Multi-scale modelling of multi-physics flow in coal seams

Zakhar Lanetc, Aleksandr Zhuravljov, Kunning Tang, Ryan T. Armstrong, Peyman Mostaghimi

aSchool of Minerals and Energy Resources Engineering, University of New South Wales, Sydney, NSW 2052, Australia
bInstitute of Environmental and Agricultural Biology, University of Tyumen, Tyumen 625003, Russia

Abstract

The understanding and quantitative analysis of multi-physics flow in coal seam gas reservoirs are of importance for estimating gas production or assessing the feasibility of carbon dioxide sequestration and hydrogen storage projects. Thus, such phenomena as two-phase flow, gas and rock compressibility, as well as sorption and diffusion and their relative contributions to flow characteristics, should be quantitatively analysed. To develop an appropriate hybrid numerical solution, the two-phase Darcy-Brinkman flow model is employed as a basis. The gas phase is considered compressible while another incompressible phase represents water. The sorption processes are introduced by the Langmuir isotherm, while the transient nature of sorption is captured by the implicit combination of the Langmuir and pressure equations in the Darcy-Brinkman model. The surface diffusion is embedded in the proposed hybrid model explicitly by using the second Fick’s law. The matrix swelling-shrinkage phenomenon and its impact on the coal porosity and absolute permeability is accounted for by using the Palmer-Masoori analytical model. The proposed hybrid numerical solution is implemented by employing the OpenFoam open-source libraries. Several illustrative synthetic and realistic simulations are presented to demonstrate the capability of the developed solver to capture complex coal multi-physics. Moreover, the employment of numerical irregular meshes for saving computational resources is also exemplified.

Keywords: Pore-scale simulation, Coal seam gas, Transient multiphase flow in fractures, Darcy-Brinkman model, Sorption and diffusion
1. Introduction

Natural gas stored in coal seams is often considered as a potential hazard for coal mining and vented out before the coal extraction commences [1]. The gas venting is undesirable procedure since methane (CH$_4$) global warming potential is significantly higher than for carbon dioxide (CO$_2$) [2]. Therefore, it is currently preferred to produce natural gas from coal seams rather than venting it out to the atmosphere. Moreover, coal seam gas (CSG) can be economically extracted as an independent natural resource. Countries such as the US, China, India and Australia have made substantial investments to CSG exploration projects [3, 4, 5, 6]. There are also environmental benefits associated with CSG reservoirs. Among them, the injection of carbon dioxide CO$_2$ into coal seams are of particular research interest [7, 8, 9]. This may not only allow to enhance the methane CH$_4$ recovery but also provides the possibility to store a significant amount of CO$_2$ since its affinity to coal matrix is several times stronger than CH$_4$ [10, 11, 12]. Nevertheless, the transport mechanisms taking place during CSG production are complex which makes quantitative analysis challenging [13, 14, 15]. The development of numerical methods allowing to improve the understanding of multi-physics transport in coal are crucial to enhance the natural gas production and achieve above-mentioned environmental benefits.

Digital Rock Physics (DRP) combines a family of methods allowing to utilise the micro-computed tomography (micro-CT) of the rock to visualise 3D geometries of the pore space to be used as an input for flow simulations [16, 17, 18, 19]. Direct numerical simulations (DNS) conducted on the micro-CT images of a rock allow operating on a pore-scale where the competition between various multi-physics phenomena is better understood [20, 21, 22, 23]. The upscaling procedure can follow DNS to estimate macroscopic properties such as absolute and relative permeability curves [24, 25, 26, 27, 28]. Micro-CT imaging of coal has been extensively utilised in various research applications including statistical analysis of cleat systems, predicting sorption-induced swelling and bulk moduli, and diffusion modelling [1, 29, 30, 31, 32, 33].

It is particularly challenging to predict multi-phase displacement occurring in coal seams due to the multi-scale nature of coal which consists of matrix and fractures. Coal matrix is very low permeable and mainly composed of macerals and organic minerals [34, 35, 36]. In turn, the fluid flow conduit in coal seams is provided by a system of hydrodynamically connected fractures [37, 38]. While larger coal fractures can be resolved on micro-CT images, smaller fractures and micro-pores falls below the micro-CT resolution [31, 39]. The interaction between gas molecules...
occurring in the nano- and meso-pores can be characterised by the molecular-level mechanisms including surface and Knudsen diffusion, as well as gas sorption [14, 40, 41, 42]. At the same time, coal permeability has a considerable dependence upon the sorption-induced swelling and effective stress [43, 44, 45, 46, 47]. As a result, it is extremely difficult to account and evaluate the contribution of such multi-physics phenomena in both experimental and simulation studies.

In such circumstance, the hybrid image-based solvers are of particular interest.

The hybrid solvers allow to model multi-scale flow phenomena in and between resolved and unresolved domains [48, 49, 50, 51, 52]. Such solvers are based on two conceptually different methods: pore-network modelling (PNM) and direct numerical simulations (DNS) [53, 54, 55, 56, 57]. In PNM, porous media is treated by geometric primitives (e.g., spheres and cylindrical tubes) which represent pore bodies and throats [58, 59, 60]. Dual-porosity in PNM can be modelled by stitching the pore-networks extracted from the resolved regions with the additional finer-scale networks representing sub-resolved domains [61, 62]. Likewise, the connectivity between resolved pores via sub-resolved regions can be established by cubic lattices both in parallel and in series [56, 63, 64]. Alternatively, PNM can be coupled with continuum diffusivity or Darcy-type models, or free (Navier-) Stokes flow to account for multi-scale physics [53, 55, 69]. The additional physics phenomena including sorption, diffusion, reactive transport and slippage effect can then be introduced to the region of interest (e.g., microporous domain) [67, 68, 69, 70].

DNS are superior in comparison with PNM due to the ability to preserve the fine detail obtained from micro-CT imaging and no need to introduce geometric simplifications [55, 71]. Generalised Lattice Boltzmann (LB) models were utilised to account for single-phase flow in dual-scale medium by employing the partial bouncing-back scheme in gray-scale regions of micro-CT images [72, 73, 74, 75, 76]. The Darcy-Brinkman method belongs to the classic mesh-based CFD approaches and has been utilised to couple Darcy flow component in porous region with the volume of fluid (VOF) advection scheme in the void space [77, 78]. Thus, the flow in both void and gray-scale domains can be described by a single equation with variable parameters for relative velocity and permeability [71, 79]. There is a number of papers which show applicability of the DB method for predicting multi-physics transport in heterogeneous media under one- and two-phase flow conditions [22, 80, 81, 82]. For instance, Carrillo et. al., 2022 [83] utilised the multiphase DB solver to evaluate the impact of sub-resolution porosity on resulting dynamic
relative permeability curves. Furthermore, Soulaine et. al., 2019 [84] developed a micro-
continuum DB framework to simulate multiphase transport in shales with the inclusion of various
physical mechanisms including Knudsen and surface diffusion, sorption and slip effects.

In this paper, we adapt a DB approach to simulate multi-physics processes taking place
in coal seams during fluid transport. Our model incorporates multiphase flow in the resolved
pore-space (VOF) and unresolved (Darcy) regions. Moreover, the additional physics inherent
to coal is incorporated into the solver allowing to account for sorption, surface, Knudsen and
free diffusion, gas and rock compressibility, as well as sorption-induced swelling. We create
several 2D demo simulations to show the applicability of the developed solver to address multi-
physics processes in coal. Likewise, we also conduct a more complex study to demonstrate
model feasibility for realistic applications. The developed framework can be used to model CSG
production mechanisms in micro-CT images of coal.

2. Methods

Mathematical model

This section contains a mathematical and numerical description of the modified multiphase
DB model which is based on the combination of the two-phase Darcy equation, single-phase
compressible Navier–Stokes and continuity equations, and VOF advection scheme [79, 85]. This
modified model allows to simulate two-phase flow in both resolved pores and sub-resolved pores
(continuum). Moreover, gas and coal compressibility, Fick’s 2nd law of diffusion and Langmuir
sorption equation are included in the developed model in order to account for multi-physics
phenomena taking place in coal seam gas reservoirs. A detailed description of the employed
as a basis multi-phase DB solver with correspondent mathematical model, initial and boundary
conditions, as well as its finite volume representation, software implementation and validation
can be found in [79, 86]. The main governing equations and key assumptions which allow the
numerical implementation of various multi-physics phenomena are described below.

The proposed model accounts for two-phase immiscible flow of Newtonian incompressible
and compressible fluids in pore- and continuum scales (fractures and permeable matrix). Thereby,
it is convenient to commence the mathematical description with continuity equation which is taken
in a compressible single-phase form:

\[
\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \vec{v}) + S_n = 0,
\]

(1)
where \( S_g = S_g(p, C_g) \) is a gas sorption source term which is conventionally defined using the Langmuir equation, \( p \) is pressure of a mixture, \( C_g \) is concentration of the adsorbed gas, \( \phi \) is porosity which equals 1 in fractures (unless fracture compressibility is accounted for), \( \rho \) and \( \tilde{v} \) are density and velocity of a fluid mixture, respectively. Langmuir isotherm is defined through the equilibrium gas surface concentration \( C_g \) and is pressure dependent:

\[
C_g = \frac{C_L p}{p_L + p}
\]  

(2)

where \( C_L \) and \( p_L \) are isotherm constants. In turn, the compressible phase is represented by using the equation of state in the following form:

\[
\rho_g = a_g p_g + b_g,
\]  

(3)

where \( a_g \) and \( b_g \) are the equation of state constants, while \( p_g \) is pressure in the gas phase. In turn, pressure of the mixture is defined by pressures in the phases \( p_g \) and \( p_l \) as follows:

\[
p = \begin{cases} 
p_l = p_g : \text{fracture}, \\
\alpha_l p_l + \alpha_g p_g : \text{matrix}, 
\end{cases}
\]  

(4)

Surface diffusion is given by the Fick’s 2nd law:

\[
\frac{\partial C_g}{\partial t} - \tilde{\nabla} \cdot D_g \tilde{\nabla} C_g = S_g,
\]  

(5)

where \( D_g \) is the surface diffusion coefficient while source term \( S_g \), which is also presented in continuity Eq. (1), allows to numerically relate the surface diffusion with advection and sorption.

The equation of the VOF advection algorithms can be introduced in its conventional form:

\[
\frac{\partial \phi_{i,j}}{\partial t} + \tilde{\nabla} \cdot \phi_{i,j} \tilde{v} + \tilde{\nabla} \cdot \phi_{i,j} \alpha_i \tilde{v}_r = 0,
\]  

(6)

where subscript indices \( i \) and \( j \) denote liquid or gas phases (\( l \) or \( g \)), while \( \alpha \) is the volume fraction of a particular phase. The relative velocity \( \tilde{v}_r \) is considered as a difference between fluid velocities and can be defined as follows:

\[
\tilde{v}_r = \begin{cases} 
\lambda \max(|\tilde{v}|) \tilde{n}_{lg} : \text{fracture}, \\
\left( \frac{k_{kg}}{\mu_g} - \frac{k_{kg}}{\mu_l} \right) \tilde{\nabla} p_l + \frac{k_{kg}}{\mu_g} \tilde{\nabla} p_c : \text{matrix},
\end{cases}
\]  

(7)

where \( \lambda \) is a model parameter which is used to control the interface compression, \( \tilde{n}_{lg} \) is an average unit normal vector of the liquid-gas interface while subscript indices \( l \) and \( g \) denote liquid and gas phases, respectively.
The modification of single-phase Navier–Stokes equations utilised in the DB model is expressed as follows:

\[
\frac{1}{\phi} \left( \frac{\partial \rho \ddot{v}}{\partial t} + \nabla \cdot \rho \ddot{v} \ddot{v} \right) = -\ddot{v} p_t + \frac{1}{\phi} \nabla \cdot F_k \mu \ddot{v} + \ddot{f}_c - \psi \ddot{v},
\]

(8)

where \( \gamma \) is water-gas interfacial tension, \( \mu \) is dynamic viscosity of fluids mixture, while factor \( F_k \) can be used to account for absolute permeability variation due to coal compressibility. Capillary forces \( \ddot{f}_c \) and total porous conductance \( \psi \) are defined differently in fractures and matrix:

\[
\ddot{f}_c = \begin{cases} 
\gamma \ddot{v}, & \text{fracture}, \\
\frac{\partial p_c}{\partial n} \ddot{v}, & \text{matrix}, 
\end{cases}
\]

(9)

\[
\psi = \begin{cases} 
0, & \text{fracture}, \\
\left( \frac{k_{kr_L}}{\mu} + \frac{k_{kr_R}}{\mu} \right)^{-1}, & \text{matrix}, 
\end{cases}
\]

(10)

where flow characteristics inside the matrix are defined by absolute permeability \( k \), relative permeability \( k_{ri} \) and capillary pressure \( p_c \) through the Brooks-Corey model:

\[
k_{ri} = A_i \left( \frac{\alpha_{rL} - \alpha_{ri}}{1 - \alpha_{rL} - \alpha_{gr}} \right)^{m_i}, \quad k_{rg} = A_g \left( \frac{I - \alpha_{ri} - \alpha_{gr}}{I - \alpha_{rL} - \alpha_{gr}} \right)^{m_g}, \quad p_c = A_c \left( \frac{\alpha_{rL} - \alpha_{ri}}{I - \alpha_{rL} - \alpha_{gr}} \right)^{-m_c},
\]

(11)

where \( A_i, A_c, \alpha_{ri}, m_i, m_c \) are the parameters of the Brooks-Corey models.

Compressibility of gas phase is accounted for by the first and second terms of Eqs. (1) and (8) while sorption is modelled by the third terms of Eqs. (1) and (5). The numerical representation of the first and second terms of Eqs. (1) and (8) can be found in Carrillo et al. [79], while the implicit expression of the sorption term is derived using the Newton’s linearization method [87]:

\[
\frac{\partial S_g(p^n, C_g^n)}{\partial p^n} (p^{n+1} - p^n) + S_g(p^n, C_g^n),
\]

(12)

where subscript index \( n \) denotes time and sorption rate \( S_g(p^n, C_g^n) \) is expressed through the Langmuir equation [2] as follows:

\[
S_g(p^n, C_g^n) = \frac{C_{Lp}^n}{\frac{C_{Lp}^n}{p^n} - C_{eq}^n},
\]

(13)

where \( \Delta t^n \) is a numerical time step for \( n \) time moment. In turn, the surface diffusion equation [5] is embedded in the described DB numerical scheme sequentially and, thus, accounted for explicitly by the source term in the continuity equation [1].

This combination of gas compressibility, explicit simulation of surface diffusion and implicit inclusion of sorption term allows obtaining a stable numerical solution for adsorption and desorption phenomena. The aim of these modifications is an achievement of unsteady-state balance.
between pressure \( p \), gas surface concentration \( C_g \) and surface diffusion by avoiding numerical oscillations for a wide range of simulation parameters. The implicit implementation of the sorption term within the numerical scheme, allows us to accurately estimate pressure values with respect to the current time step \( n + 1 \).

The developed mathematical model is also able to account for the matrix swelling-shrinkage phenomena by incorporating the existing empirical or analytical models. In our case, the Palmer-Mansoori model \((14)\) which considers the elastic deformation of coal under uniaxial stress conditions is employed:

\[
\frac{\phi}{\phi_0} = 1 + \frac{1}{M \phi_0} (p - p_0) + \frac{\varepsilon_L}{3 \phi_0} \left( \frac{K}{M} - 1 \right) \left( \frac{p}{p_L + p} - \frac{p_0}{p_L + p_0} \right),
\]

\[(14)\]

where \( \phi_0 \) is porosity at pressure \( p_0 \), constrained axial modulus \( M = \frac{E}{1 - 2\nu} \) \((1 - 2\nu)\), \( E \) is Young’s modulus, \( \nu \) is Poisson’s ratio, bulk modulus \( K = \frac{E}{3(1 - 2\nu)} \), \( \varepsilon_L \) is Langmuir volumetric strain. This empirical equation is incorporated to the mathematical model by considering porosity \( \phi \) as a function of pressure \( p \) explicitly: \( \phi = \phi(p^n) \). The fracture permeability variation during swelling-shrinkage processes is modelled by considering the correction factor \( F_k \) in the fourth term of Eq. (8) as follows:

\[
F_k = \left( \frac{\phi_0}{\phi} \right)^m,
\]

\[(15)\]

where \( m \) can be equal 2 or 3 depending on the considered case: 2D or 3D, accordingly. Such factor is introduced in order to achieve the correspondence between the permeability variation and stress change described by Palmer-Mansoori \((44, 45)\).

The developed solver ’HybridDDSInterFoam’ is based on the open source project ’Hybrid-PorousInterFoam’ developed by Carrillo et al. \((86)\). This open source project contains the software implementation of the basic multi-scale two-phase incompressible DB numerical model \((79)\) and a wide range of correspondent validation tests which are directly applicable to our solver. The implemented additional multi-physics modifications of the DB method are presented in mathematical and numerical forms in this section. The numerical solution of the diffusion equation \((5)\) is provided by the ’OpenFoam’ solver ’LaplacianFoam’ \((88)\).

3. Results and Discussion

The developed solver ’hybridDDSInterFoam’ is used to capture multiphase multi-scale processes of fluid displacement in coal. The simulation is initially based on the multiphase Darcy-
Brinkman open-source implementation which accounts for immiscible two-phase flow in hybrid systems containing both resolved void regions and non-resolved porous matrices [79]. Since coal matrix stores most of the gas deposits and significantly affects the displacement dynamics, its contribution should not be overlooked during numerical simulations. Thus, the additional physics phenomena inherent to coal including sorption and surface diffusion in coal matrix along with the gas and rock compressibility is then built upon the basic DB model.

Another important aspect of the proposed numerical solution is a gradual local grid refinement which is implemented by the `snappyHexMesh` [89] ‘OpenFoam’ utility. Such refinement allows avoiding a situation where neighbouring grid-blocks significantly differ in size. The initial cell size, which is assigned before refinement, should provide satisfactory accuracy in the presence of numerical diffusion with respect to the Darcy flow in matrix regions. In turn, local grid refinement is applied for fractures and should provide satisfactory accuracy regarding Poiseuille-like flow.

To ensure the mesh quality, the grid-independence test was conducted by increasing the minimum characteristic size of numerical cells in the fractures and calculating the average velocity and flux errors. Additionally, the gradual transition between refined and unrefined regions provides the convergence of simulation results obtained with locally refined and entirely refined meshes.

To demonstrate an ability of the developed numerical solution in capturing the above-mentioned coal multi-physics phenomena, we firstly construct a simple two-dimensional (2D) geometry consisting of one fracture within matrix (Fig. 1). This geometry is processed by two numerical meshes (Fig. 2): simple regular (consists of 6400 cells and requires 95.3 MB of RAM) and irregular with local grid refinement (consists of 1750 cells and requires 57.5 MB of RAM). All simulation for these meshes are conducted on one high-performance core of Apple M1 processor. The different numerical meshes are used to demonstrate the computational benefits and numerical accuracy provided by the implemented local grid refinement.
Figure 1: Geometry utilised in demo cases 1–4 where blue central domain represents fracture while red domain belongs to matrix. A central vertical line depicts the cross-section from which the data for 1D plots (Figs. 4 and 5) is obtained.

Figure 2: Two meshes utilised in demo cases 1–4: left is regular (6400 cells), right is irregular (1750 cells).

There are several demo simulations conducted to demonstrate the functional of the developed solver. The main characteristics of simulations with respect to the physical phenomena involved are listed in Tab. 1. Firstly, we demonstrate the ability of proposed numerical solution to capture the gas compressibility by introducing the dependency between gas density and pore
pressure (Case 1, Fig. 3). Secondly, the interrelation between rock compressibility and its porosity and absolute permeability is presented in Fig. 4 (Case 2). The multi-physics processes occurring alongside with desorption in coals are exemplified by demo Case 3 which is illustrated in Fig. 5. Finally, the effect of surface diffusion on pore pressure and surface gas concentration is depicted Figs. 6 and 7 (Cases 4 and 5, respectively). In all simulations, we assign realistic fluid and rock properties obtained in the literature (Tabs 2, 3, and 4).

Table 1: Main characteristics of conducted demo simulations

<table>
<thead>
<tr>
<th>Characteristics</th>
<th>Demo cases</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>1</td>
</tr>
<tr>
<td>Dimensions</td>
<td>2D</td>
</tr>
<tr>
<td>Synthetic/Realistic (S/R)</td>
<td>S</td>
</tr>
<tr>
<td>One-phase</td>
<td>+</td>
</tr>
<tr>
<td>Two-phase</td>
<td>-</td>
</tr>
<tr>
<td>Gas compressibility</td>
<td>+</td>
</tr>
<tr>
<td>Rock compressibility</td>
<td>-</td>
</tr>
<tr>
<td>Sorption</td>
<td>-</td>
</tr>
<tr>
<td>Surface diffusion</td>
<td>-</td>
</tr>
<tr>
<td>Regular mesh</td>
<td>+</td>
</tr>
<tr>
<td>Irregular mesh</td>
<td>-</td>
</tr>
</tbody>
</table>
To demonstrate the correctness of gas compressibility modelling in both fracture and matrix domains, a single-phase simulation is conducted for Case 1 (Fig. 3). The Dirichlet boundary conditions regarding pressure are imposed. In Fig. 3, the change in pore pressure is reflected by the gas density which is consistent with equation of state (3). The presented case has a relatively small pressure drop and density gradient which is relevant to realistic values for the utilised geometric domain. However, considering a high pressure drop at a larger scale, gas compressibility can have a notable impact on fluid displacement dynamics which can be accounted for using the developed solver.

Table 2: Fluid properties

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>( \rho_l )</td>
<td>( 10^3 \text{ kg/m}^3 )</td>
</tr>
<tr>
<td>( a_g )</td>
<td>( 7.667 \times 10^{-6} \text{ s}^2/\text{m}^2 )</td>
</tr>
<tr>
<td>( b_g )</td>
<td>( -2.333 \text{ kg/m}^3 )</td>
</tr>
<tr>
<td>( \mu_l )</td>
<td>( 10^{-5} \text{ Pa s} )</td>
</tr>
<tr>
<td>( \mu_g )</td>
<td>( 10^{-5} \text{ Pa s} )</td>
</tr>
<tr>
<td>( \gamma^2 )</td>
<td>( 7 \times 10^{-2} \text{ kg/s}^2 )</td>
</tr>
</tbody>
</table>

*1 - [90]; *2 - [91]

Table 3: Matrix characteristics

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>( D_g )</td>
<td>( 5 \times 10^{-9} \text{ m}^2/\text{sec} )</td>
</tr>
<tr>
<td>( k^{s1} )</td>
<td>( 10^{-15} \text{ m}^2 )</td>
</tr>
<tr>
<td>( k^{s2} )</td>
<td>( 10^{-19} \text{ m}^2 )</td>
</tr>
<tr>
<td>( A_c )</td>
<td>( 0 \text{ Pa} )</td>
</tr>
<tr>
<td>( A_i, m_i, m_c )</td>
<td>( 1 )</td>
</tr>
<tr>
<td>( \alpha_{ir} )</td>
<td>( 0 )</td>
</tr>
</tbody>
</table>

*1 - [92]; *2 - [8, 15, 38, 93]

Table 4: Palmer-Mansoori and Langmuir constants

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>( p_0 )</td>
<td>( 10^6 \text{ Pa} )</td>
</tr>
<tr>
<td>( \varepsilon )</td>
<td>( 0.035 )</td>
</tr>
<tr>
<td>( E )</td>
<td>( 1.38 \times 10^{9} \text{ Pa} )</td>
</tr>
<tr>
<td>( \phi_0 )</td>
<td>( 0.01 )</td>
</tr>
<tr>
<td>( \nu )</td>
<td>( 0.35 )</td>
</tr>
<tr>
<td>( p_L )</td>
<td>( 2.1 \times 10^6 \text{ Pa} )</td>
</tr>
<tr>
<td>( C_L )</td>
<td>( 230 \text{ kg/m}^3 )</td>
</tr>
</tbody>
</table>

*1 - [94]; *2 - [47]; *3 - [95]
Same initial and boundary conditions as in Case 1 are used in Case 2 to demonstrate the ability of the proposed numerical solution to account for the dependence between fracture absolute permeability, porosity and effective stress (Fig. 4). The dependence between fracture porosity and effective stress is explicitly calculated during the numerical modelling by utilising the Palmer-Mansoori model (Eq. (14)), while the correspondent absolute permeability variation is accounted for by the correction factor $F_k$ (Eqs. (8) and (15)). Since Palmer-Mansoori porosity model is non-linear regarding pore pressure and introduced explicitly, it can be replaced by any other available empirical or analytical models. Five simulations are conducted at different pore pressures from 1 to $5 \, MPa$ which is in a range reported in the literature [96, 97]. The relative absolute permeability $k/k_0$ is calculated for each simulation using analytical solution for planar Poiseuille flow [98] and compared with dimensionless porosity $\phi/\phi_0$. As can be observed in Fig. 4, there is a close match between numerically predicted $k/k_0$ and expected $\phi/\phi_0$ squared value [46, 47] where both fracture shrinkage and matrix swelling phenomena due to coal compressibility and adsorption are accounted for.
Regarding Case 3 (Fig. 5), the model is initially filled with water while gas is stored in the matrix in the adsorbed state. The amount of gas that can be stored in the matrix at particular pressure is determined by the Langmuir isotherm embedded in the numerical solution. Initially, there is more gas adsorbed in the matrix than its equilibrium amount calculated by the Langmuir equation (Eq. (2), Table 4). In such circumstances, the excessive amount of the adsorbed gas is released to the matrix in a free state and then transports towards the fracture following the computed pressure gradient and displacing presented water. Thus, the amount of water stored in the fracture is gradually decreased and replaced by the gaseous phase (Fig. 5a, b and c). The Dirichlet boundary conditions for pressure are imposed in this demo case. However, there is no initial pressure drop between the inlet (left) and outlet (right) boundaries of the simulation. The liquid is able to leave the simulation domain since zero gradient boundary conditions for saturation are enforced at the inlet and outlet of the model. This simulation demonstrates a complex transient desorption process where the numerically stable results are achieved in a presence of two competitive interrelated phenomena: pressure growths due to desorption and
variation of the desorption rate due to pressure increment.

Figure 5: Demo Case 3. Two-phase simulation, gas desorption. The first and second rows correspond to regular and irregular meshes, respectively. Initial liquid saturation is 1. Inlet and outlet boundary conditions are Dirichlet-type regarding pressure. Pressure drop from 4 MPa to 3 MPa is applied. The depicted figures reflect times equal 0.02 s (a), 0.04 s (b), and 0.06 s (c). Execution times are 172 s and 88 s for regular and irregular meshes, correspondingly.

Cases 4 and 5 (Figs. 6 and 7) demonstrate the potential contribution of the surface diffusion between the adsorbed gas molecules to the gas displacement dynamics. The boundary conditions imposed are similar to Case 3, while the sample is initially saturated by the gaseous phase only and the amount of gas adsorbed in the matrix is lower than its equilibrium calculated by the Langmuir equation (Eq. 2, Table 4). Under such circumstances, gas firstly starts to adsorb into the matrix at the matrix/fracture interface. The adsorption process leads to an occurrence of pressure gradient and, as a result, gas also transports into the matrix in a free state due to advection. The only difference between Case 4 and 5 is that surface diffusion is not accounted ($D_g = 0$) for Case 5. The comparison between pressure and surface gas concentration profiles depicted in Figs. 6 and 7 shows that surface diffusion can potentially affect the transient nature of fluid transport in the coal matrix. This is quantitatively exemplified in Fig. 8 where the propagation of pressure and adsorbed gas concentration into the matrix is more considerable for Case 4 which accounts for...
the contribution of surface diffusion.

Figure 6: Demo Case 4. One-phase, gas adsorption including surface diffusion. First and second rows depict pore pressure and surface gas concentration, respectively. The first and second columns correspond to regular and irregular meshes, respectively. Liquid saturation is 0. Inlet and outlet boundary conditions are Dirichlet-type regarding pressure. Vertical pressure gradient from 4 MPa (inside fracture) to 3 MPa (inside matrix) is applied. The depicted figures reflect time equals 100s. Execution times are 8356 s and 1175 s for regular and irregular meshes, correspondingly.
Figure 7: Demo Case 5. One-phase, gas adsorption excluding surface diffusion. First and second rows depict pore pressure and surface gas concentration, respectively. The first and second columns correspond to regular and irregular meshes, respectively. Liquid saturation is 0. Inlet and outlet boundary conditions are Dirichlet-type regarding pressure. Vertical pressure gradient from 4 MPa (inside fracture) to 3 MPa (inside matrix) is applied. The depicted figures reflect time equals 100s. Execution times are 8229s and 1730s for regular and irregular meshes, correspondingly.
To demonstrate the applicability of the developed multi-physics solver to realistic coal geometries, we took a 2D micro-CT slice with dimension 2001 × 2501 voxels where voxel resolution equals $2.8 \times 10^{-5}$ m (Fig. 9a). For this, the dry micro-CT image of coal cored from an exploration well in the Gloucester Basin in Australia is taken. More details regarding micro-CT imaging, sample preparation and its petrophysical characteristics can be found in [99]. The segmentation of this slice is conducted using Trainable Weka Segmentation (TWS) through ImageJ software [100]. In TWS, the segmentation is performed by training with a few number of manually labeled pixels. The output of such segmentation can be found in Fig. 9b. We then selected and crop a section of this slice with well-developed cleat network to perform numerical simulations (Fig. 9c). The cropped micro-CT slice is used to create the irregular numerical 2D mesh (Fig. 10) consisting of 54778 grid blocks and requiring 3.3 GB of RAM to run a simulation by a developed solver. The simulation for this mesh is conducted on 35 cores by Message Passing Interface (MPI) of processor Intel Xeon Gold 6242R. The decomposition is made by ‘decomposePar’ ‘openFOAM’ utility with scotch algorithm assigned [89]. This irregular mesh is used to decrease the number of
numerical grid blocks and, thus, reduce the execution time since the regular mesh would require 412672 cells. If the 3D geometry was considered, the difference in the number of grid blocks between the regular and irregular meshes would approximately increase by an order of magnitude.

Figure 9: Realistic 2D geometry extraction workflow: a) Raw; b) Segmented; c) Cropped 2D micro-CT images of coal.
The numerical simulation for Case 6 is similar to Case 3 with respect to initial and boundary conditions. The whole void space available in fracture and matrix is initially filled with water while gaseous phase is only existing in the adsorbed state inside the coal matrix. Since there is more gas adsorbed in the matrix than its equilibrium value determined by the Langmuir equation (Eq. 2, Table 4), the gas starts to displace water from coal matrix and from the fractures edges while the water phase is situated at the centre of the cleats (Fig. 11a). Considering a second depicted time moment (Fig. 11b), the water saturation in the matrix is significantly declined as well as the surface gas concentration due to the gas desorption. Likewise, the flow regimes inside the fractures is similar to the segregated two-phase flow with large gas and water regions. At the final moment (Fig. 11c), the gaseous phase prevails in both matrix and cleats. Water in fractures is presented in form of unevenly distributed bubbles and plugs while the water saturation is also not constant inside the matrix due to the pore pressure distribution which dictates the spacial adsorption dynamics. Such uneven saturation distribution inside the coal sample under two-phase flow is inline with the dynamic micro-CT study [101] where spontaneous water imbibition in coals is researched. There are few other micro-CT-based studies conducted to analyse multi-physics flow and sorption processes in coals, although they only consider one-phase gas flow [30, 33, 102].
Figure 11: Demo Case 6. Two-phase simulation, gas desorption. The first and second columns correspond to liquid saturation and surface gas concentration, respectively. Initial liquid saturation is 1. All boundary conditions are Dirichlet-type regarding pressure. Pressure drop from 4 MPa to 3 MPa is applied. The depicted figures reflect times equal 0.01 s (a), 0.02 s (b), and 0.04 s (c). Execution times is 44,485 s for irregular mesh.

4. Conclusion

In this paper we demonstrated the capacity of the developed 'HybridDDSInterFoam' solver to model various multi-physics phenomena inherent in coal. These phenomena include multiphase flow in multi-scale media, gas and rock compressibility, as well as sorption and surface diffusion in the coal matrix. We conducted demo simulation using both simple synthetic 2D geometry and a more complex realistic image of coal. We made the following observations regarding the numerical simulations:

- The effect of gas compressibility is negligible on gas density and displacement profile during pore-scale experiment with realistic flow characteristics. However, if the nature of numerical experiment requires a pressure gradient which can result in density variation exceeding several percent, the gas compressibility should not be overlooked.

Electronic copy available at: https://ssrn.com/abstract=4298771
The simulator is flexible in terms of empirical or analytical models which can be used to account for the dependence between fracture porosity/absolute permeability and effective stress. Thus, both fracture shrinkage and matrix swelling phenomena can be incorporated into the numerical simulation.

By implicitly introducing the sorption term into the numerical solution using the Newton’s linearisation, we achieved the numerical stability when modelling complex sorption physics under multi-phase flow conditions. The numerical stability is ensured by the absence of computational oscillations and the ability to simulate sorption processes under a wide range of pressure gradients utilised throughout this study.

Surface diffusion is taken into account when modelling sorption processes in coals since it may impact the adsorption dynamics and flow direction inside the matrix. The relative impact of surface diffusion would depend upon the competition between diffusive and advective processes.

The usage of a local grid refinement significantly reduces computational time and memory requirements.

Future work will be focused on the multi-component extension of the current solver for the implementation of competitive sorption mechanisms. This would allow to estimate $CO_2$ and hydrogen storage capacities and mechanisms in CSG formations. For this, the dynamic synchrotron experiments are going to be conducted.

References

URL https://linkinghub.elsevier.com/retrieve/pii/S0166516220305486

URL https://ACP.COPERNICUS.ORG/ARTICLES/20/15487/2020/


Electronic copy available at: https://ssrn.com/abstract=4298771

URL https://linkinghub.elsevier.com/retrieve/pii/S0301420716300769

URL https://linkinghub.elsevier.com/retrieve/pii/B9780128008805000188

URL https://pubs.acs.org/doi/10.1021/acs.energyfuels.9b01190

URL https://linkinghub.elsevier.com/retrieve/pii/S0166516205001527


URL https://linkinghub.elsevier.com/retrieve/pii/S0016236115007838

URL https://linkinghub.elsevier.com/retrieve/pii/S0166516213001833

URL https://linkinghub.elsevier.com/retrieve/pii/S0166516211001832

URL https://linkinghub.elsevier.com/retrieve/pii/S187551020300668

URL https://linkinghub.elsevier.com/retrieve/pii/S0016236115007838

Electronic copy available at: https://ssrn.com/abstract=4298771

URL: https://onepetro.org/SPEATCE/proceedings/09ATCE/All-09ATCE/New%20Orleans,%20%20Louisiana/147347


URL: https://linkinghub.elsevier.com/retrieve/pii/S0309170814001730


URL: https://onepetro.org/SPEATCE/proceedings/09ATCE/All-09ATCE/New%20Orleans,%20%20Louisiana/147347


URL: https://linkinghub.elsevier.com/retrieve/pii/S0016236119317387


URL: https://linkinghub.elsevier.com/retrieve/pii/S0016236117312723


URL: https://linkinghub.elsevier.com/retrieve/pii/S18755100163000343


URL: https://linkinghub.elsevier.com/retrieve/pii/S016516215300197


URL: https://linkinghub.elsevier.com/retrieve/pii/S016516217301726


URL: https://linkinghub.elsevier.com/retrieve/pii/S0016236114010412
URL: https://linkinghub.elsevier.com/retrieve/pii/S0016236115006394


URL: https://pubs.acs.org/doi/10.1021/ef100165w

URL: https://linkinghub.elsevier.com/retrieve/pii/S0166516215300694

URL: https://linkinghub.elsevier.com/retrieve/pii/S0166516218306541

URL: https://academic.oup.com/jge/article/15/2/315-329/5078496

URL: https://linkinghub.elsevier.com/retrieve/pii/S0969209016300555

URL: https://academic.oup.com/jge/article/15/2/315-329/5078496

URL: https://onepetro.org/SJ/article/15/01/152/114777/Predicting-Sorption-Induced-Strain-and

URL: https://linkinghub.elsevier.com/retrieve/pii/S0166516210000131

URL: https://linkinghub.elsevier.com/retrieve/pii/S1365160907001876

[47] E. P. Robertson, R. L. Christiansen, Modeling Laboratory Permeability in Coal Using Sorption-Induced-Strain


URL https://linkinghub.elsevier.com/retrieve/pii/S2590055220300251


URL https://linkinghub.elsevier.com/retrieve/pii/S0309170821002451


URL http://link.springer.com/10.1007/BF02120313


URL https://xlink.rsc.org/?DOI=D0RA07967G


URL http://www.nature.com/articles/s41598-017-14678-1

URL http://journals.sagepub.com/doi/10.1260/0144-5987.32.6.927


URL https://linkinghub.elsevier.com/retrieve/pii/S0166516211000619


URL https://linkinghub.elsevier.com/retrieve/pii/S0016236119306738

URL https://academic.oup.com/bioinformatics/article/33/15/2424/3692362

URL https://linkinghub.elsevier.com/retrieve/pii/S0960180521000949

URL https://linkinghub.elsevier.com/retrieve/pii/S0166516215300963

URL https://academic.oup.com/bioinformatics/article/33/15/2424/3692362

URL https://linkinghub.elsevier.com/retrieve/pii/S0960180521000949

URL https://linkinghub.elsevier.com/retrieve/pii/S0166516215300963