is shown in Fig. A.4b.

Algorithm 6: Stiffness matrix for the SM-CVFE method

```

1: Initialize stiffness mass matrix ( $\mathbf{B}$ )
2: for  $e_i = 1$  to number of elements  $e_n$  do
3:   for  $e_j = 1$  to number of adjacent elements to  $e_i$  ( $e_{i,adj}$ ) do
4:     add jump term contribution in stiffness matrix  $\mathbf{B}$  for rows corresponding to  $e_i$ 
5:   end for
6: end for

```

The divergence-free operator matrix for the SM-CVFE approach is described in Algorithm 7 such that the element mesh is utilized to construct a continuous velocity field along element boundaries, refer to Section 6.2.4 for further details. The corresponding sparsity pattern is shown in Fig. A.4c.

Algorithm 7: Divergence-free matrix for the SM-CVFE method

-
- 1: Initialize divergence-free matrix ($\mathbf{C}$)
 - 2: **for** $e_i = 1$ to number of elements e_n **do**
 - 3: **for** $e_j = 1$ to number of adjacent elements to e_i ($e_{i,adj}$) **do**
 - 4: add continuity term contributions in divergence-free operator matrix $\mathbf{B}$ for row corresponding to e_i
 - 5: **end for**
 - 6: **end for**
-

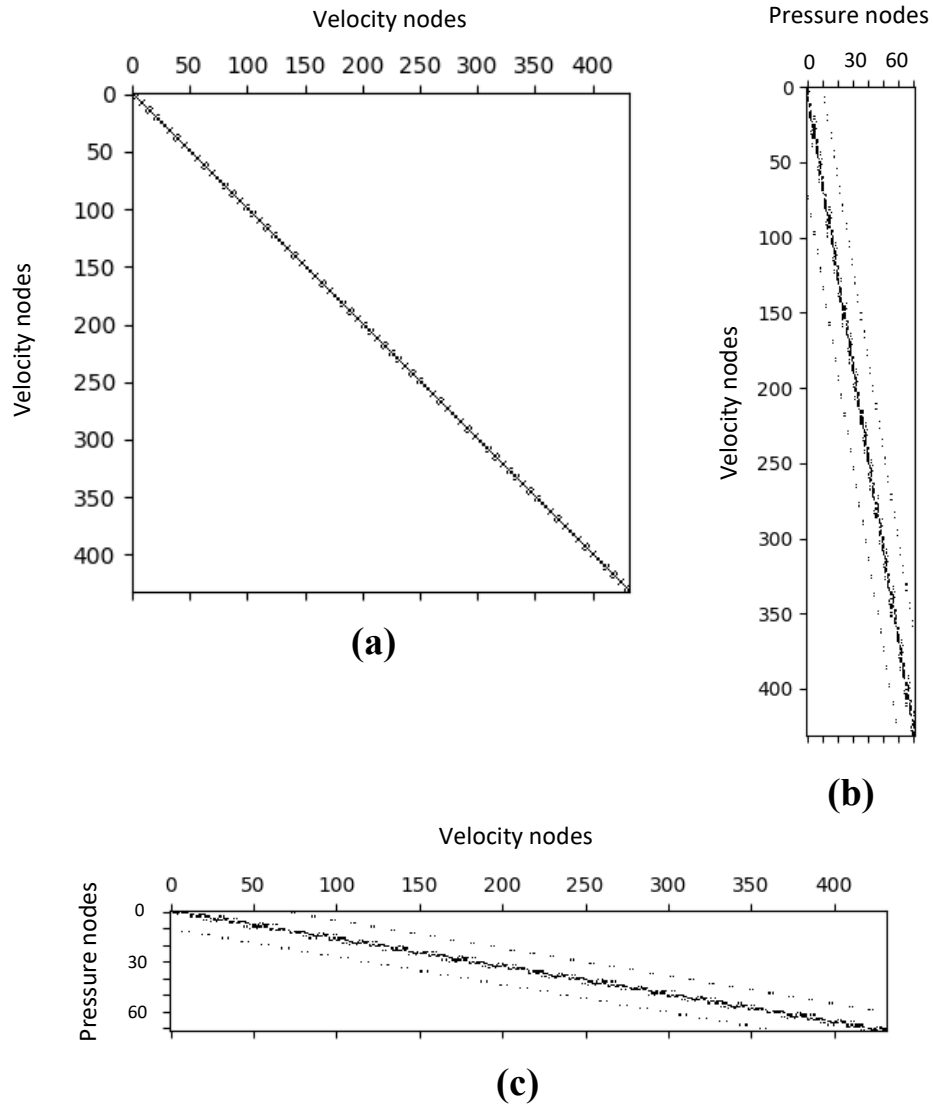


Figure A.4: The sparsity pattern obtained from setting up the SM-CVFE approach for the mesh shown in Fig. A.1a. The mass matrix in (a), the stiffness matrix in (b), and the divergence-free operator matrix in (c).

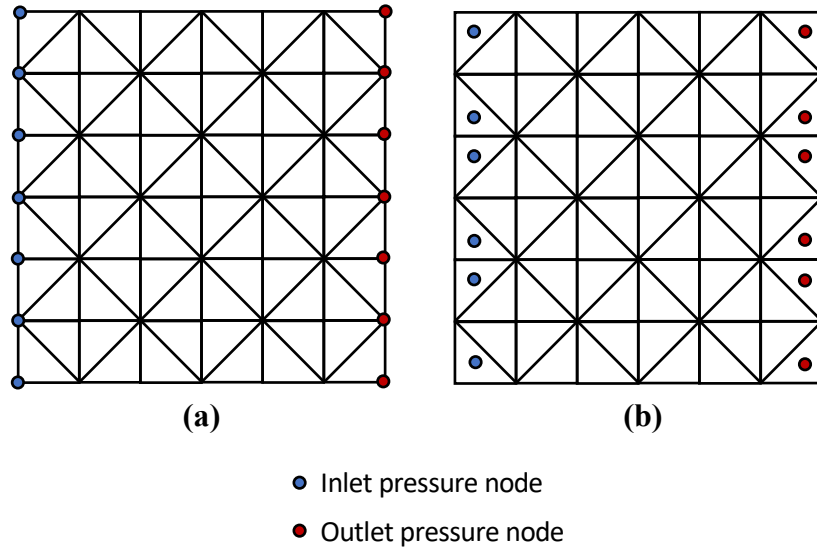


Figure A.5: Comparison of the boundary node implementation in (a) CVFE and HyCVFE methods, and (b) SM-CVFE method.

A.3.1 Pressure boundary conditions

We describe the differences in implementation for prescribing boundary conditions in the SM-CVFE compared to the classical CVFE and HyCVFE methods. The SM-CVFE employs an element-wise approximation of pressure, with the pressure node positioned at the barycenter of the element. When prescribing pressure boundary conditions, due to the lack of a pressure node on the boundary, our implementation utilizes the pressure node from the boundary element, as illustrated in Fig. A.5b, contrasting with the approach used in the CVFE and HyCVFE methods (Fig. A.5a). A potential improvement could involve implementing the ghost-cell approach [LeVeque, 2002] to provide a more effective mechanism for applying boundary conditions to the computational domain.

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