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Upscaling Poromechanical Models of Coalbed Methane Reservoir Incorporating the Interplay between Non-linear Cleat Deformation and Solvation Forces

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Abstract

We construct herein a three-scale coupled mechanical model for naturally fractured coalbed methane reservoir with the ability of describing the stress balance between the solvation force, arising from the gas adsorption in nanopores, and the restoration stress stemming from the elastic response of the cleats. To determine the cleat porosity, the non-linear hyperbolic Barton-Bandis (BB) law, which captures increase in joint stiffness induced by the cleat closure due to matrix swelling, is postulated for the fracture mechanical response. At the microscale, the theory incorporates the coupling between the effects of the solvation force and the elastic response of the

matrix. Such system of governing equations is coupled with the fluid pressure in the discrete cleat system with dependency of aperture with the normal stress dictated by the aforementioned BB-model. A reiterated homogenized procedure is pursued and capable of providing the constitutive response of the homogenized poromechanical parameters on gas pressure. Numerical simulations illustrate the performance of the proposed model.

keywords: Three-scale poromechanical model; Enhanced Coalbed Methane Recovery; Non-linear Barton-Bandis law; Adsorption effects

1 Introduction

It has been well documented that gradual increase of carbon dioxide concentration in the atmosphere induces global warming. Several procedures, commonly adopted to mitigate such an undesirable phenomenon, consist in the long-term storage of supercritical CO₂ in underground geological sites, such as active or depleted oil and gas fields, deep saline aquifers, methane hydrate formations, coal seams and salt caverns [1, 2, 3]. Among the aforementioned sequestration scenarios, we are particularly interested in the enhanced coalbed methane recovery (ECBMR) in unmineable coal seams combined with CO₂ sequestration [4, 5, 6, 7, 8, 9]. Such an attractive combination is motivated by the large quantities of sorbed methane in coal, combined with the high capacity of the coal matrix for storing large amounts of carbon dioxide and consequently generating revenue that mitigates the expenses of sequestration [4, 5]. In coalbed methane reservoirs, the primary production stage is dictated by traditional pressure drawdown which induces methane desorption from the nanopores, with subsequent diffusion in the matrix and flow through the higher permeability layers (cleats) toward the production wells [4, 10]. Owing to the higher affinity with the solid phase, particularly higher adsorption capacity, injected CO₂ maintains the reservoir pressure but decreases the partial pressure of methane causing desorption from the surfaces of the coal matrix. In addition, subsequently CO₂ displaces methane

17 towards the production wells enhancing gas production [4, 5].

18 Fractured coalbed matrix consists of a canonical example of a system characterized by a bimodal
19 structure with two distinct porous systems commonly referred to as cleat (natural fracture) and ma-
20 trix. The former is associated with the gas (and water) percolation whereas the latter dominates
21 the storativity along with slow diffusion within the matrix [4]. Owing to the molecular nature of
22 adsorption, the description requires the use of discrete models or intermediate statistical mechanics
23 tools. Moreover, multiscale flow and diffusion patterns are ruled by phenomena described in terms
24 of continuum physics at two coarser natural scales associated with the expansive matrix intertwined
25 by the cleat system (micro), and the entire macroscopic picture of the homogenized system (macro)
26 characterized by juxtaposed different continua (see Figure 1).

27 A peculiar feature regarding coalbed methane reservoir modeling is the necessity of introducing
28 hydro-mechanical coupled phenomena in order to describe, in an accurate manner, the evolution
29 of the cumulative production curves along with the performance of injector wells [11, 7, 8]. In
30 this context, inclusion of matrix swelling containing nanopores is of utmost importance and appears
31 strongly correlated with the anomalous behavior of the confined fluid [12, 13]. In such a context, it
32 becomes mandatory to develop an accurate description of the fluid-solid intermolecular interaction
33 with the ability to capture local adsorption in the vicinity of the nanopore walls in conjunction
34 with efficient up-scaling methods to propagate the local information to the macroscopic scale. In a
35 sequence of papers [14, 15, 16], the authors have combined the Density Functional Theory (DFT) with
36 formal homogenization methods to derive three-scale methods for expansive porous media containing
37 **nanopores and natural fractures**. More specifically in [15] the authors constructed a new three-scale
38 geomechanical approach for an anomalous mixture of gases in nanopores with spherical geometry
39 coupled with a cleat system of totally open fractures with zero traction on the boundary. In addition to
40 the strong fluid-solid interaction within the coal matrix, competitive mechanisms between desorption
41 induced swelling and the restoring incremental elastic stress due to the mechanical interaction between

42 opposite cleat asperities tend to provide asymptotic stable values of cleat porosity and permeability
43 [12, 17, 15, 14]. Thus, understanding and quantifying accurately the gas-matrix-cleat interactions are
44 crucial for reliable long-term predictions of methane withdrawal and carbon dioxide retention in coal
45 seams.

46 A particular feature of jointed rocks lies in the description of the non-linear stresses induced by
47 the progressive contact between opposite rough-walled surfaces [18, 19, 20]. In this setting, the
48 underlying fine-scale model must have the ability to incorporate the constitutive response of normal
49 and tangential stresses of the joint network, which are strongly dependent on joint closure. The mutual
50 mechanical contact between adjacent asperities in opposite faces gives rise to enhancement in joint
51 stiffness as the gap progressively moves towards the range of very small apertures. Such a non-linear
52 elastic response has been reported in the literature as a cornerstone of a general model commonly
53 referred to as Barton-Bandis model [21, 19]. In this context, the joint-normal stress behaves in a
54 hyperbolic fashion with the displacement jump, whereas the shear component exhibits a quasi-linear
55 dependence on the tangential jump up to a peak, where strong softening inelastic behavior followed
56 by dilatancy takes place [22].

57 In this work, our goal consists in the development of a three-scale poromechanical model with
58 capabilities of capturing the interplay between matrix swelling and non-linear cleat restoring force
59 dictated by the Barton-Bandis law. In order to accomplish this task, we begin by constructing the
60 two-scale poromechanical model for the expansive matrix by combining the results obtained with the
61 DFT for the solvation force with a formal homogenization of an elastic matrix perforated by nanopores
62 saturated by an anomalous adsorbed gas. Such an upscaling provides incremental constitutive laws
63 with additional features such as pore pressure dependency of the elastic modulus and Biot-Willis
64 coefficient stemming from the solvation force. Subsequently, we proceed within the context of a
65 reiterated homogenization procedure [23, 24] in the sense of [25, 26, 27] to incorporate discontinuities
66 inherent to the cleat network ruled by the non-linear constitutive law of Barton-Bandis type giving

67 rise to a three-scale homogenized incremental poromechanical model. A remarkable consequence
 68 of the three-scale approach relies in the construction of the local closure problems for the effective
 69 parameters in the incremental laws, whose solution provides the underlying characteristic function
 70 profiles. Unlike previous work [14, 15, 16], the new closure problems show ability to capture the
 71 interplay between solvation forces and the corresponding counter force in the cleat system dictated by
 72 the non-linear elastic law.

73 Numerical results illustrate the evolution of cleat closure and poromechanical parameters in an
 74 example of CO₂ sequestration in a box-shaped reservoir with a prescribed pore pressure evolution,
 highlighting the potential of the new model proposed herein.

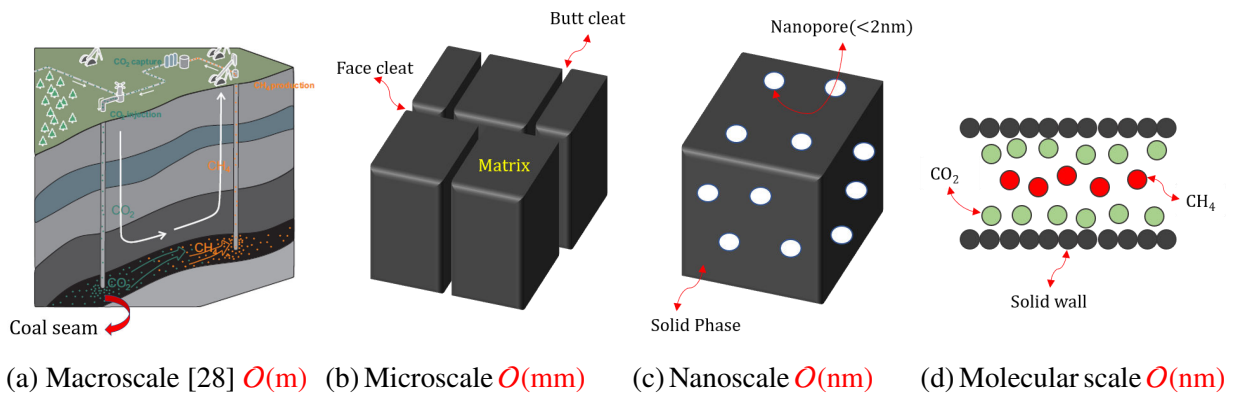


Figure 1: Natural length scales of a coalbed methane reservoir

75

76 2 Review of the Constitutive Laws at the Different Scales

77 We consider a mixture of gases (CH₄ and CO₂) in a coal seam characterized by a bimodal structure
 78 composed of nanopores within the matrix intertwined by a discrete periodic network of cleats. The
 79 gases are thermodynamically adsorbed within the nanopores. The coal skeleton is assumed elastic
 80 and submitted to a stress field induced by solvation forces stemming from intermolecular interactions
 81 between gas molecules and the walls of the nanopore system. Such a mechanical interaction induces

82 swelling/shrinking of the coal skeleton which gives rise to mechanical perturbations in the fracture
 83 aperture consequently modifying cleat permeability. The cleat network is treated as a lower $n - 1$ -
 84 dimensional object for $n = 2, 3$ with the constitutive response of the averaged normal and tangential
 85 stresses ruled by the non-linear hyperbolic law postulated by Barton and Bandis (BB) [19, 22, 29, 21].

86 For the sake of completeness, we begin by reviewing the underlying constitutive response of the
 87 poromechanical variables considered in our subsequent developments, namely the solvation force
 88 induced by the adsorption and the restoring non-linear BB law for the cleats.

89 **2.1 Solvation force**

90 Our nanoscopic picture consists of a confined mixture of N_g gases distributed in a heterogeneous
 91 fashion in nanopores in equilibrium with an outer bulk solution. Unlike bulk fluids, confined gases
 92 commonly exhibit anomalous behavior in nanopores [16]. In this setting the solid surfaces of the
 93 nanopores interact with the gas molecules through a prescribed Lennard-Jones potential, repulsive
 94 and attractive at short and long distances respectively [30]. Such an interaction induces a stress field
 95 in the fluid σ_n . In order to compute its distribution in the nanopores, we begin by denoting Ω_n the
 96 sub-domain occupied by the heterogeneous gas (see Figure 2), in which under absence of gravitational
 97 forces satisfies the local equilibrium

$$\nabla \cdot \sigma_n = 0 \quad \text{in } \Omega_n \quad (1)$$

98 In addition, at the solid/fluid interface Γ_{ns} , by invoking the definition of the solvation force $\mathbf{\Pi}$
 99 exerted on the solid surface by the confined fluids, as an excess quantity with respect to a reference
 100 pressure p_m associated with the non-perturbed bulk state, continuity of the traction reads as

$$\sigma_n \cdot \mathbf{n} = -(\mathbf{\Pi} + p_m \mathbf{n}) \quad \text{on } \Gamma_{ns} \quad (2)$$

101 where \mathbf{n} is the unit normal pointing outward to the sub-domain occupied by the fluid phase.

102 For the sake of completeness, we proceed straightforward from our previous Density Functional
 103 Theory-based framework constructed in [16]. In such a thermodynamically based context applied
 104 to a pore of arbitrary geometry, by postulating proper representation of the grand potential along
 105 with fluid-fluid and fluid-solid Lennard-Jones based potentials in the grand canonical ensemble, the
 106 derivatives with respect to changes in pore volume furnish the solvation force. It should be noted that
 107 due to the complex nanopore geometry (see Figure 2 for example), the distribution of the solvation
 108 force can be non-uniform on the solid wall.

109 To illustrate the numerical outcome of this methodology, let consider a fluid (CO_2) confined in a
 110 spherical nanopore of radius $R_p = 2.5 d_{\text{CO}_2}$ where d_{CO_2} refers to the diameter of the CO_2 molecule.
 111 Figures 3(a) and (b) show the variation of the solvation force as a function of the CO_2 bulk pressure and
 112 the radial distribution function for three values of the CO_2 bulk pressure denoted by A, B, C. It should
 113 be noted that, owing to the adsorption of gas molecules at the vicinity of the solid surface, the solvation
 114 force tends to "pull" the pore wall acting as a traction in the direction to close the nanopores. This
 115 yields a negative value of Π with $\mathbf{\Pi} = \Pi \mathbf{n}$ in (2) with a magnitude much higher than the bulk pressure.
 116 More specifically, at low CO_2 pressures, the gas molecules tend to move towards the attractive zone
 117 inside the nanopores, located in the vicinity of the repulsive boundary layer adjacent to the wall.
 118 Consequently the solid attracts the gas molecules which counter exert an increasing traction force on
 119 the wall as the number of molecules (bulk gas pressure) increases. As the molecules fill completely
 120 this zone, the coupled system reaches the most attractive thermodynamic state at point B in Figure 3.
 121 On the other hand, with further increase in pressure from the critical point B, the gas gradually moves
 122 towards the repulsive zone, with molecules partitioned between the two zones. Therefore the value
 123 of Π decreases in magnitude, the traction exerted by the gas molecules on the wall also diminishes.
 124 Consequently, the path B→C is intrinsically linked to matrix swelling.

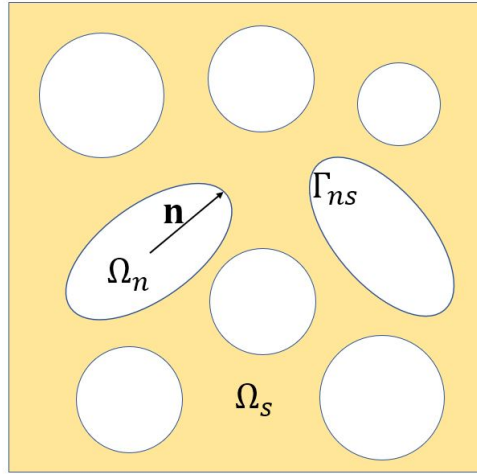


Figure 2: Illustration of the sub-domains in the coal matrix

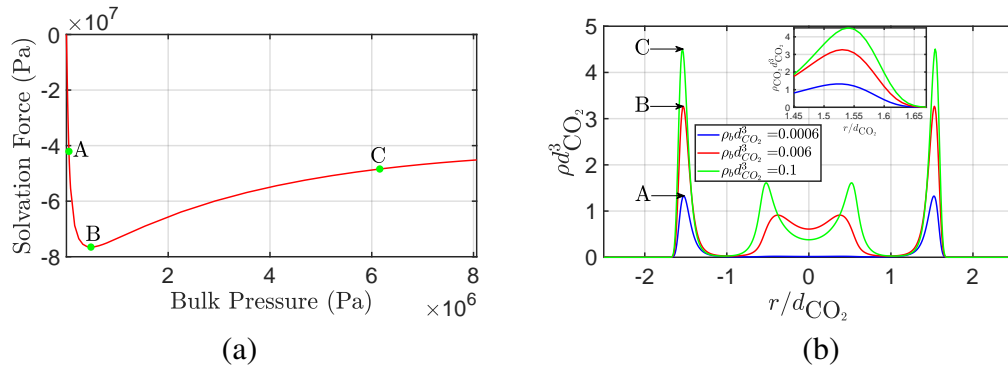


Figure 3: (a) Solvation force versus CO_2 bulk pressure in a spherical pore of radius $R = 2.5 d_{\text{CO}_2}$. (b) Gas density profiles corresponding to three points for low (A), transition (B) and high (C) bulk pressures [16].

125 2.2 Non-linear elastic stress in the cleats

In addition to the aforementioned response of the solvation force, one also needs to postulate a constitutive law for the contact stress at the coarser scale. As stated previously, in contrast to earlier work [15], we proceed within a more realistic experimentally-based framework proposed by Barton-Bandis [19, 22, 29, 21]. In this approach, the contact stress is represented in terms of perturbations in the mechanical aperture, characterized by the mean point-wise distance between opposite faces

denoted + and – (see Figure 4). The joint closure due to compression, denoting herein in terms of a

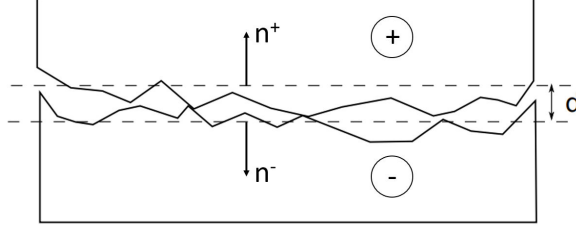


Figure 4: Illustration of the mechanical interaction between opposite joint surfaces.

displacement jump, is defined as the difference between the maximum aperture V_m , measured at the traction-free state, and the crack opening d associated to a loaded state. We have

$$[[u_n]] = d - V_m \quad (3)$$

126 where $[[u_n]] := \mathbf{u}^+ \cdot \mathbf{n}^+ + \mathbf{u}^- \cdot \mathbf{n}^- = (\mathbf{u}^+ - \mathbf{u}^-) \cdot \mathbf{n}^+$ with \mathbf{u}^\pm and \mathbf{n}^\pm the displacements and the normal
 127 vectors on each edge of the cleat (see Figure 4) From the above relation, the bounds $d = V_m$ and $d = 0$,
 128 corresponding to $[[u_n]] = 0$ and $[[u_n]] = -V_m$, naturally appear inherent to the cases of totally open
 129 (unloaded) and closed joints respectively. Thus, following Barton and Bandis [19], the constitutive
 130 relation between joint closure and contact stress is ruled by the hyperbolic equations

$$[[u_n]] = \frac{\bar{\sigma}_n^{\text{BB}} V_m}{K_{ni} V_m - \bar{\sigma}_n^{\text{BB}}} \quad (4)$$

$$\bar{\sigma}_n^{\text{BB}} = \frac{K_{ni} V_m [[u_n]]}{V_m + [[u_n]]} \quad (5)$$

with $\bar{\sigma}_n^{\text{BB}}$ the contact stress and $K_{n,i}$ the initial normal stiffness. Hence, in incremental form we have

$$d\bar{\sigma}_n^{\text{BB}} = K_n d[[u_n]] \quad \text{with} \quad K_n := \frac{K_{ni} V_m^2}{(V_m + [[u_n]])^2} \quad (6)$$

131 the normal stiffness of the joint. Figure 5 shows a typical profile associated with the Barton-Bandis law. One can easily observe a tremendous increase in stiffness K_n as $[[u_n]] \rightarrow -V_m$.

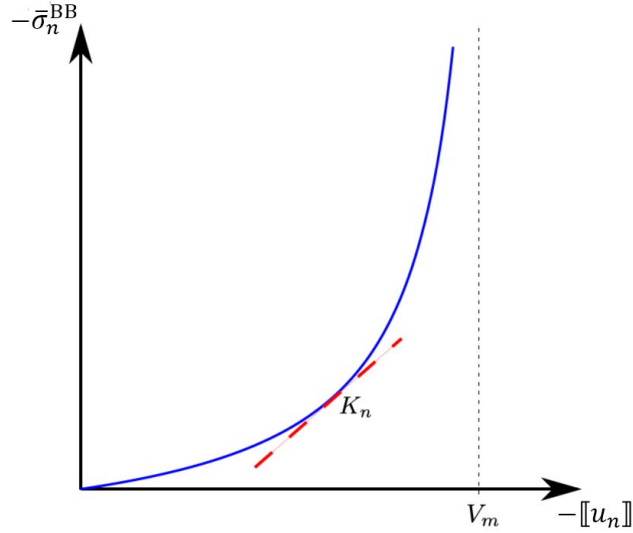


Figure 5: Typical curve associated with the Barton-Bandis constitutive law.

132

133 In addition to the normal stress, the shear component admits complex behavior mainly characterized
 134 by a peak value and subsequent softening behavior [19, 31]. In particular, in the range of small
 135 tangential displacement jump $[[\mathbf{u}_\tau]]$ (lower than 30% of the peak value), the elastic behavior behaves
 136 in a nearly linear fashion solely induced by friction mobilization. For simplicity, in our subsequent
 137 developments we restrict our analysis to the range of linear dependence of shear stress on tangential
 138 displacement ruled by a constant **proportionality** coefficient $0 < \mu_c \leq 1$ which dictates the ratio
 139 between tangential and normal stiffness. Thus, denoting $K_{\tau i}$ the initial shear stiffness we have

$$\frac{K_\tau}{K_{\tau i}} = \frac{K_n}{K_{ni}}, \quad \text{with} \quad \mu_c := \frac{K_{\tau i}}{K_{ni}} = \frac{K_\tau}{K_n} \quad (7)$$

140

Finally, denoting σ^+ and σ^- the stresses on the two sides + and - of the fracture, the traction

141 vector \mathbf{t}_f is given by the projection

$$\mathbf{t}_f = \boldsymbol{\sigma}^+ \cdot \mathbf{n}^+ = \boldsymbol{\sigma}^- \cdot \mathbf{n}^+ \equiv \boldsymbol{\sigma} \cdot \mathbf{n}^+ \quad (8)$$

142 whose increment can be represented as

$$\begin{aligned} d\boldsymbol{\sigma}^+ \cdot \mathbf{n}^+ &= d\boldsymbol{\sigma}^- \cdot \mathbf{n}^+ \equiv d\boldsymbol{\sigma} \cdot \mathbf{n}^+ \\ d\boldsymbol{\sigma} \cdot \mathbf{n}^+ &= K_n \llbracket d\mathbf{u}_n \rrbracket + K_\tau \llbracket d\mathbf{u}_\tau \rrbracket \\ \text{with } \llbracket d\mathbf{u}_n \rrbracket &= (d\mathbf{u}^+ \cdot \mathbf{n}^+ + d\mathbf{u}^- \cdot \mathbf{n}^-) \mathbf{n}^+ = [(d\mathbf{u}^+ - d\mathbf{u}^-) \cdot \mathbf{n}^+] \mathbf{n}^+ \\ \text{and } \llbracket d\mathbf{u}_\tau \rrbracket &= d\mathbf{u}^+ - d\mathbf{u}^- - \llbracket d\mathbf{u}_n \rrbracket \end{aligned} \quad (9)$$

143 **3 Reiterated Homogenization**

144 Hereafter we pursue the upscaling of the nanoscopic description to the microscale aiming at construct-
 145 ing incremental constitutive law for the effective stress and Lagrangian porosity in the coal matrix.
 146 Subsequently the microscopic model is homogenized in a reiterated fashion with the cleat system
 147 considering the normal traction on the cleat surface ruled by the BB law.

148 **3.1 Nanoscopic Model**

149 By invoking the previous nanoscopic description, our fine scale scenario is characterized by a coal
 150 matrix composed of a nanopore system occupied by a mixture of adsorbed gases. The locations
 151 associated with the pore space are denoted by the sub-domain Ω_n whereas the complementary solid
 152 phase occupies the volume Ω_s . The interface between them is denoted by Γ_{ns} . Under the absence of

153 gravitational forces, mechanical equilibrium reads as

$$\begin{cases} \nabla \cdot \boldsymbol{\sigma}_n = 0 & \text{in } \Omega_n \\ \nabla \cdot \boldsymbol{\sigma}_s = 0 & \text{in } \Omega_s \end{cases} \quad (10)$$

154 supplemented by the aforementioned interface conditions

$$\boldsymbol{\sigma}_n \cdot \mathbf{n} = \boldsymbol{\sigma}_s \cdot \mathbf{n} = -(\boldsymbol{\Pi} + p_m \mathbf{n}), \quad \text{on } \Gamma_{ns} \quad (11)$$

155 In addition, the stress tensor in the solid phase is given by

$$\boldsymbol{\sigma}_s = \mathbf{c}_s : \boldsymbol{\mathcal{E}}(\mathbf{u}) \quad \text{in } \Omega_s \quad (12)$$

156 where \mathbf{c}_s is the elastic modulus of the solid phase, \mathbf{u} the displacement and $\boldsymbol{\mathcal{E}}(\mathbf{u}) = (\nabla \mathbf{u} + (\nabla \mathbf{u})^T)/2$
157 the linearized deformation.

158 **3.2 Two-scale homogenization**

159 After establishing the nanoscopic model, we proceed within a formal homogenization procedure in
160 order to construct the poromechanics of the coal matrix. Thus, adopting the usual nomenclature,
161 assign a periodic structure to the overall nanoscopic domain $\Omega_n \cup \Omega_s$ which can be reconstructed by
162 replication of a representative unit cell $Z = Z_s \cup Z_n$ along with the solid-fluid interface ∂Z_{ns} . Denoting
163 ℓ_z and L_y the respective characteristic length-scales of the cell and the homogenized matrix, introduce
164 the small perturbation parameter $\varepsilon = \ell_z/L_y$ along with the slow and fast coordinates \mathbf{y} and $\mathbf{z} = \mathbf{y}/\varepsilon$.
165 We postulate the ansatz

$$f^\varepsilon(\mathbf{y}, \mathbf{z}) = \sum_{k=0}^{\infty} \varepsilon^k f^{(k)}(\mathbf{y}, \mathbf{z}) \quad (13)$$

166 Under the macroscopic point of view, the spatial operators are given by

$$\nabla f^\varepsilon(\mathbf{y}, \mathbf{z}) = \nabla_{\mathbf{y}} f^\varepsilon(\mathbf{y}, \mathbf{z}) + \frac{1}{\varepsilon} \nabla_{\mathbf{z}} f^\varepsilon(\mathbf{y}, \mathbf{z}) \quad (14)$$

167 We now proceed by collecting the terms in the different powers of ε . For the solid phase, we have

$$\begin{cases} \nabla_{\mathbf{z}} \cdot [\mathbf{c}_s : \mathcal{E}_{\mathbf{z}}(\mathbf{u}^{(0)})] = 0 \\ \nabla_{\mathbf{z}} \cdot \boldsymbol{\sigma}_s^{(0)} = 0 \\ \nabla_{\mathbf{y}} \cdot \boldsymbol{\sigma}_s^{(0)} + \nabla_{\mathbf{z}} \cdot \boldsymbol{\sigma}_s^{(1)} = 0 \\ \boldsymbol{\sigma}_s^{(0)} = \mathbf{c}_s : [\mathcal{E}_{\mathbf{y}}(\mathbf{u}^{(0)}) + \mathcal{E}_{\mathbf{z}}(\mathbf{u}^{(1)})] \end{cases} \quad \text{in } Z_s \quad (15)$$

168 and for the gas phase

$$\begin{cases} \nabla_{\mathbf{z}} \cdot \boldsymbol{\sigma}_n^{(0)} = 0 \\ \nabla_{\mathbf{y}} \cdot \boldsymbol{\sigma}_n^{(0)} + \nabla_{\mathbf{z}} \cdot \boldsymbol{\sigma}_n^{(1)} = 0 \end{cases} \quad \text{in } Z_n \quad (16)$$

169 supplemented by the interface conditions

$$\begin{cases} \boldsymbol{\sigma}_n^{(0)} \cdot \mathbf{n} = \boldsymbol{\sigma}_s^{(0)} \cdot \mathbf{n} = -(p_m^{(0)} \mathbf{n} + \boldsymbol{\Pi}^{(0)}) & \text{on } \partial Z_{ns} \\ \boldsymbol{\sigma}_n^{(1)} \cdot \mathbf{n} = \boldsymbol{\sigma}_s^{(1)} \cdot \mathbf{n} \end{cases} \quad (17)$$

170 From (15), we have the local rigid motion $\mathbf{u}^{(0)}(\mathbf{y}, \mathbf{z}) = \mathbf{u}^{(0)}(\mathbf{y})$. In addition, the fluctuations satisfy

171 the local problem

$$\begin{cases} \nabla_{\mathbf{z}} \cdot (\mathbf{c}_s : \mathcal{E}_{\mathbf{z}}(\mathbf{u}^{(1)})) = 0 & \text{in } Z_s \\ \mathbf{c}_s : [\mathcal{E}_{\mathbf{y}}(\mathbf{u}^{(0)}) + \mathcal{E}_{\mathbf{z}}(\mathbf{u}^{(1)})] \cdot \mathbf{n} = -(p_m^{(0)} \mathbf{n} + \boldsymbol{\Pi}^{(0)}) & \text{on } \partial Z_{ns} \end{cases} \quad (18)$$

172 Hence, by invoking linearity, postulate the decomposition of the displacement at order $\mathcal{O}(\varepsilon)$, $\mathbf{u}^{(1)} =$

173 $\mathbf{u}_e^{(1)} + p_m^{(0)} \boldsymbol{\eta} + \mathbf{u}_\pi^{(1)}$ with the right hand side satisfying the local problems

$$\begin{cases} \nabla_z \cdot (\mathbf{c}_s : \boldsymbol{\mathcal{E}}_z(\mathbf{u}_e^{(1)})) & = 0 \quad \text{in } Z_s \\ \mathbf{c}_s : [\boldsymbol{\mathcal{E}}_y(\mathbf{u}^{(0)}) + \boldsymbol{\mathcal{E}}_z(\mathbf{u}_e^{(1)})] \cdot \mathbf{n} & = 0 \quad \text{on } \partial Z_{ns} \end{cases} \quad (19)$$

174 along with

$$\begin{cases} \nabla_z \cdot (\mathbf{c}_s : \boldsymbol{\mathcal{E}}_z(\boldsymbol{\eta})) & = 0 \quad \text{in } Z_s \\ (\mathbf{c}_s : \boldsymbol{\mathcal{E}}_z(\boldsymbol{\eta}) + \mathbf{I}) \cdot \mathbf{n} & = 0 \quad \text{on } \partial Z_{ns} \end{cases} \quad (20)$$

175 and

$$\begin{cases} \nabla_z \cdot (\mathbf{c}_s : \boldsymbol{\mathcal{E}}_z(\mathbf{u}_\pi^{(1)})) & = 0 \quad \text{in } Z_s \\ \mathbf{c}_s : \boldsymbol{\mathcal{E}}_z(\mathbf{u}_\pi^{(1)}) \cdot \mathbf{n} & = -\boldsymbol{\Pi}^{(0)} \quad \text{on } \partial Z_{ns} \end{cases} \quad (21)$$

176 It should be noted that non-slit and non-spherical pore geometries imply in a non-uniform solvation
177 force profile which inherits the local dependency $\boldsymbol{\Pi}^{(0)} = \boldsymbol{\Pi}^{(0)}(\mathbf{z})$. Consequently, from (21), the
178 component $\mathbf{u}_\pi^{(1)}$ does not admit a straightforward decomposition. Conversely, from classical linear
179 elasticity we have

$$\mathbf{u}_e^{(1)} = \boldsymbol{\xi}(\mathbf{z}) : \boldsymbol{\mathcal{E}}_y(\mathbf{u}^{(0)}(\mathbf{y})) \quad (22)$$

180 where the third order tensor $\boldsymbol{\xi}(\mathbf{z})$ satisfies the closure problem

$$\begin{cases} \nabla_z \cdot (\mathbf{c}_s : \boldsymbol{\mathcal{E}}_z(\boldsymbol{\xi})) & = 0 \quad \text{in } Z_s \\ \mathbf{n} \cdot \mathbf{c}_s : [\mathbb{I} + \boldsymbol{\mathcal{E}}_z(\boldsymbol{\xi})] & = 0 \quad \text{on } \partial Z_{ns} \end{cases} \quad (23)$$

181 with \mathbb{I} the fourth-order identity tensor, $\mathbb{I}_{ijkl} := (\delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk})/2$ and δ_{ij} the Kronecker delta symbol.

182 Given the local closure problems for the fluctuations we now pursue the derivation of the upscaled
 183 equations. To this end, the total stress tensor for the matrix is defined as

$$\boldsymbol{\sigma}_m^{(0)} = \langle \boldsymbol{\sigma}_n^{(0)} \rangle + \langle \boldsymbol{\sigma}_s^{(0)} \rangle \quad (24)$$

with $\langle \cdot \rangle$ designating the average operator over the unit cell. A straightforward calculation from the equilibrium condition at $\mathcal{O}(\varepsilon^0)$ shows $\nabla_y \cdot \boldsymbol{\sigma}_m^{(0)} = 0$. Hence, introducing the effective modulus of the matrix

$$\mathbf{C}_m := \langle \mathbf{c}_s : (\mathbb{I} + \mathcal{E}_z(\boldsymbol{\xi})) \rangle \quad (25)$$

184 by averaging (15) and using the above-mentioned decompositions we infer

$$\begin{aligned} \langle \boldsymbol{\sigma}_s^{(0)} \rangle &= \langle \mathbf{c}_s : (\mathbb{I} + \mathcal{E}_z(\boldsymbol{\xi})) \rangle : \mathcal{E}_y(\mathbf{u}^{(0)}) + \langle \mathbf{c}_s : \mathcal{E}_z(\boldsymbol{\eta}) \rangle p_m^{(0)} + \langle \mathbf{c}_s : \mathcal{E}_z(\mathbf{u}_\pi^{(1)}) \rangle \\ &= \mathbf{C}_m : \mathcal{E}_y(\mathbf{u}^{(0)}) + \langle \mathbf{c}_s : \mathcal{E}_z(\boldsymbol{\eta}) \rangle p_m^{(0)} + \langle \mathbf{c}_s : \mathcal{E}_z(\mathbf{u}_\pi^{(1)}) \rangle \end{aligned} \quad (26)$$

185 It remains to compute the component $\langle \boldsymbol{\sigma}_n^{(0)} \rangle$ induced by the solvation force. For the sake of simplicity,
 186 the problem here is limited to the case of closed-pore system. By exploring the local equilibrium
 187 $\nabla_z \cdot \boldsymbol{\sigma}_n^{(0)} = 0$ and the symmetry of the Cauchy stress tensor, the third order tensor $\boldsymbol{\sigma}_n^{(0)} \otimes \mathbf{z}$ satisfies
 188 the relation

$$\nabla_z \cdot (\boldsymbol{\sigma}_n^{(0)} \otimes \mathbf{z}) = \boldsymbol{\sigma}_n^{(0)} \quad (27)$$

189 By using the divergence theorem along with the interface condition (17) we obtain

$$\begin{aligned}
\langle \boldsymbol{\sigma}_n^{(0)} \rangle &= \langle \nabla_z \cdot (\boldsymbol{\sigma}_n^{(0)} \otimes \mathbf{z}) \rangle = \frac{1}{|Z|} \int_{\partial Z_{ns}} \mathbf{n} \cdot (\boldsymbol{\sigma}_n^{(0)} \otimes \mathbf{z}) \, dS \\
&= \frac{1}{|Z|} \int_{\partial Z_{ns}} (\boldsymbol{\sigma}_n^{(0)} \cdot \mathbf{n}) \otimes \mathbf{z} \, dS = -\frac{1}{|Z|} \int_{\partial Z_{ns}} (p_m^{(0)} \mathbf{n} + \boldsymbol{\Pi}^{(0)}) \otimes \mathbf{z} \, dS \\
&= -\phi_m p_m^{(0)} \mathbf{I} - \frac{1}{|Z|} \int_{\partial Z_{ns}} \boldsymbol{\Pi}^{(0)} \otimes \mathbf{z} \, dS
\end{aligned} \tag{28}$$

190 with $|Z|$ the local cell volume. Finally, by collecting our previous results, the total stress tensor in the
191 matrix admits the generalized effective stress decomposition

$$\boldsymbol{\sigma}_m^{(0)} = \mathbf{C}_m : \boldsymbol{\mathcal{E}}_y(\mathbf{u}^{(0)}) - \alpha_m p_m^{(0)} + \langle \mathbf{c}_s : \boldsymbol{\mathcal{E}}_z(\mathbf{u}_\pi^{(1)}) \rangle - \frac{1}{|Z|} \int_{\partial Z_{ns}} \boldsymbol{\Pi}^{(0)} \otimes \mathbf{z} \, dS \tag{29}$$

Hence, using the classical relation $\langle \mathbf{c}_s : \boldsymbol{\mathcal{E}}_z(\boldsymbol{\eta}) \rangle = \langle \nabla_z \cdot \boldsymbol{\xi} \rangle$ along with the definition of the Biot-Willis tensor [32]

$$\alpha_m = \phi_m \mathbf{I} - \langle \mathbf{c}_s : \boldsymbol{\mathcal{E}}_z(\boldsymbol{\eta}) \rangle = \phi_m \mathbf{I} - \langle \nabla_z \cdot \boldsymbol{\xi} \rangle \tag{30}$$

and defining the swelling tensor as

$$\mathbf{F}_S = \langle \mathbf{c}_s : \boldsymbol{\mathcal{E}}_z(\mathbf{u}_\pi^{(1)}) \rangle - \frac{1}{|Z|} \int_{\partial Z_{ns}} \boldsymbol{\Pi}^{(0)} \otimes \mathbf{z} \, dS \tag{31}$$

192 the total stress tensor admits the representation

$$\boldsymbol{\sigma}_m^{(0)} = \mathbf{C}_m : \boldsymbol{\mathcal{E}}_y(\mathbf{u}^{(0)}) - \alpha_m p_m^{(0)} + \mathbf{F}_S \tag{32}$$

193 which consists of the classical effective stress principle with the additional component involving the
194 solvation force.

195 We are now ready to state the two-scale poromechanical model for the coal matrix. Let Ω_m be
196 the domain occupied by the matrix. Given the usual local representations of the pair of poroelastic

197 coefficients $\{\alpha_m, \mathbf{C}_m\}$ along with the nanoscopic representation for the solvation force and the pore
 198 pressure profile in the reference bulk gas in the matrix $p_m^{(0)} = p_m^{(0)}(\mathbf{y})$, we seek the pair $\{\boldsymbol{\sigma}_m^{(0)}, \mathbf{u}^{(0)}\}$
 199 satisfying

$$\begin{cases} \nabla_{\mathbf{y}} \cdot \boldsymbol{\sigma}_m^{(0)} = 0 \\ \boldsymbol{\sigma}_m^{(0)} = \mathbf{C}_m : \boldsymbol{\mathcal{E}}_{\mathbf{y}}(\mathbf{u}^{(0)}) - \alpha_m p_m^{(0)} + \mathbf{F}_S \end{cases} \quad \text{in } \Omega_m \quad (33)$$

200 By comparing with the effective stress principle of traditional poroelasticity, the novelty here is
 201 the inclusion of the solvation force component, which, for a given pore geometry, can be accurately
 202 computed from the nanoscopic representation.

203 3.3 Incremental formulation

204 The appearance of the solvation force induces a strong non-linearity as \mathbf{F}_S depends in a non-linear
 205 fashion on the partial pressure of each gas in a mixture of N components $p_{m,i}$, ($i = 1, \dots, N$) along with
 206 the Lagrangian porosity of the matrix ϕ_m . Whence, following the traditional framework of non-linear
 207 solid mechanics, we proceed by rephrasing the modified effective stress principle in incremental form
 208 from a prescribed reference state.

209 3.3.1 General setting

210 Without loss of generality, consider the swelling tensor \mathbf{F}_S depending only on the pressures $p_{m,i}$ and
 211 the porosity ϕ_m . This yields

$$d\boldsymbol{\sigma}_m^{(0)} = \mathbf{C}_m : \boldsymbol{\mathcal{E}}(d\mathbf{u}^{(0)}) - \alpha_m dp_m^{(0)} + \sum_{i=1}^N \gamma_i dp_{m,i}^{(0)} + \nu d\phi_m \quad (34)$$

with

$$\gamma_i := \frac{\partial \mathbf{F}_S}{\partial p_{m,i}^{(0)}} \quad \text{and} \quad \nu := \frac{\partial \mathbf{F}_S}{\partial \phi_m} \quad (35)$$

212 Given the incremental form of the total stress in the matrix, to complete the two-scale model, it
 213 remains to establish the constitutive law for the Lagrangian porosity relative to the reference state. To
 214 this end, one needs to characterize an extension of the displacement of the solid phase over the fluid
 215 phase. This can be accomplished by simply filling the voids with a fictitious poroelastic system with
 216 negligible stiffness which plays none role in the equilibrium. This yields the extension

$$\begin{cases} \mathbf{u} := \mathbf{u}_s & \text{in } Z_s \\ \mathbf{u} := \mathbf{u}_n & \text{in } Z_n \end{cases} \quad (36)$$

217 together with the continuity condition at the interface $\mathbf{u}_s \cdot \mathbf{n}_{ns} = \mathbf{u}_n \cdot \mathbf{n}_{ns}$.

218 By definition, the incremental Lagrangian porosity is given by

$$d\phi_m = \frac{d|Z_n|}{|Z|} = \frac{1}{|Z|} \int_{\partial Z_n} d\mathbf{u}_n \cdot \mathbf{n}_n dS \quad (37)$$

219 Considering the closed-pore domain Z_n of external surface $\partial Z_n = \partial Z_{ns}$ inside the unit cell $Z = Z_n \cup Z_s$,
 220 we have

$$\begin{aligned} d\phi_m &= \frac{1}{|Z|} \int_{\partial Z_{ns}} d\mathbf{u}_n \cdot \mathbf{n}_{ns} dS = \frac{1}{|Z|} \int_{Z_n} \nabla \cdot d\mathbf{u}_n dV \\ &= \frac{1}{|Z|} \int_Z \nabla \cdot d\mathbf{u} dV - \frac{1}{|Z|} \int_{Z_s} \nabla \cdot d\mathbf{u}_s dV \\ &= \langle \nabla \cdot d\mathbf{u} \rangle - (1 - \phi_m) \langle \nabla \cdot d\mathbf{u}_s \rangle^s \end{aligned} \quad (38)$$

where $\langle \cdot \rangle^s = \langle \cdot \rangle / (1 - \phi_m)$ is the intrinsic volume average over the solid phase. Thus, after invoking periodicity together with the rigid motion at $\mathcal{O}(1)$, the first term in the r.h.s. can be rewritten as

$$\langle \nabla \cdot d\mathbf{u} \rangle = \langle \nabla_y \cdot d\mathbf{u}^{(0)} + \nabla_z \cdot d\mathbf{u}^{(1)} \rangle = \nabla_y \cdot d\mathbf{u}^{(0)} + \frac{1}{|Z|} \int_{\partial Z} d\mathbf{u}^{(1)} \cdot \mathbf{n}_e dS = \nabla_y \cdot d\mathbf{u}^{(0)} = \nabla_y \cdot d\mathbf{u}_s^{(0)} \quad (39)$$

where the integral term vanishes invoking periodicity. The intrinsic average of the divergence of the

solid displacement can be written

$$\langle \nabla \cdot \mathbf{d}\mathbf{u}_s \rangle^s = \nabla_y \cdot \mathbf{d}\mathbf{u}_s^{(0)} + \langle \nabla_z \cdot \mathbf{d}\mathbf{u}_s^{(1)} \rangle^s \quad (40)$$

²²¹ Inserting the above results in (38) we obtain

$$d\phi_m = \phi_m \nabla_y \cdot \mathbf{d}\mathbf{u}^{(0)} - \langle \nabla_z \cdot \mathbf{d}\mathbf{u}^{(1)} \rangle \quad (41)$$

By invoking the aforementioned decomposition for the displacement fluctuation

$$\mathbf{d}\mathbf{u}^{(1)} = \boldsymbol{\xi} : \mathcal{E}_y \left(\mathbf{d}\mathbf{u}^{(0)} \right) + dp_m^{(0)} \boldsymbol{\eta} + \mathbf{d}\mathbf{u}_\pi^{(1)} \quad (42)$$

we infer

$$\langle \nabla_z \cdot \mathbf{d}\mathbf{u}^{(1)} \rangle = \langle \nabla_z \cdot \boldsymbol{\xi} \rangle : \mathcal{E}_y \left(\mathbf{d}\mathbf{u}^{(0)} \right) + dp_m^{(0)} \langle \nabla_z \cdot \boldsymbol{\eta} \rangle + \langle \nabla_z \cdot \mathbf{d}\mathbf{u}_\pi^{(1)} \rangle \quad (43)$$

²²² Recalling the representation for the Biot-Willis parameter (30)

$$\langle \nabla_z \cdot \boldsymbol{\xi} \rangle = \phi_m \mathbf{I} - \boldsymbol{\alpha}_m \quad (44)$$

²²³ and combining relations (41) and (43) lead to

$$d\phi_m = \boldsymbol{\alpha}_m : \mathcal{E}_y \left(\mathbf{d}\mathbf{u}^{(0)} \right) - dp_m^{(0)} \langle \nabla_z \cdot \boldsymbol{\eta} \rangle - \langle \nabla_z \cdot \mathbf{d}\mathbf{u}_\pi^{(1)} \rangle \quad (45)$$

Introducing the **matrix compressibility** with respect to each partial gas pressure, including mechanical and solvation components in the form

$$\beta_i = -\frac{\partial}{\partial p_{m,i}^{(0)}} \left(\langle \nabla_z \cdot \mathbf{u}_\pi^{(1)} \rangle \right) - \langle \nabla_z \cdot \boldsymbol{\eta} \rangle \quad (46)$$

224 and considering $p_m = \sum_i p_{m,i}$, we obtain

$$d\phi_m = \alpha_m : \mathcal{E}_y \left(d\mathbf{u}^{(0)} \right) + \sum_{i=1}^N \beta_i dp_{m,i}^{(0)} \quad (47)$$

225 Hence, combination with (34) gives the incremental form of the effective stress principle

$$d\sigma_m^{(0)} = \mathbf{C}_m^* : \mathcal{E} \left(d\mathbf{u}^{(0)} \right) + \sum_{i=1}^N (\gamma_i + \nu \beta_i - \alpha_m) dp_{m,i}^{(0)} \quad (48)$$

$$\text{with } \mathbf{C}_m^* = \mathbf{C}_m + \nu \otimes \alpha_m \quad (49)$$

which leads to a new tangent modulus for the matrix including the component of the solvation force associated with changes in matrix porosity. Moreover, the modified Biot-Willis parameter which also incorporates the effects of the solvation force reads as

$$\alpha_{m,i}^* := \alpha_m - \gamma_i - \nu \beta_i \quad (50)$$

Thus, in terms of an effective stress, the incremental decomposition (48) can be rewritten as

$$d\sigma_m^{(0)} = \mathbf{C}_m^* : \mathcal{E} \left(d\mathbf{u}^{(0)} \right) - \sum_{i=1}^N \alpha_{m,i}^* dp_{m,i}^{(0)} \quad (51)$$

226 It is noteworthy that, unlike α_m , the modified parameter $\alpha_{m,i}^*$ is not a single property of the matrix but
227 also carries the index associated with each gas in the mixture.

228 3.3.2 Isotropic configuration of spherical nanopores

229 For the sake of simplicity and without loss of generality, hereafter we consider the scenario of spherical
230 pores. In this configuration, isotropy implies in reduction of both $\mathbf{\Pi}^{(0)}$ to a scalar quantity acting in
231 the normal direction to the surface $\mathbf{\Pi}^{(0)} = \Pi^{(0)} \mathbf{n}$, and the tensorial swelling stress to a spherical scalar

232 quantity $\mathbf{F}_S = F_S \mathbf{I}$. Thus, denoting R the radius of the sphere and \mathbf{n} the unit outward normal, by
 233 invoking (28) along with the relation

$$\int_S \mathbf{n} \otimes \mathbf{n} \, dS = \frac{4}{3} \pi R^2 \mathbf{I} \quad (52)$$

234 we infer

$$\begin{aligned} \langle \boldsymbol{\sigma}_n^{(0)} \rangle &= -\phi_m p_m^{(0)} - \frac{1}{|Z|} \int_{\partial Z_{ns}} \Pi^{(0)} \otimes \mathbf{z} \, dS = -\phi_m p_m^{(0)} - \Pi^{(0)} \frac{1}{|Z|} \int_{\partial Z_{ns}} \mathbf{n} \otimes (R \mathbf{n}) \, dS \\ &= -\phi_m (p_m^{(0)} + \Pi^{(0)}) \mathbf{I} \end{aligned} \quad (53)$$

Further, since Π is constant for spherical pores, by invoking definition (20), the closure problem (21) for $\mathbf{u}_\pi^{(1)}$ admits the decomposition

$$\mathbf{u}_\pi^{(1)} = \Pi^{(0)} \boldsymbol{\eta} \quad (54)$$

235 The above result can be explored to obtain the reduced representation for the first term of the r.h.s. of
 236 (31) in the form

$$\langle \mathbf{c}_s : \boldsymbol{\mathcal{E}}_z(\mathbf{u}_\pi^{(1)}) \rangle = \langle \mathbf{c}_s : \boldsymbol{\mathcal{E}}_z(\boldsymbol{\eta}) \rangle \Pi^{(0)} \quad (55)$$

237 Combining with (30), the swelling tensor (31) becomes

$$\mathbf{F}_s = (\langle \mathbf{c}_s : \boldsymbol{\mathcal{E}}_z(\boldsymbol{\eta}) \rangle - \phi_m \mathbf{I}) \Pi^{(0)} = -\alpha_m \Pi^{(0)} \quad (56)$$

238 Using the above representation in the modified effective stress principle (32) gives

$$\begin{aligned} \boldsymbol{\sigma}_m^{(0)} &= \mathbf{C}_m : \boldsymbol{\mathcal{E}}_y(\mathbf{u}^{(0)}) - (p_m^{(0)} + \Pi^{(0)}) (\phi_m \mathbf{I} - \langle \mathbf{c}_s : \boldsymbol{\mathcal{E}}_z(\boldsymbol{\eta}) \rangle) \\ &= \mathbf{C}_m : \boldsymbol{\mathcal{E}}_y(\mathbf{u}^{(0)}) - (p_m^{(0)} + \Pi^{(0)}) \alpha_m \end{aligned} \quad (57)$$

239 In addition, under isotropy, the tensorial coefficients of the incremental effective stress principle (48)
 240 reduce to scalars (denoted herein without boldface), leading to

$$d\boldsymbol{\sigma}_m = \mathbf{C}_m^* : \boldsymbol{\mathcal{E}}(d\mathbf{u}) - \sum_{i=1}^N \alpha_{m,i}^* dp_{m,i} \mathbf{I} \quad (58)$$

$$\text{with } \mathbf{C}_m^* = \mathbf{C}_m + \nu \alpha_m \mathbf{I} \otimes \mathbf{I} \quad \text{and} \quad \alpha_{m,i}^* = \alpha_m - \gamma_i - \nu \beta_i \quad (59)$$

241 Finally, by invoking (45) together with the relation $\langle \nabla_z \cdot \mathbf{u}_\pi^{(1)} \rangle = \Pi^0 \langle \nabla_z \cdot \boldsymbol{\eta} \rangle$, this yields

$$\begin{aligned} d\phi_m &= \alpha_m \nabla_y \cdot d\mathbf{u}^{(0)} - dp_m^{(0)} \langle \nabla_z \cdot \boldsymbol{\eta} \rangle - \left\langle \nabla_z \cdot d\mathbf{u}_\pi^{(1)} \right\rangle \\ &= \alpha_m \nabla_y \cdot d\mathbf{u}^{(0)} - \sum_{i=1}^N \langle \nabla_z \cdot \boldsymbol{\eta} \rangle (dp_{m,i}^{(0)} + d\Pi^0) \end{aligned} \quad (60)$$

242 Hence, by invoking the constitutive dependency $d\Pi^0 = d\Pi^0(d\mathbf{u}^{(0)}, dp_{m,i}^{(0)})$, the last term in the r.h.s.
 243 can be rephrased in the form $d\Pi^0 = \sum_{i=1}^N (\partial\Pi/\partial p_{m,i}) dp_{m,i}$. By comparing with (47) we have

$$d\phi_m = \alpha_m \nabla_y \cdot d\mathbf{u}^{(0)} + \sum_{i=1}^N \beta_i dp_{m,i}^{(0)} \quad (61)$$

with β_i given by (46). Further, denoting k_s the bulk modulus of the solid grains [32], under isotropy
 we have $\langle \nabla_z \cdot \boldsymbol{\eta} \rangle = -(\alpha_m - \phi_m)/k_s$. Whence, the overall undrained compressibility is given by

$$\beta_i = \left(\frac{\partial\Pi}{\partial p_{m,i}} + 1 \right) \frac{\alpha_m - \phi_m}{k_s} \quad (62)$$

244 which consists of the traditional poroelastic value supplemented by an additional component involving
 245 the response of the solvation force with gas pressure under isochoric conditions.

246 **3.4 Homogenization with the cleat network**

247 We shall henceforth discuss the micro-macro upscaling by incorporating the discrete cleat network in
 248 the poromechanical model. To this end, we combine the aforementioned poromechanical description
 249 of the matrix with the non-linear elastic response of cleats described by the Barton-Bandis (BB)
 250 law. It is worth mentioning the mixed-dimensional nature of the coupled problem, since the cleats
 251 are treated as $(n - 1)$ -manifolds ($n = 2, 3$) governed by a reduced poromechanics model ruled by
 252 the BB law. Thus denoting ℓ_y and L_x the respective characteristic length-scales of the micro and
 253 macroscopic descriptions, the perturbation parameter is rephrased as $\varepsilon = \ell_y/L_x$, whereas the slow
 254 and fast coordinates are now denoted by \mathbf{x} and $\mathbf{y} = \mathbf{x}/\varepsilon$ respectively. The microscopic periodic cell,
 255 designated by Y is occupied by the matrix domain Y_m which is intertwined by interface ∂Y_{mf} associated
 256 with the lower dimension cleat network.

257 **3.4.1 Microscopic model**

258 For the sake of completeness and conciseness of notation, the incremental microscopic formulation is
 259 revisited herein with subscripts and superscripts omitted for convenience. We then have

$$\left\{ \begin{array}{l} \nabla \cdot \mathbf{d}\boldsymbol{\sigma}_m = 0 \\ \mathbf{d}\boldsymbol{\sigma}_m = \mathbf{C}_m^* : \boldsymbol{\mathcal{E}}(\mathbf{d}\mathbf{u}) - \sum_{i=1}^N \boldsymbol{\alpha}_{m,i}^* \mathbf{d}p_{m,i} \\ \mathbf{d}\phi_m = \boldsymbol{\alpha}_m : \boldsymbol{\mathcal{E}}_y(\mathbf{d}\mathbf{u}) + \sum_{i=1} \beta_i \mathbf{d}p_{m,i} \end{array} \right. \quad (63)$$

260 We now invoke continuity of normal component of the total matrix stress and the fluid pressure at
 261 the matrix/cleat interface. Considering the traction given by the Bandis-Barton law in Section 2.2,
 262 denoting $p_{f,i}$, p_f and α_f the partial pressure, total pressure and Biot coefficient of the fracture, the

263 incremental form of transmission condition reads as

$$\begin{aligned} d\boldsymbol{\sigma}_m \cdot \mathbf{n}^+ &= K_n \llbracket d\mathbf{u}_n \rrbracket + K_\tau \llbracket d\mathbf{u}_\tau \rrbracket - \alpha_f dp_f \mathbf{n}^+ \\ dp_{m,i} &= dp_{f,i} \end{aligned} \quad (64)$$

264 It is noteworthy that the last term in the r.h.s embodies the Biot-Willis coefficient of the cleats α_f . The
 265 BB law (64) underlying this parameter may bring an extra dependence on gas pressure. More precisely
 266 in D we deduce the relation between α_f and the BB-parameters. A value $\alpha_f = 1$ corresponds to the
 267 case where the strain induced by the gas pressure is entirely associated with the cleat/matrix interface.

268 Further, in order to restrict the effects of the BB law to stress fluctuations within each cell at $\mathcal{O}(\varepsilon)$,
 269 the first term in r.h.s shall be re-scaled. This yields

$$d\boldsymbol{\sigma}_m^{(\varepsilon)} \cdot \mathbf{n}^+ = \varepsilon^{-1} \left(K_n \llbracket d\mathbf{u}_n^{(\varepsilon)} \rrbracket + K_\tau \llbracket d\mathbf{u}_\tau^{(\varepsilon)} \rrbracket \right) - \alpha_f dp_f^{(\varepsilon)} \mathbf{n}^+ \quad (65)$$

270 3.4.2 Micro-Macro Homogenization

271 By writing the above results at successive orders of ε gives

$$\left\{ \begin{array}{l} \mathcal{O}(\varepsilon^{-2}) : \nabla_y \cdot [\mathbf{C}_m^* : \mathcal{E}_y(d\mathbf{u}^{(0)})] = 0 \\ \mathcal{O}(\varepsilon^{-1}) : \nabla_y \cdot d\boldsymbol{\sigma}_m^{(0)} = 0 \\ \quad d\boldsymbol{\sigma}_m^{(0)} = \mathbf{C}_m^* : [\mathcal{E}_x(d\mathbf{u}^{(0)}) + \mathcal{E}_y(d\mathbf{u}^{(1)})] - \sum_{i=1}^N \alpha_{m,i}^* dp_{m,i}^{(0)} \\ \mathcal{O}(\varepsilon^0) : \nabla_x \cdot d\boldsymbol{\sigma}_m^{(0)} + \nabla_y \cdot d\boldsymbol{\sigma}_m^{(1)} = 0 \end{array} \right. \quad (66)$$

272 along with perturbed boundary conditions at the matrix/cleat interface

$$\left\{ \begin{array}{l} O(\varepsilon^{-1}) : \mathbf{C}_m^* : \mathcal{E}_y(\mathbf{du}^{+(0)}) \cdot \mathbf{n}^+ = \\ \quad \mathbf{C}_m^* : \mathcal{E}_y(\mathbf{du}^{-(0)}) \cdot \mathbf{n}^+ = K_n \llbracket \mathbf{du}_n^{(0)} \rrbracket + K_\tau \llbracket \mathbf{du}_\tau^{(0)} \rrbracket \\ O(\varepsilon^0) : \mathbf{C}_m^* : [\mathcal{E}_x(\mathbf{du}^{+(0)}) + \mathcal{E}_y(\mathbf{du}^{+(1)})] \cdot \mathbf{n}^+ = \\ \quad \mathbf{C}_m^* : [\mathcal{E}_x(\mathbf{du}^{-(0)}) + \mathcal{E}_y(\mathbf{du}^{-(1)})] \cdot \mathbf{n}^+ = K_n \llbracket \mathbf{du}_n^{(1)} \rrbracket + K_\tau \llbracket \mathbf{du}_\tau^{(1)} \rrbracket \\ \quad \quad \quad - \sum_{i=1}^N (\alpha_f \mathbf{I} - \alpha_{m,i}^*) dp_{m,i}^{(0)} \cdot \mathbf{n}^+ \end{array} \right. \quad (67)$$

273 By invoking (66a) and (67a), our macroscopic slow variables are $\mathbf{du}^{(0)}(\mathbf{x}, \mathbf{y}, t) = \mathbf{du}^{(0)}(\mathbf{x}, t)$ and
 274 $\llbracket \mathbf{du}_n^{(0)} \rrbracket = \llbracket \mathbf{du}_\tau^{(0)} \rrbracket = 0$. Such a result induced by the re-scaling in (65) implies that, at $O(\varepsilon^0)$, cleats
 275 and matrix behave as a rigid body in each cell and consequently the BB closure affects only the
 276 displacement fluctuations. In addition, the closure problem for $\mathbf{u}^{(1)}$ reads as

$$\left\{ \begin{array}{l} \nabla_y \cdot [\mathbf{C}_m^* : \mathcal{E}_y(\mathbf{du}^{(1)})] = \sum_{i=1}^N \nabla_y \cdot (\alpha_{m,i}^* dp_{m,i}^0) \quad \text{in } Y_m \\ \mathbf{C}_m^* : [\mathcal{E}_x(\mathbf{du}^{(0)}) + \mathcal{E}_y(\mathbf{du}^{+(1)})] \cdot \mathbf{n}^+ = \\ \mathbf{C}_m^* : [\mathcal{E}_x(\mathbf{du}^{(0)}) + \mathcal{E}_y(\mathbf{du}^{-(1)})] \cdot \mathbf{n}^+ = K_n \llbracket \mathbf{du}_n^{(1)} \rrbracket + K_\tau \llbracket \mathbf{du}_\tau^{(1)} \rrbracket \\ \quad \quad \quad - \sum_{i=1}^N (\alpha_f \mathbf{I} - \alpha_{m,i}^*) dp_{f,i}^{(0)} \cdot \mathbf{n}^+ \quad \text{on } \partial Y_{mf} \end{array} \right. \quad (68)$$

277 Since our aim is to focus on the poromechanics, for a prescribed macroscopic gas pressure path in the
 278 time-domain $p_{f,i}^{(0)} = p_{f,i}^{(0)}(\mathbf{x}, t)$, under local equilibrium condition equilibrium we have $p_{m,i}^{(0)} = p_{f,i}^{(0)} =$
 279 $p_{f,i}^{(0)}(\mathbf{x}, t)$. Such a hydraulic communication between the pore pressures precludes the local variability
 280 $p_{m,i}^{(0)}(\mathbf{y})$ implying that the r.h.s of (68a) vanishes. It should be noted that under unsteady conditions
 281 where $p_{m,i}^{(0)} = p_{m,i}^{(0)}(\mathbf{x}, \mathbf{y}, t)$, an additional source term related to the matrix/cleat pressure difference,
 282 which commonly appears in double-porosity-type models shall be added [33, 14].

283 By adopting a superposition analogous to the two-scale problem, by linearity $\mathbf{du}^{(1)}$ can be decom-
 284 posed in the form $\mathbf{du}^{(1)} = \mathbf{du}_e^{(1)} + \mathbf{du}_\pi^{(1)}$ corresponding to the elastic and solvation components. This

285 yields

$$\left\{ \begin{array}{ll} \nabla_y \cdot [\mathbf{C}_m^* : \mathcal{E}_y(\mathbf{du}_e^{(1)})] & = 0 & \text{in } Y_m \\ \mathbf{C}_m^* : [\mathcal{E}_x(\mathbf{du}_e^{(0)}) + \mathcal{E}_y(\mathbf{du}_e^{+(1)})] \cdot \mathbf{n}^+ & = \mathbf{C}_m^* : [\mathcal{E}_x(\mathbf{du}_e^{(0)}) + \mathcal{E}_y(\mathbf{du}_e^{-(1)})] \cdot \mathbf{n}^+ & \\ & = K_n \llbracket \mathbf{du}_{e,n}^{(1)} \rrbracket + K_\tau \llbracket \mathbf{du}_{e,\tau}^{(1)} \rrbracket & \text{on } \partial Y_{mf} \end{array} \right. \quad (69)$$

286 and

$$\left\{ \begin{array}{ll} \nabla_y \cdot [\mathbf{C}_m^* : \mathcal{E}_y(\mathbf{du}_\pi^{(1)})] & = 0 & \text{in } Y_m \\ \mathbf{C}_m^* : [\mathcal{E}_y(\mathbf{du}_\pi^{+(1)})] \cdot \mathbf{n}^+ & = \mathbf{C}_m^* : [\mathcal{E}_y(\mathbf{du}_\pi^{-(1)})] \cdot \mathbf{n}^+ & \\ & = K_n \llbracket \mathbf{du}_{\pi,n}^{(1)} \rrbracket + K_\tau \llbracket \mathbf{du}_{\pi,\tau}^{(1)} \rrbracket & \\ & - \sum_{i=1}^N (\alpha_f \mathbf{I} - \boldsymbol{\alpha}_{m,i}^*) dp_{f,i}^{(0)} \cdot \mathbf{n}^+ & \text{on } \partial Y_{mf} \end{array} \right. \quad (70)$$

287 where $\llbracket \mathbf{du}_{e,n}^{(1)} \rrbracket$, $\llbracket \mathbf{du}_{e,\tau}^{(1)} \rrbracket$, $\llbracket \mathbf{du}_{\pi,n}^{(1)} \rrbracket$ and $\llbracket \mathbf{du}_{\pi,\tau}^{(1)} \rrbracket$ are the normal/tangential displacement jumps corre-
 288 sponding to the elastic and solvation effects respectively. Likewise, as $\mathbf{du}_e^{(1)}$ depends linearly on
 289 $\mathcal{E}_x(\mathbf{du}^{(0)})$ we infer

$$\mathbf{du}^{(1)} = \boldsymbol{\xi} : \mathcal{E}_x(\mathbf{du}^{(0)}) + \mathbf{du}_\pi^{(1)} \quad (71)$$

290 Unlike the two-scale counterpart in (23), where the third-order tensor consists of a purely geometrical
 291 quantity, here the third-order tensor $\boldsymbol{\xi}$ also incorporates dependence on the non-linear joint BB-stiffness
 292 which brings indirect dependence on the partial gas pressures

$$\left\{ \begin{array}{ll} \nabla_y \cdot [\mathbf{C}_m^* : \mathcal{E}_y(\boldsymbol{\xi})] & = 0 & \text{in } Y_m \\ \mathbf{n}^+ \cdot \mathbf{C}_m^* : [\mathbb{I} + \mathcal{E}_y(\boldsymbol{\xi}^+)] & = \mathbf{n}^+ \cdot \mathbf{C}_m^* : [\mathbb{I} + \mathcal{E}_y(\boldsymbol{\xi}^-)] & \\ & = K_n \llbracket \boldsymbol{\xi}_n \rrbracket + K_\tau \llbracket \boldsymbol{\xi}_\tau \rrbracket & \text{on } \partial Y_{mf} \end{array} \right. \quad (72)$$

293 with $[[\boldsymbol{\xi}_n]] = \mathbf{n}^+ (\mathbf{n}^+ \cdot \boldsymbol{\xi}^+ + \mathbf{n}^- \cdot \boldsymbol{\xi}^-)$ and $[[\boldsymbol{\xi}_\tau]] = \boldsymbol{\xi}^+ - \boldsymbol{\xi}^- - [[\boldsymbol{\xi}_n]]$. Thus, defining the total macroscopic
 294 stress $\boldsymbol{\sigma}_T^{(0)}$ as the average of $\boldsymbol{\sigma}_m^{(0)}$ ($\boldsymbol{\sigma}_T^{(0)} = \langle \boldsymbol{\sigma}_m^{(0)} \rangle$), by integrating (66d) over Y and using (71) and (66)
 295 gives

$$\nabla_x \cdot d\boldsymbol{\sigma}_T^{(0)} = 0$$

where

$$d\boldsymbol{\sigma}_T^{(0)} = \mathbb{C}^{eff} : \boldsymbol{\mathcal{E}}_x(d\mathbf{u}^{(0)}) + \langle \mathbf{C}_m^* : \boldsymbol{\mathcal{E}}_y(d\mathbf{u}_\pi^{(1)}) \rangle - \sum_{i=1}^N \boldsymbol{\alpha}_{m,i}^* dp_{f,i}^{(0)} \quad (73)$$

296 with the three-scale effective elasticity tensor inheriting the same dependence on $\boldsymbol{\xi}$ of the two-scale
 297 problem

$$\mathbb{C}^{eff} = \mathbf{C}_m^* : \langle [\mathbb{I} + \boldsymbol{\mathcal{E}}_y(\boldsymbol{\xi})] \rangle \quad (74)$$

298 which brings extra dependence on fluid pressure through the BB-dependent $\boldsymbol{\xi}$. Equation (73) consists
 299 of the incremental form of the macroscopic effective stress principle. It is remarkable to see that, in
 300 contrast to the linear poroelastic case, solvation forces do not limit the fluid pressure effects to the
 301 Biot-Willis term but also affect the effective stress.

302 We are now left to compute perturbations in the volume fraction of the cleats $d\phi_{cleat}$ induced by
 303 pore pressure changes. To this end, we begin by computing variations in the cleat aperture profile
 304 $H(\mathbf{y})$ which is engendered by the jump of the normal fluctuation displacements $\mathbf{u}^{(1)}$. From (71) this
 305 yields

$$dH = \mathbf{n}^+ \cdot [[\boldsymbol{\xi}]] : \boldsymbol{\mathcal{E}}_x(d\mathbf{u}^{(0)}) + \mathbf{n}^+ \cdot [[d\mathbf{u}_\pi^{(1)}]] \quad (75)$$

with

$$\begin{aligned} \llbracket \boldsymbol{\xi} \rrbracket &= \boldsymbol{\xi}^+ - \boldsymbol{\xi}^- \\ \llbracket \mathbf{d}\mathbf{u}_\pi^{(1)} \rrbracket &= \mathbf{d}\mathbf{u}_\pi^{(1)+} - \mathbf{d}\mathbf{u}_\pi^{(1)-} \end{aligned} \quad (76)$$

306 Hence, integration over the cleat/matrix interface ∂Y_{mf} within each cell furnishes

$$d\phi_{cleat} = \frac{1}{|Y|} \int_{\partial Y} dH \, d\Gamma \quad (77)$$

307 Thus, by combining the above results we have from the divergence theorem and periodicity

$$d\phi_{cleat} = - \left[\langle \nabla_y \cdot \boldsymbol{\xi} \rangle : \boldsymbol{\mathcal{E}}_x \left(\mathbf{d}\mathbf{u}^{(0)} \right) + \langle \nabla_y \cdot \mathbf{d}\mathbf{u}_\pi^{(1)} \rangle \right] \quad (78)$$

308 The above incremental relation provides the desired result for any nanopore geometry.

309 3.4.3 Application to spherical-nanopore geometry

310 The aforementioned isotropic representation for the solvation force also allows to simplify the three-
311 scale closure relations for the poromechanical coefficients. In a similar fashion to the local problem
312 (72) for the third-order characteristic function $\boldsymbol{\xi}$, we introduce the three-scale vectorial function $\boldsymbol{\eta}$.

$$\left\{ \begin{array}{ll} \nabla_y \cdot [\mathbf{C}_m^* : \boldsymbol{\mathcal{E}}_y(\boldsymbol{\eta})] &= 0 & \text{in } Y_m \\ \mathbf{C}_m^* : \boldsymbol{\mathcal{E}}_y(\boldsymbol{\eta}^+) \cdot \mathbf{n}^+ &= \mathbf{C}_m^* : \boldsymbol{\mathcal{E}}_y(\boldsymbol{\eta}^-) \cdot \mathbf{n}^+ \\ &= K_n \llbracket \boldsymbol{\eta}_n \rrbracket + K_\tau \llbracket \boldsymbol{\eta}_\tau \rrbracket - \mathbf{n}^+ & \text{on } \partial Y_{mf} \end{array} \right. \quad (79)$$

313 with $\llbracket \boldsymbol{\eta}_n \rrbracket = \mathbf{n}^+ (\mathbf{n}^+ \cdot \boldsymbol{\eta}^+ + \mathbf{n}^- \cdot \boldsymbol{\eta}^-)$ and $\llbracket \boldsymbol{\eta}_\tau \rrbracket = \boldsymbol{\eta}^+ - \boldsymbol{\eta}^- - \llbracket \boldsymbol{\eta}_n \rrbracket$. Under the spherical representation for
314 the scalar $\alpha_{m,i}^*$ in (59), we can explore the above definition along with the linearity in (70) to reduce

315 (71) to the form

$$\mathbf{du}^{(1)} = \boldsymbol{\xi} : \boldsymbol{\mathcal{E}}_x(\mathbf{du}^{(0)}) + \boldsymbol{\eta} \sum_{i=1}^N (\alpha_f - \alpha_{m,i}^*) \mathbf{d}p_{f,i}^{(0)} \quad (80)$$

316 In addition, the reduced representation for \mathbf{u}_π^1 in the last term in r.h.s can be combined with (73) to
317 infer for the total stress

$$\mathbf{d}\boldsymbol{\sigma}_T^{(0)} = \mathbb{C}^{eff} : \boldsymbol{\mathcal{E}}_x(\mathbf{du}^{(0)}) - \sum_{i=1}^N [\bar{\boldsymbol{\alpha}}(\alpha_f - \alpha_{m,i}^*) + \alpha_{m,i}^* \mathbf{I}] \mathbf{d}p_{f,i}^{(0)} \quad (81)$$

318 with

$$\bar{\boldsymbol{\alpha}} := -\langle \mathbf{C}_m^* : \boldsymbol{\mathcal{E}}_y(\boldsymbol{\eta}) \rangle = -\langle \boldsymbol{\nabla}_y \cdot \boldsymbol{\xi} \rangle \quad (82)$$

319 The last equality between the characteristic functions $\boldsymbol{\eta}$ and $\boldsymbol{\xi}$ is well established in the traditional
320 context of poroelasticity where it leads to symmetry in the governing equations (see e.g. [32]). The
321 extension of such property to the present more complex case, with underlying dependence on the
322 BB-stiffness, requires further elaboration (see A).

The fluid pressure dependent macroscopic effective stress is defined as

$$\boldsymbol{\sigma}_{eff}^{(0)} := \mathbb{C}^{eff} : \boldsymbol{\mathcal{E}}_x(\mathbf{du}^{(0)}) \quad (83)$$

323 whereas the Biot-Willis parameter reads as

$$\begin{aligned} \boldsymbol{\alpha}_i^T &:= \bar{\boldsymbol{\alpha}}(\alpha_f - \alpha_{m,i}^*) + \alpha_{m,i}^* \mathbf{I} \\ &= \underbrace{\alpha_f \bar{\boldsymbol{\alpha}} + \alpha_m (\mathbf{I} - \bar{\boldsymbol{\alpha}})}_{\text{Non-linear poroelasticity}} - \underbrace{(\gamma_i + \nu \beta_i) (\mathbf{I} - \bar{\boldsymbol{\alpha}})}_{\text{Solvation effects}} \end{aligned} \quad (84)$$

324 The above underlying decomposition suggests the additive sum of the effects stemming from poroelas-
 325 ticity in conjunction with the BB effects in the cleats, and the contribution arising from the solvation
 326 force. In particular, unlike poroelasticity, the magnitude of the latter swelling component is not
 327 constrained to unitary interval.

328 Finally, we address the modeling of the perturbations in cleat porosity $H(\mathbf{y})$ induced by increment in
 329 pore pressure. By incorporating the jumps in the decomposition (80) for the displacement fluctuations
 330 we have

$$dH = \mathbf{n}^+ \cdot \llbracket \boldsymbol{\xi} \rrbracket : \boldsymbol{\mathcal{E}}_x(\mathbf{d}\mathbf{u}^{(0)}) + \mathbf{n}^+ \cdot \llbracket \boldsymbol{\eta} \rrbracket \sum_{i=1}^N (\alpha_f - \alpha_{m,i}^*) dp_{f,i}^{(0)} \quad (85)$$

331 which by the divergence theorem leads to the incremental cleat volume fraction ϕ_{cleat} given by

$$\begin{aligned} d\phi_{cleat} &= - \left[\langle \nabla_{\mathbf{y}} \cdot \boldsymbol{\xi} \rangle : \boldsymbol{\mathcal{E}}_x(\mathbf{d}\mathbf{u}^{(0)}) + \langle \nabla_{\mathbf{y}} \cdot \boldsymbol{\eta} \rangle \sum_{i=1}^N (\alpha_f - \alpha_{m,i}^*) dp_{f,i}^{(0)} \right] \\ &= \bar{\boldsymbol{\alpha}} : \boldsymbol{\mathcal{E}}_x(\mathbf{d}\mathbf{u}^{(0)}) - \langle \nabla_{\mathbf{y}} \cdot \boldsymbol{\eta} \rangle \sum_{i=1}^N (\alpha_f - \alpha_{m,i}^*) dp_{f,i}^{(0)} \end{aligned} \quad (86)$$

332 When compared to the more general constitutive law (78), the above result explores the linear decom-
 333 position underlying $\mathbf{u}_{\pi}^{(1)}$ to obtain a reduced representation.

334 3.5 Summary of three-scale poromechanical model

335 We are now in position of stating the three-scale poromechanical model in the case of spherical
 336 nanopores. Given the set of parameters $\{\mathbf{c}_s, \boldsymbol{\alpha}_m, \phi_m^{ref}, k_s, \boldsymbol{\gamma}_i, \boldsymbol{\nu}\}$ for the coal matrix, compute the
 337 homogenized parameters $\{\mathbf{C}_m^*, \boldsymbol{\alpha}_{m,i}^*, \beta_i\}$ by invoking the two-scale closure relations (25), (50), and
 338 (62).

339 Further, given the pair of BB-stiffness $\{K_n, K_{\tau}\}$, solve (72) and (79) for the pressure-dependent
 340 characteristic functions $\boldsymbol{\xi}$ and $\boldsymbol{\eta}$ and (82) and for $\bar{\boldsymbol{\alpha}}$. Our three-scale incremental poromechanical

341 model consists in, given the values of the macroscopic poromechanical variables at the reference
 342 configuration along with the perturbations in the fluid pressure field of each gas $p_{f,i}^{(0)}$, compute the the
 343 triplet increments $\{\mathbf{d}\boldsymbol{\sigma}_T^{(0)}, \mathbf{d}\mathbf{u}^{(0)}, \mathbf{d}\phi_{cleat}\}$ satisfying

$$\left\{ \begin{array}{l} \nabla_x \cdot \mathbf{d}\boldsymbol{\sigma}_T^{(0)} = 0 \\ \mathbf{d}\boldsymbol{\sigma}_T^{(0)} = \mathbb{C}^{eff} : \boldsymbol{\mathcal{E}}_x(\mathbf{d}\mathbf{u}^{(0)}) - \sum_{i=1}^N \boldsymbol{\alpha}_i^T \mathbf{d}p_{f,i}^{(0)} \\ \mathbf{d}\phi_{cleat} = \bar{\boldsymbol{\alpha}} : \boldsymbol{\mathcal{E}}_x(\mathbf{d}\mathbf{u}^{(0)}) - \langle \nabla_y \cdot \boldsymbol{\eta} \rangle \sum_{i=1}^N (\alpha_f - \alpha_{m,i}^*) \mathbf{d}p_{f,i}^{(0)} \end{array} \right.$$

344 with the homogenized coefficients $\{\mathbb{C}^{eff}, \boldsymbol{\alpha}_i^T\}$ given by (74 and (84).

345 Note that for a non-porous matrix ($\alpha_m \simeq 0$), in the absence of solvation force effects ($\gamma_i = \nu \simeq 0$)
 346 and a Biot coefficient of the cleats $\alpha_f = 1$, the symmetry of the Biot relations is recovered:

$$\mathbf{d}\boldsymbol{\sigma}_T^{(0)} = \mathbb{C}^{eff} : \boldsymbol{\mathcal{E}}_x(\mathbf{d}\mathbf{u}^{(0)}) - \bar{\boldsymbol{\alpha}} \mathbf{d}p_f^{(0)} \quad (87)$$

$$\mathbf{d}\phi_{cleat} = \bar{\boldsymbol{\alpha}} : \boldsymbol{\mathcal{E}}_x(\mathbf{d}\mathbf{u}^{(0)}) - \langle \nabla_y \cdot \boldsymbol{\eta} \rangle \mathbf{d}p_f^{(0)} \quad (88)$$

347 4 Computational Simulations

348 Hereafter we present numerical experiments of the constitutive response of the homogenized coeffi-
 349 cients along with preliminary simulations of a CO₂ injection in a coalbed methane reservoir.

350 4.1 Two-scale coefficients for the coal matrix

351 We begin by presenting the numerical results for the two-scale problem by quantifying the effects
 352 of the solvation force upon the magnitude of the homogenized coefficients in the coal matrix. In
 353 the simulations that follow, we consider the periodic cell with a single nanopore at the center with a
 354 given matrix porosity ϕ_m and pore radius R filled by CO₂. To simplify notation, the single subscript

355 $i = \text{CO}_2$ is hereafter omitted. In addition, for a given matrix porosity ϕ_m the traditional poromechanical
 356 constant values are assessed using Mori-Tanaka approach [34].

357 The input data for the simulations that follow are shown in Table 1. **Particularly, the pair of elastic**
 358 **parameters of the solid phase $\{v_s, k_s\}$ are typically selected within the range of values for a coal matrix**
 359 **(see [35]).** Our first target is to quantify the sensitivity of the solvation force with changes in pressure
 p_m which is dictated by the coefficient γ . In Figure 6a we display the behavior of γ with changes in

Parameters	Unit	Value
Temperature T	K	318
Molecular diameter d_{CO_2}	m	3.9×10^{-10}
Pore diameter $D_p = 2R$	m	$5 d_{\text{CO}_2}$
Reference bulk pressure p_m^{ref}	MPa	0.5
Bulk modulus of solid phase k_s	GPa	4.5
Poisson coefficient of solid phase v_s		0.4
Reference matrix porosity ϕ_m	%	18.5
Biot coefficient of matrix α_m		0.5
Young's modulus of matrix E_m	GPa	1.86
Poisson's ratio of matrix v_m		0.36

Table 1: Parameters used in numerical simulations **of the two-scale parameters.**

360

361 the CO_2 pressure. We may observe initially a sharp decrease stemming from the abrupt appearance
 362 of attractive forces followed by a gradual increase as the effects of the solvation force tend to diminish
 363 with the increase in gas pressure. Such a latter behavior induces swelling of the matrix blocks leading
 364 to the closure of the cleats. Further, by invoking (50), the aforementioned behavior in γ engenders
 365 perturbations in the magnitude of the modified Biot coefficient of the matrix as shown in Figure 6b .
 366 It is remarkable to see the tremendous increase in α_m^* for low pressure values which allows the coal
 367 matrix to sustain substantial increase in gas pressure during CO_2 injection. After reaching the peak,
 368 the effects of the solvation force tend to decrease in the range of high gas pressure leading to a decrease
 369 in α_m^* but nevertheless still bigger than unit, which is commonly envisioned as an upper bound in
 370 traditional poroelasticity.

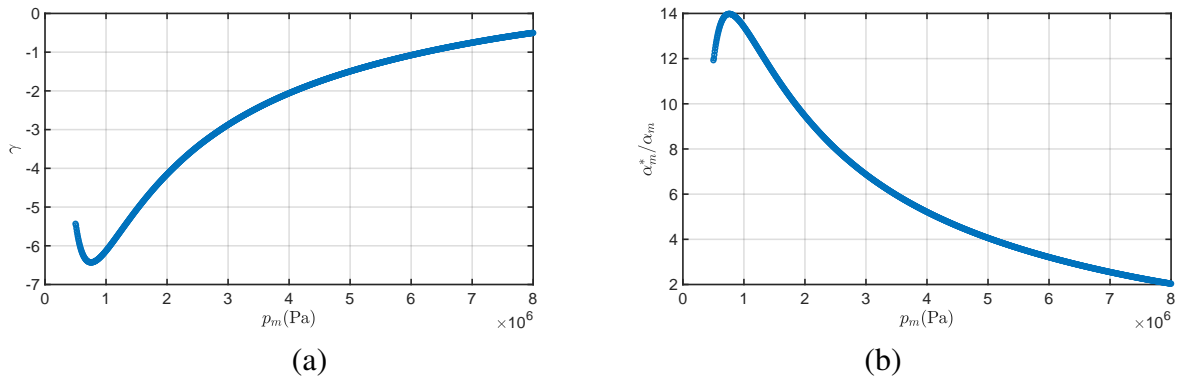


Figure 6: Dependence of γ (a); and α_m^*/α_m (b) on the CO₂ pressure.

371 We display the bulk modulus $9K_m^* := \mathbf{C}_m^* : \mathbf{I} : \mathbf{I}$ as a function of the pore diameter parametrized by
 372 the gas pressure. By comparing the microscopic representations (50) and (49), we may observe that,
 373 unlike α_m^* , which is highly sensitive to γ_i , the profiles of K_m^* show weaker dependence on both pore
 374 diameter and gas pressure as depicted in Figure 7. The dependence of the ratio K_m^*/K_m with increase
 375 in pore size shows mild deviations from the unit value, which suggests adopting the approximation
 376 $\mathbf{C}_m^* \simeq \mathbf{C}_m$ in the subsequent simulations. In addition, owing to the volumetric influence of the
 377 solvation force in the isotropic scenario, from (59) the modified Lamé's second parameter μ_m^* remains
 378 insensitive to solvation effects.

379 Finally, the two-scale poromechanical model is illustrated in a canonical swelling example induced
 380 by CO₂ injection. Our selected scenario comprises a coal sample immersed in a chamber filled by
 381 CO₂ at thermodynamic equilibrium under an homogeneous bulk pressure, which is increased quasi-
 382 statically and parametrized by a sequence of equilibrium states. Input parameters are shown in Table
 383 1. In Figure 8, we display the dependence of the volumetric strain of the coal sample according with
 384 the CO₂ bulk pressure. As expected, rapid increase of the volumetric strain dominates at low pressure
 385 tending asymptotically to a plateau at high pressures owing to the attenuation of the solvation force.

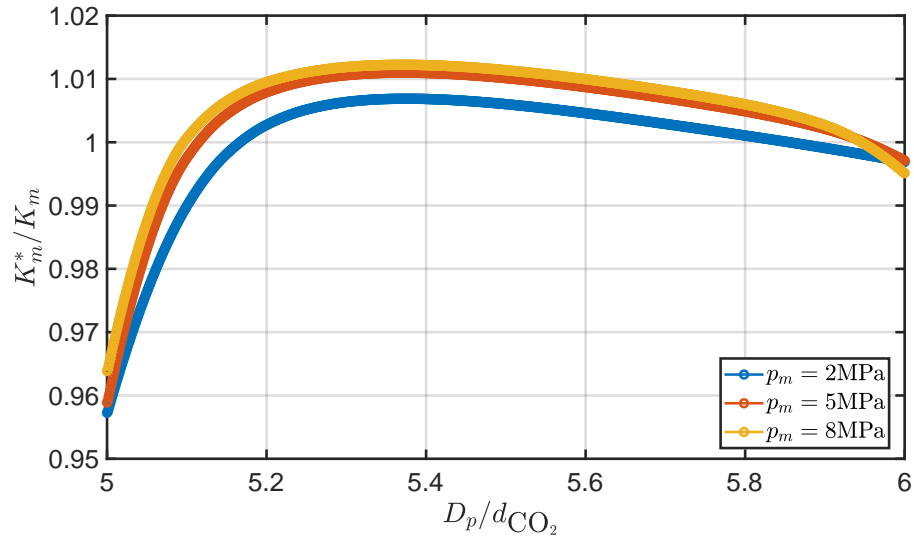


Figure 7: Dependence of K_m^*/K_m on the pore diameter for different values of the CO₂ pressure.

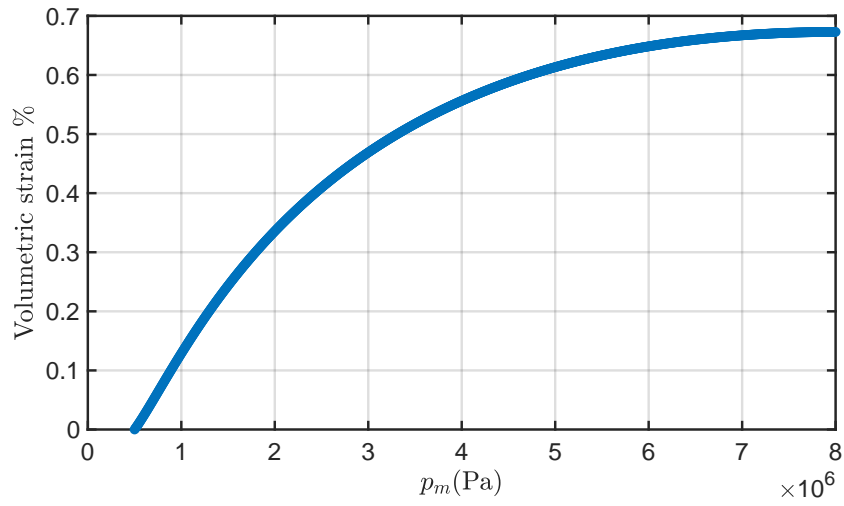


Figure 8: Volumetric strain vs CO₂ bulk pressure

386 4.2 Three-scale poromechanical parameters

387 We now proceed towards the computation of the three-scale poromechanical parameters, whose
 388 magnitude now incorporates the non-linear BB-stiffness $\{K_n, K_\tau\}$ inherent to the cleat system. Our
 389 simulations are carried out for the two cell configurations depicted in Figure 9, based on a simple cross
 arrangement and two face/butt cleats [4]. We remark that, in spite of selecting simple cell-geometries,

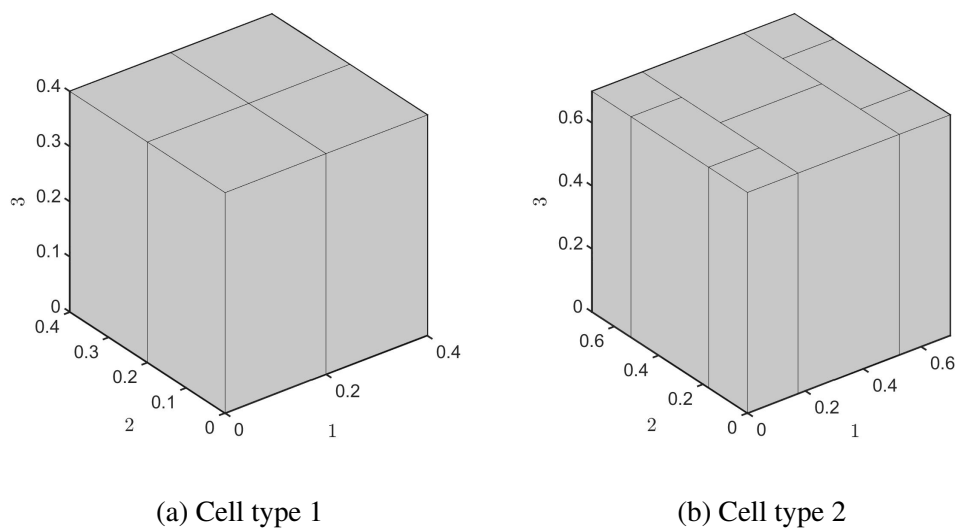


Figure 9: Cell configurations exhibiting cross arrangement and face/butt cleats

390

391 the upscaling may lead to a highly anisotropic medium induced by the distinct properties between the
 392 two orthogonal cleat families (see B). In addition, the tangential cleat stiffness K_τ usually exhibits a
 393 different constitutive response compared to the normal counterpart K_n leading to additional sources
 394 of anisotropy. **For the sake of simplicity, the cleat parameters are suitably chosen in order to enforce**
 395 **transverse isotropy of the homogenized medium (see Table 2). The other parameters associated with**
 396 **the matrix are presented in Table 1.**

397

Both configurations in Figure 9 have the same initial cleat porosity and BB-stiffness parameters.
 398 The geometry is chosen to ensure the continuity of the cleat network. Periodic conditions are imposed
 399 on the boundaries. For cell 1, the auxiliary problems (72) and (79) admit the analytical solutions

Parameters	Unit	Value
Initial normal stiffness K_{ni} [36]	GPa/m	6.6
Initial tangential stiffness $K_{\tau i}$ [36]	GPa/m	6.6
Initial aperture V_m [36]	m	107×10^{-6}
Reference normal stiffness K_n^{ref}	GPa/m	1111
Reference tangential stiffness K_τ^{ref}	GPa/m	6.6
Reference aperture V_m^{ref}	m	8.25×10^{-6}
Cleat porosity at reference ϕ_{cleat}^{ref}	%	0.41

Table 2: Parameters used in numerical simulations for the cleats.

400 given in B and C. Due to the complexity of the cleat network in the cell 2, calculations are performed
 401 numerically using the Structural Mechanics Module implemented in COMSOL Multiphysics software.

402 In Figure 10 we plot the horizontal ($\alpha_{11}^T = \alpha_{22}^T$) and vertical (α_{33}^T) components of the macroscopic
 403 Biot-Willis coefficient as a function of the gas pressure for cell type-1. Firstly, α^T augments in
 404 magnitude due to the increase of the solvation force for low pressures, reaching a peak in the vicinity
 405 of the value of 1 MPa, and subsequently followed by a gradual decrease as the solvation force tends to
 406 diminish with the CO₂ pressure build-up. In addition, the cleat closure driven by the raise in pressure
 407 increases the stiffness of the fractured coal matrix, as shown in Figure 10b which displays the evolution
 of the horizontal stiffness C_{1111}^{eff} with the gas pressure.

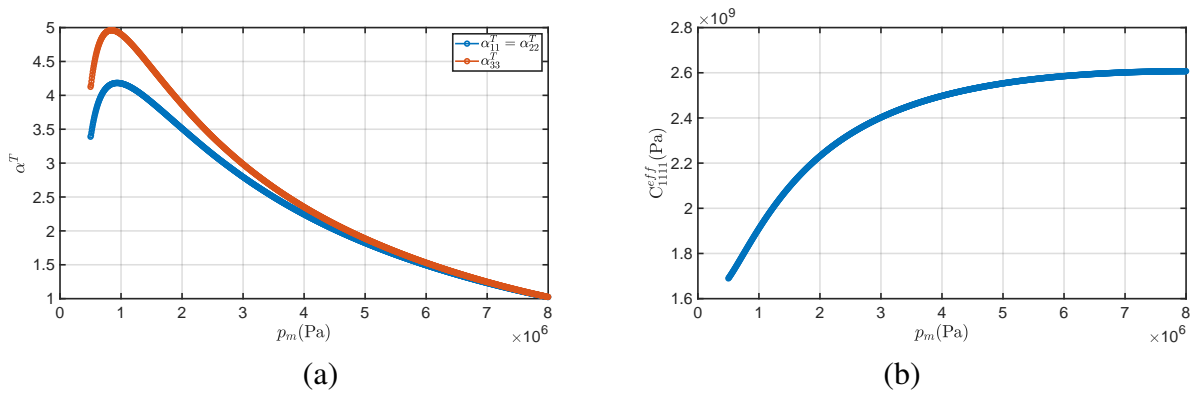


Figure 10: Dependence of (a) α^T and (b) C_{1111}^{eff} on the gas pressure

408

409 We now analyze the effects of the cell geometry on cleat porosity. Considering both arrangements

410 in Figure 9, in Figure 11 we display the dependence of cleat closure on the gas pressure. Despite
 411 both cells exhibiting strong dissimilarities in local geometry, we observe minor differences between
 412 the two arrangements for a wide-range of pore pressures. Such a result motivates the use of a simple
 type 1 cell to reproduce patterns commonly encountered in more complex geometries.

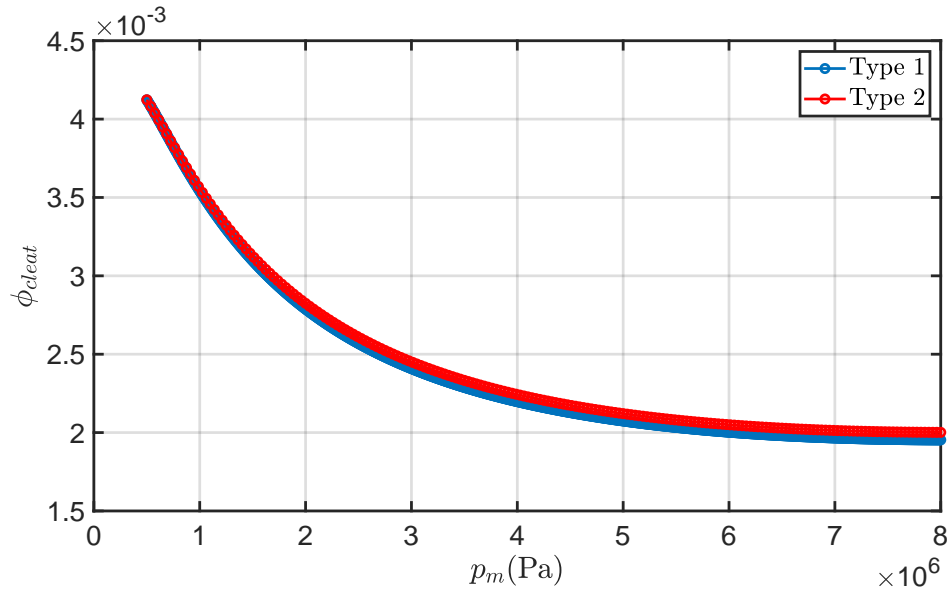


Figure 11: Decrease of ϕ_{cleat} with CO₂ pressure build-up for two cell configurations

413

414 **4.3 Macroscopic example of CO₂ injection**

415 We now illustrate the performance of the three-scale model proposed herein in a macroscopic example
 416 of CO₂ sequestration. The sketch in Figure 12 shows two injection wells located at opposite corners
 417 of the reservoir. The calculations are performed in a 100 m x 100 m x 2 m (sugar-box reservoir).
 418 Our subsequent calculations are carried out in COMSOL Multiphysics software, considering zero
 419 displacement at the external boundaries, so that matrix and cleats interchange the perturbations in
 420 strain. The input parameters used in the simulations are listed in Table 1 and Table 2.

421 It should be noted that the full coupling between hydrodynamics and poromechanics is not con-

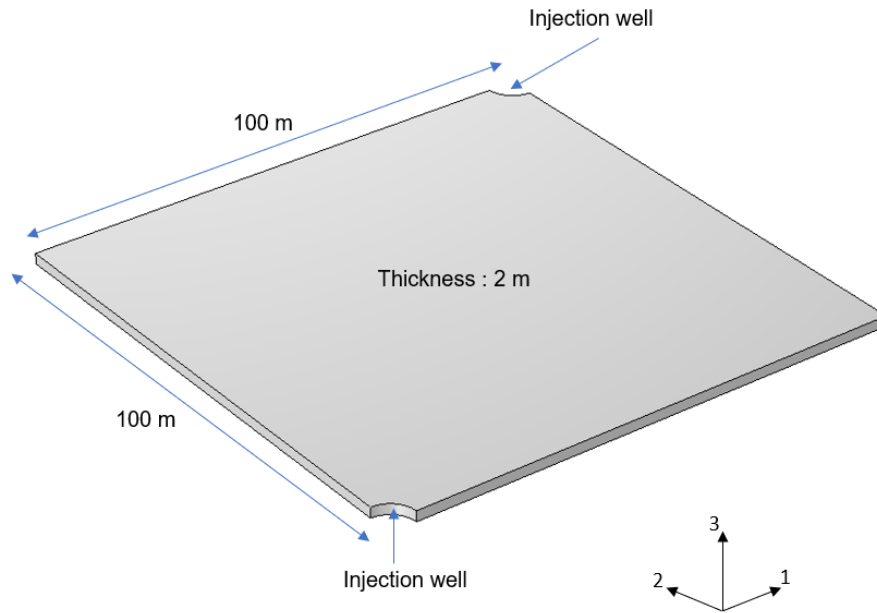


Figure 12: Sketch of the macroscopic example of CO₂ injection

422 sidered in this work. Hence, the input pressure evolving profiles shown in Figure 13 are assumed
 423 solution of a linear diffusion equation at some discrete times considering initial and well pressures
 424 $p_f(t = 0) = 0.5$ MPa and $p_f = 8$ MPa respectively. In regards to the boundary conditions for the
 425 flow problem, Dirichlet conditions for the pressure are enforced at the wells combined with no-flux
 426 conditions at the edges of the reservoir. The horizontal component profile of α_{11}^T is shown in Figure 14
 427 for two times. We can observe a peak in four orders of magnitude for low pressure values compared to
 428 the unit of incompressible poroelasticity. The pressure build-up tends to further reduce the magnitude
 429 particularly propagating from the injection wells. For large times, lower and higher values of the
 430 horizontal component of α^T tend to clusterize in the vicinity of the injectors and in the center of the
 431 reservoir respectively.

432 Figure 15 and Figure 16 depict the variability of the macroscopic stiffness \mathbb{C}_{1111}^{eff} and cleat porosity
 433 ϕ_{cleat} . Near the injection well, in contrast to non-swelling media, the cleat porosity decreases counter-
 434 intuitively implying in strong decrease in permeability and increase in macroscopic stiffness induced

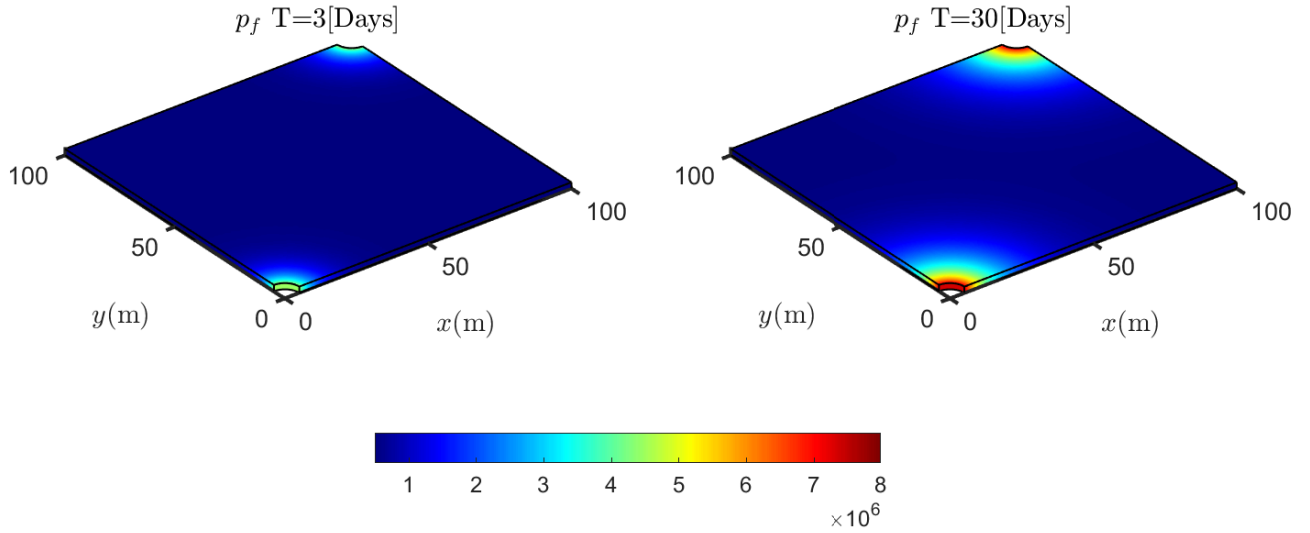


Figure 13: Input CO₂ pressure profiles in the reservoir, computed from a simple diffusion equation for different times

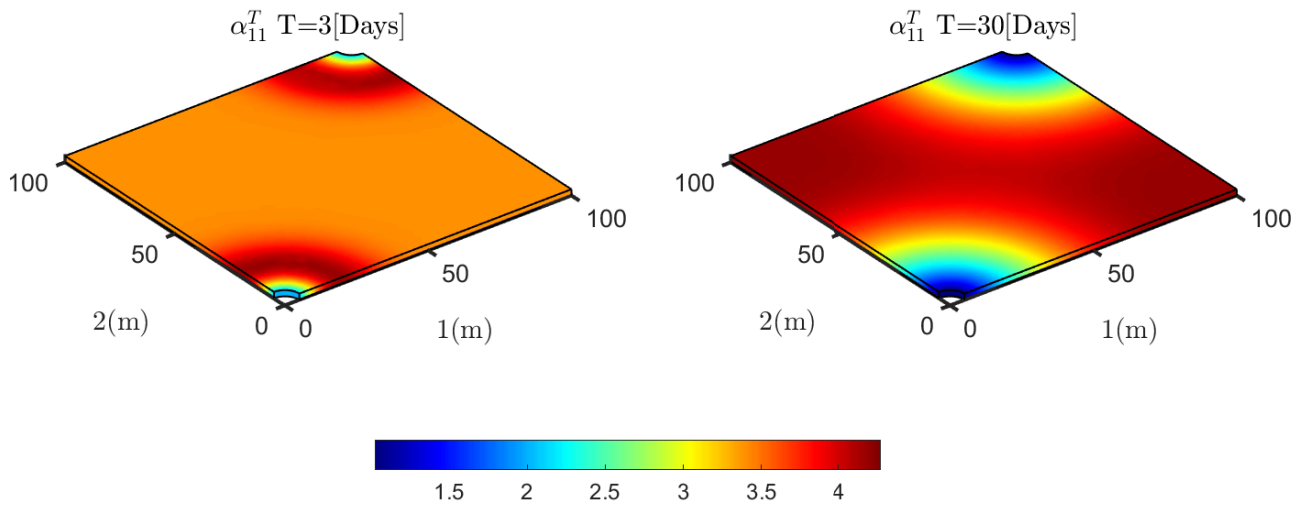


Figure 14: Variability of α_{11}^T for different times

435 by matrix swelling. Subsequently, as time and gas pressure increase, such a low porosity sub-region
 436 is propagated towards the center of the reservoir mainly through the diagonal connecting the two
 437 injection wells and afterwards spreading to other locations. It is remarkable to see the essential role
 438 played by the non-linear Barton-Bandis law to counterbalance the cleat closure due to matrix swelling.
 439 The non-linear behavior of the stress in the cleat network is crucial to preserve residual values of the
 cleat porosity consequently avoiding interpenetration of adjacent matrix blocks.

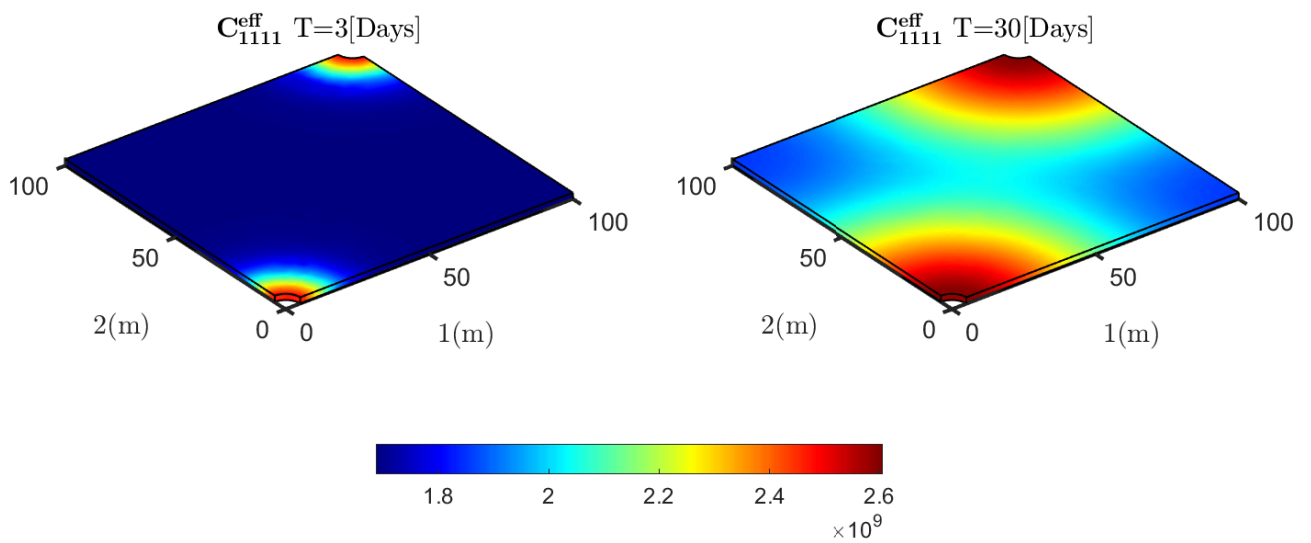


Figure 15: Variability of C_{1111}^{eff} for different times

440

441 5 Conclusions

442 We developed an innovative three-scale poromechanical model for coalbed methane reservoirs com-
 443 posed of the coal matrix containing nanopores intertwined by a network of lower dimensional cleats
 444 saturated by a gas mixture. By exploring the DFT approach, the solvation force induces modified
 445 effective stress principle including the effects of the attractive solvation forces. Within the framework
 446 of the incremental formulation, the effects of the solvation force are mainly manifested in a modified
 447 Biot-Willis parameter with magnitude dictated by the sensitivity of the solvation force with changes

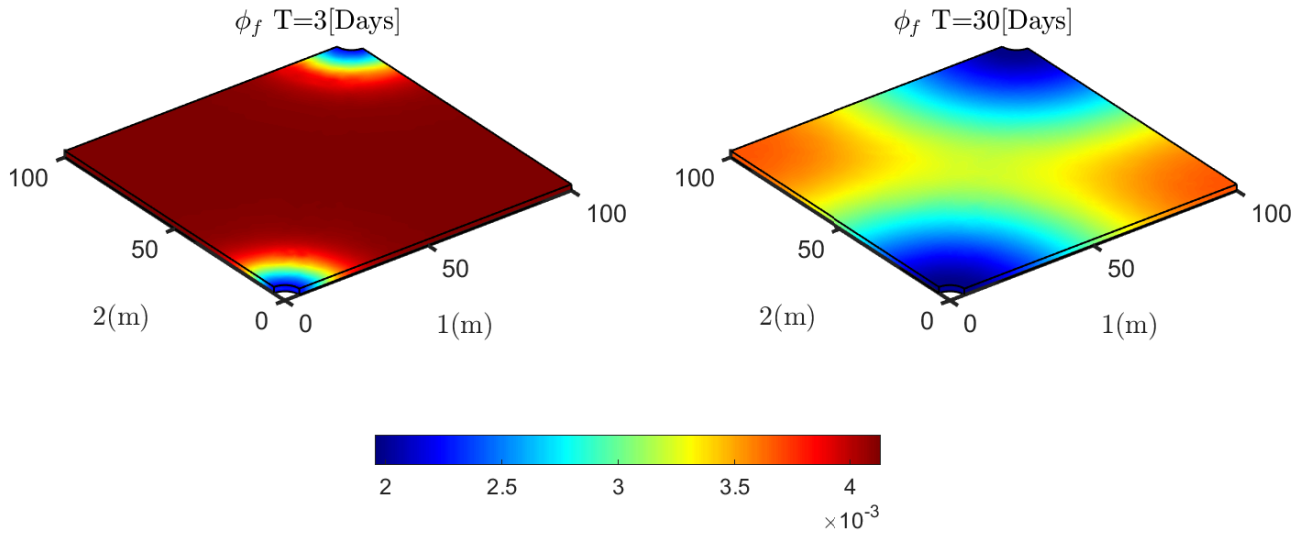


Figure 16: Variability of ϕ_{cleat} for different times

448 in gas pressure. In particular, at low pressures, we observed a tremendous increase in $\alpha_{m,i}^*$, which may
 449 achieve up to ten times the unit value of classical poroelasticity. Such a non-intuitive pattern suggests
 450 that, for a fixed reservoir volume, small variations in the pressure in the cleats may imply in large
 451 variations in total stress of the matrix.

452 In contrast to previous approaches, the cleat system is supposed to withstand normal and tangential
 453 stresses, which act to counterbalance the effects of the solvation force in the matrix blocks. By
 454 postulating a non-linear hyperbolic law in the sense of Barton and Bandis for the normal stress, within
 455 the framework of reiterated homogenization, the role of the BB component is manifested in the profile
 456 of the characteristic functions. In this context, the increase in the normal BB-stiffness of the cleats
 457 tends to reduce the jumps of these functions at the matrix/cleat interfaces which are propagated to the
 458 macroscale in terms of perturbations in the macroscopic poromechanical parameters.

459 In addition to the overall three-scale decomposition of the total macroscopic stress, we constructed
 460 a new constitutive law for the Lagrangian cleat porosity. Moreover, a new undrained-type coefficient
 461 naturally arises in the constitutive response of the cleat porosity which plays a central role in the cleat
 462 permeability response. The dependence of the two- and three-scale homogenized poromechanical

463 coefficients on the gas pressure is reconstructed numerically quantifying precisely the influence of the
464 solvation force.

465 To the authors best knowledge, the paper is the first attempt to address the important mechanical
466 interaction between solvation force and BB restoring stresses in nanoporous jointed rocks. Ongoing
467 work will incorporate the full coupling with the flow equations in the cleat system.

468 Acknowledgement

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470 computer resources necessary to perform the numerical simulations. Q D Ha also thanks the ‘Grand
471 Est’ Region for the research grant allowing him to carry out his PhD thesis.

472 A Proof of Symmetry

473 In the classical poromechanics, it has been proved that [32]

$$\langle \nabla \cdot \xi \rangle = \langle \sigma(\eta) \rangle \quad (89)$$

474 The aim of this appendix is to verify this relation in the case of non-linear BB law for the mechanical
475 behavior of the cleats.

476 ξ is a third-order tensor. If the two last indices p and q are kept fixed, from (72), by using tensor
477 notation the problem for the vector ξ^{pq} is written as

$$\left\{ \begin{array}{ll} \frac{\partial}{\partial y_j} \left[C_{ijkl}^* \mathcal{E}_{kl}(\xi^{pq}) \right] = 0 & \text{in } Y_m \\ C_{ijkl}^* \left[\mathcal{E}_{kl}(\xi^{pq+}) + \delta_{kp} \delta_{lq} \right] n_j^+ = C_{ijkl}^* \left[\mathcal{E}_{kl}(\xi^{pq-}) + \delta_{kp} \delta_{lq} \right] n_j^+ & \\ = K_n \llbracket \xi_i^{pq} \rrbracket_n + K_\tau \llbracket \xi_i^{pq} \rrbracket_\tau & \text{on } \partial Y_{fm} \end{array} \right. \quad (90)$$

478 with $[[\xi^{pq}]]_n = \mathbf{n}^+ (\mathbf{n}^+ \cdot \xi^{pq+} + \mathbf{n}^- \cdot \xi^{pq-})$ and $[[\xi^{pq}]]_\tau = \xi^{pq+} - \xi^{pq-} - [[\xi^{pq}]]_n$ where the indices n
 479 and τ designates respectively the normal and the tangential component of the jump of ξ^{pq} on the two
 480 faces \pm of the cleat (see Figure 4).

481 The problem for the vector $\boldsymbol{\eta}$ is expressed as

$$\left\{ \begin{array}{l} \frac{\partial}{\partial y_j} [C_{ijkl}^* \mathcal{E}_{kl}(\boldsymbol{\eta})] = 0 \quad \text{in } Y_m \\ [C_{ijkl}^* : \mathcal{E}_{kl}(\boldsymbol{\eta}^+) + \delta_{ij}] n_j^+ = [C_{ijkl}^* : \mathcal{E}_{kl}(\boldsymbol{\eta}^-) + \delta_{ij}] n_j^+ \quad \text{on } \partial Y_{fm} \\ = K_n [[\eta_i]]_n + K_\tau [[\eta_i]]_\tau \end{array} \right. \quad (91)$$

482 with $[[\boldsymbol{\eta}]]_n = (\mathbf{n}^+ \cdot \boldsymbol{\eta}^+ + \mathbf{n}^- \cdot \boldsymbol{\eta}^-) \mathbf{n}^+$ and $[[\boldsymbol{\eta}]]_\tau = \boldsymbol{\eta}^+ - \boldsymbol{\eta}^- - [[\boldsymbol{\eta}]]_n$.

483 The cleat network splits the matrix Y_m into M sub-domains Y_{m_α} with $1 \leq \alpha \leq M$. For any
 484 Y -periodic displacement field \mathbf{u} satisfying on each part Y_{m_α} of the unit cell, $\nabla \cdot \boldsymbol{\sigma}(\mathbf{u}) = 0$ and for any
 485 Y -periodic vector $\boldsymbol{\omega}$ differentiable on each part Y_{m_α} , we have (noting that the normal exterior to Y_{m_α}
 486 on $\partial Y_{m_\alpha}^\pm$ is \mathbf{n}^\mp)

$$\begin{aligned} 0 &= \int_{Y_m} \frac{\partial \sigma_{ij}(\mathbf{u})}{\partial y_j} \omega_i \, dV = \sum_\alpha \int_{Y_{m_\alpha}} \frac{\partial \sigma_{ij}(\mathbf{u})}{\partial y_j} \omega_i \, dV \\ &= \sum_\alpha \int_{\partial Y_{m_\alpha}^-} \sigma_{ij}(\mathbf{u}) \omega_i^- n_j^+ \, dS + \sum_\alpha \int_{\partial Y_{m_\alpha}^+} \sigma_{ij}(\mathbf{u}) \omega_i^+ n_j^- \, dS - \sum_\alpha \int_{Y_{m_\alpha}} \sigma_{ij}(\mathbf{u}) \frac{\partial \omega_i}{\partial y_j} \, dV \\ &= - \sum_\alpha \int_{\partial Y_{m_\alpha}} \sigma_{ij}(\mathbf{u}) [[\omega_i]] n_j^+ \, dS - \sum_\alpha \int_{Y_{m_\alpha}} \sigma_{ij}(\mathbf{u}) \frac{\partial \omega_i}{\partial y_j} \, dV \end{aligned} \quad (92)$$

487 with $\partial Y_{m_\alpha}^+ \equiv \partial Y_{m_\alpha}^-$ and $[[\boldsymbol{\omega}]] = \boldsymbol{\omega}^+ - \boldsymbol{\omega}^-$.

488 Finally using the symmetry of $\boldsymbol{\sigma}(\mathbf{u}) = \mathbf{C}^* : \boldsymbol{\mathcal{E}}(\mathbf{u})$ gives

$$\sum_\alpha \int_{Y_{m_\alpha}} C_{ijkl}^* \mathcal{E}_{kl}(\mathbf{u}) \mathcal{E}_{ij}(\boldsymbol{\omega}) \, dV = - \sum_\alpha \int_{\partial Y_{m_\alpha}^+} \sigma_{ij}(\mathbf{u}) [[\omega_i]] n_j^+ \, dS \quad (93)$$

Applying the preceding relation for $\mathbf{u} = \boldsymbol{\eta}$ and $\boldsymbol{\omega} = \xi^{pq}$, using the boundary condition (91) on ∂Y_{fm} ,

the orthogonality of the normal and tangential components, the divergence theorem and the periodicity, we have

$$\begin{aligned}
& \sum_{\alpha} \int_{Y_{m\alpha}} \mathbf{C}_{ijkl}^* \mathcal{E}_{kl}(\boldsymbol{\eta}) \mathcal{E}_{ij}(\boldsymbol{\xi}^{pq}) \, dV \\
&= - \sum_{\alpha} \int_{\partial Y_{m\alpha}} (-n_i^+ + K_n \llbracket \eta_i \rrbracket_n + K_{\tau} \llbracket \eta_i \rrbracket_{\tau}) (\llbracket \xi_i^{pq} \rrbracket_n + \llbracket \xi_i^{pq} \rrbracket_{\tau}) \, dS \\
&= - \sum_{\alpha} \int_{\partial Y_{m\alpha}} (-n_i^+ \llbracket \xi_i^{pq} \rrbracket + K_n \llbracket \eta_i \rrbracket_n \llbracket \xi_i^{pq} \rrbracket_n + K_{\tau} \llbracket \eta_i \rrbracket_{\tau} \llbracket \xi_i^{pq} \rrbracket_{\tau}) \, dS \\
&= - \sum_{\alpha} \int_{Y_{m\alpha}} \frac{\partial \xi_i^{pq}}{\partial y_i} \, dV - \sum_{\alpha} \int_{\partial Y_{m\alpha}} (K_n \llbracket \eta_i \rrbracket_n \llbracket \xi_i^{pq} \rrbracket_n + K_{\tau} \llbracket \eta_i \rrbracket_{\tau} \llbracket \xi_i^{pq} \rrbracket_{\tau}) \, dS
\end{aligned} \tag{94}$$

Exploring the same relation but now with $\mathbf{u} = \boldsymbol{\xi}^{pq}$ and $\boldsymbol{\omega} = \boldsymbol{\eta}$ we obtain

$$\begin{aligned}
& \sum_{\alpha} \int_{Y_{m\alpha}} \mathbf{C}_{ijkl}^* \mathcal{E}_{kl}(\boldsymbol{\xi}^{pq}) \mathcal{E}_{ij}(\boldsymbol{\eta}) \, dV \\
&= - \sum_{\alpha} \int_{\partial Y_{m\alpha}} (-\mathbf{C}_{ijpq}^* n_j^+ + K_n \llbracket \xi_i^{pq} \rrbracket_n + K_{\tau} \llbracket \xi_i^{pq} \rrbracket_{\tau}) (\llbracket \eta_i \rrbracket_n + \llbracket \eta_i \rrbracket_{\tau}) \, dS \\
&= - \int_{Y_m} \mathbf{C}_{ijpq}^* \mathcal{E}_{ij}(\boldsymbol{\eta}) \, dV - \sum_{\alpha} \int_{\partial Y_{m\alpha}} (K_n \llbracket \xi_i^{pq} \rrbracket_n \llbracket \eta_i \rrbracket_n + K_{\tau} \llbracket \xi_i^{pq} \rrbracket_{\tau} \llbracket \eta_i \rrbracket_{\tau}) \, dS
\end{aligned} \tag{95}$$

489 Due to the symmetry of the elastic tensor ($\mathbf{C}_{ijkl}^* = \mathbf{C}_{klij}^*$), the two terms on the l.h.s of (94) and (95)

490 are equal and therefore

$$\begin{aligned}
\int_{Y_m} \frac{\partial \xi_i^{pq}}{\partial y_i} \, dV &= \int_{Y_m} \mathbf{C}_{ijpq}^* \mathcal{E}_{ij}(\boldsymbol{\eta}) \, dV \\
\langle \boldsymbol{\nabla}_y \cdot \boldsymbol{\xi}^{pq} \rangle &= \langle \boldsymbol{\sigma}_{pq}(\boldsymbol{\eta}) \rangle
\end{aligned} \tag{96}$$

491 which is an expected result.

492 **B Analytical solution for the closure problems and effective stiff-** 493 **ness tensor**

494 Consider the cleat network immersed in the matrix phase characterized by λ and μ for the cross
495 arrangement shown in Figure 9a. The cleat (I) described by (K_n^I, K_τ^I) is located on $y_1 = \ell/2$ whereas
496 the cleat (II) with (K_n^{II}, K_τ^{II}) is placed on $y_2 = \ell/2$. The goal now is to solve the closure problem (90)
497 with

$$C_{ijkl}^* = \lambda \delta_{ij} \delta_{kl} + \mu (\delta_{ik} \delta_{jl} + \delta_{il} \delta_{jk}) \quad (97)$$

$$\mathcal{E}_{kl}(\xi^{pq}) = \frac{1}{2} \left(\frac{\partial \xi_k^{pq}}{\partial y_l} + \frac{\partial \xi_l^{pq}}{\partial y_k} \right) \quad (98)$$

498 From (74), the effective stiffness tensor reads as

$$C_{ijpq}^{eff} = C_{ijkl}^* \left(\delta_{kp} \delta_{lq} + \frac{1}{2} \left(\frac{\partial \xi_k^{pq}}{\partial y_l} + \frac{\partial \xi_l^{pq}}{\partial y_k} \right) \right) \quad (99)$$

499 The interface condition on the matrix-cleat interface for the both cleats is written as

$$\begin{aligned} & \delta_{1j} \left[\lambda \delta_{ij} \delta_{kl} + \mu (\delta_{ik} \delta_{jl} + \delta_{il} \delta_{jk}) \right] \left[\delta_{kq} \delta_{lq} + \frac{1}{2} \left(\frac{\partial \xi_k^{pq}}{\partial y_l} + \frac{\partial \xi_l^{pq}}{\partial y_k} \right) \right] \\ & = K_n^I \Delta \xi_1^{pq} \delta_{i1} + K_\tau^I \Delta \xi_2^{pq} \delta_{i2} + K_\tau^I \Delta^I \xi_3^{pq} \delta_{i3} \end{aligned} \quad (100)$$

$$\begin{aligned} & \delta_{2j} \left[\lambda \delta_{ij} \delta_{kl} + \mu (\delta_{ik} \delta_{jl} + \delta_{il} \delta_{jk}) \right] \left[\delta_{kq} \delta_{lq} + \frac{1}{2} \left(\frac{\partial \xi_k^{pq}}{\partial y_l} + \frac{\partial \xi_l^{pq}}{\partial y_k} \right) \right] \\ & = K_n^{II} \Delta^{II} \xi_2^{pq} \delta_{i2} + K_\tau^{II} \Delta^{II} \xi_1^{pq} \delta_{i1} + K_\tau^{II} \Delta^{II} \xi_3^{pq} \delta_{i3} \end{aligned} \quad (101)$$

500 Performing normal projection gives

$$\lambda + 2\mu + \lambda \left(\frac{\partial \xi_1^{11}}{\partial y_1} + \frac{\partial \xi_2^{11}}{\partial y_2} + \frac{\partial \xi_3^{11}}{\partial y_3} \right) + 2\mu \frac{\partial \xi_1^{11}}{\partial y_1} = K_n^I \Delta^I \xi_1^{11} \quad (102)$$

$$\lambda \left(1 + \frac{\partial \xi_1^{11}}{\partial y_1} + \frac{\partial \xi_2^{11}}{\partial y_2} + \frac{\partial \xi_3^{11}}{\partial y_3} \right) + 2\mu \frac{\partial \xi_2^{11}}{\partial y_2} = K_n^{II} \Delta^{II} \xi_2^{11} \quad (103)$$

501 It should be noted that there is no displacement along the third direction because of the cleats structure.

502 Combining with the periodic conditions leads to

$$\begin{aligned} \Delta^I \xi_1^{11} + \ell \frac{\partial \xi_1^{11}}{\partial y_1} &= 0 \\ \Delta^{II} \xi_2^{11} + \ell \frac{\partial \xi_2^{11}}{\partial y_2} &= 0 \end{aligned} \quad (104)$$

503 The final solutions are

$$\frac{\partial \xi_1^{11}}{\partial y_1} = - \frac{4\mu(\lambda + \mu) + (\lambda + 2\mu)K_n^{II}\ell}{4\mu(\lambda + \mu) + (\lambda + 2\mu)(K_n^I + K_n^{II})\ell + K_n^I K_n^{II} \ell^2} \quad (105)$$

$$\frac{\partial \xi_2^{11}}{\partial y_2} = - \frac{\lambda K_n^I \ell}{4\mu(\lambda + \mu) + (\lambda + 2\mu)(K_n^I + K_n^{II})\ell + K_n^I K_n^{II} \ell^2} \quad (106)$$

504 From the definition of the effective stiffness tensor (99), the components \mathbb{C}_{1111}^{eff} and \mathbb{C}_{2211}^{eff} take the form

$$\mathbb{C}_{1111}^{eff} = \frac{K_n^I \ell [4\mu(\lambda + \mu) + (\lambda + 2\mu)K_n^{II}\ell]}{4\mu(\lambda + \mu) + (\lambda + 2\mu)(K_n^I + K_n^{II})\ell + K_n^I K_n^{II} \ell^2} \quad (107)$$

$$\mathbb{C}_{2211}^{eff} = \frac{\lambda K_n^I K_n^{II} \ell^2}{4\mu(\lambda + \mu) + (\lambda + 2\mu)(K_n^I + K_n^{II})\ell + K_n^I K_n^{II} \ell^2} \quad (108)$$

505

By proceeding in a similar way, the full solution for the effective stiffness tensor is given as follows

$$\begin{aligned}
\mathbb{C}_{1111}^{eff} &= \frac{K_n^I \ell [4\mu(\lambda + \mu) + (\lambda + 2\mu)K_n^{II} \ell]}{4\mu(\lambda + \mu) + (\lambda + 2\mu)(K_n^I + K_n^{II})\ell + K_n^I K_n^{II} \ell^2} \\
\mathbb{C}_{2222}^{eff} &= \frac{K_n^{II} \ell [4\mu(\lambda + \mu) + (\lambda + 2\mu)K_n^I \ell]}{4\mu(\lambda + \mu) + (\lambda + 2\mu)(K_n^I + K_n^{II})\ell + K_n^I K_n^{II} \ell^2} \\
\mathbb{C}_{3333}^{eff} &= \lambda + 2\mu - \frac{\lambda^2(4\mu + K_n^I \ell + K_n^{II} \ell)}{\lambda(4\mu + K_n^I \ell + K_n^{II} \ell) + (2\mu + K_n^I \ell)(2\mu + K_n^{II} \ell)} \\
\mathbb{C}_{1122}^{eff} &= \mathbb{C}_{2211}^{eff} = \frac{4\mu(\lambda + \mu) + (\lambda + 2\mu)(K_n^I + K_n^{II})\ell + K_n^I K_n^{II} \ell^2}{\lambda K_n^I K_n^{II} \ell^2} \\
\mathbb{C}_{1212}^{eff} &= \frac{\mu K_\tau^I K_\tau^{II} \ell}{\mu(K_\tau^I + K_\tau^{II}) + K_\tau^I K_\tau^{II} \ell} \\
\mathbb{C}_{1133}^{eff} &= \frac{\lambda(2\mu + K_n^{II} \ell) K_n^I \ell}{\lambda(4\mu + K_n^I \ell + K_n^{II} \ell) + (2\mu + K_n^I \ell)(2\mu + K_n^{II} \ell)} \\
\mathbb{C}_{2233}^{eff} &= \frac{\lambda(2\mu + K_n^I \ell) K_n^{II} \ell}{\lambda(4\mu + K_n^I \ell + K_n^{II} \ell) + (2\mu + K_n^I \ell)(2\mu + K_n^{II} \ell)} \\
\mathbb{C}_{1313}^{eff} &= \frac{\mu K_\tau^I \ell}{\mu + K_\tau^I \ell} \\
\mathbb{C}_{2323}^{eff} &= \frac{\mu K_\tau^{II} \ell}{\mu + K_\tau^{II} \ell}
\end{aligned} \tag{109}$$

506

C Analytical solution of η

507

The problem in η for the periodic geometry of cross arrangement shown in Figure 9a can be solved

508

analytically with the given cleat stiffness $\{K_n, K_\tau\}$. Due to the cleat structure inside the cell, there is

509

no deformation according to the third direction, *i.e.* $\epsilon_{33} = 0$.

510

The stress tensor of matrix phase reads as

$$\boldsymbol{\sigma}(\boldsymbol{\eta}) = \lambda(\epsilon_{11} + \epsilon_{22}) \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} + 2\mu \begin{pmatrix} \epsilon_{11} & 0 & 0 \\ 0 & \epsilon_{22} & 0 \\ 0 & 0 & 0 \end{pmatrix}$$

$$= \begin{pmatrix} (\lambda + 2\mu)\epsilon_{11} + \lambda\epsilon_{22} & 0 & 0 \\ 0 & (\lambda + 2\mu)\epsilon_{22} + \lambda\epsilon_{11} & 0 \\ 0 & 0 & \lambda(\epsilon_{11} + \epsilon_{22}) \end{pmatrix} \quad (110)$$

511 Noting that the cleats (I) and (II) corresponding to the normal vectors $\mathbf{n}_1^+ = (1, 0, 0)$ and $\mathbf{n}_2^+ = (0, 1, 0)$
 512 respectively, the interface condition of the closure problem (79) is written as

$$\begin{aligned} \boldsymbol{\sigma}(\boldsymbol{\eta}) \cdot \mathbf{n}_1^+ \cdot \mathbf{n}_1^+ &= K_n^I \llbracket \eta_n \rrbracket^I - 1 \\ \boldsymbol{\sigma}(\boldsymbol{\eta}) \cdot \mathbf{n}_2^+ \cdot \mathbf{n}_2^+ &= K_n^{II} \llbracket \eta_n \rrbracket^{II} - 1 \end{aligned} \quad (111)$$

513 together with the periodic conditions

$$\begin{aligned} \llbracket \eta \rrbracket^I + \epsilon_{11} \ell &= 0 \\ \llbracket \eta \rrbracket^{II} + \epsilon_{22} \ell &= 0 \end{aligned} \quad (112)$$

514 The solutions for the jumps of $\boldsymbol{\eta}$ are given by

$$\begin{aligned} \llbracket \eta \rrbracket^I &= \frac{\ell (2\mu + K_n^{II} \ell)}{\lambda (4\mu + K_n^I \ell + K_n^{II} \ell) + (2\mu + K_n^I \ell) (2\mu + K_n^{II} \ell)} \\ \llbracket \eta \rrbracket^{II} &= \frac{\ell (2\mu + K_n^I \ell)}{\lambda (4\mu + K_n^I \ell + K_n^{II} \ell) + (2\mu + K_n^I \ell) (2\mu + K_n^{II} \ell)} \end{aligned} \quad (113)$$

515 **D Biot coefficient for the cleat**

516 Let consider a cleat with an upper normal vector \mathbf{n}^+ outward to the matrix. The contact stress in
517 incremental form which is continuous through the cleat is given by

$$\begin{aligned} d\sigma_f = d\sigma_m \cdot \mathbf{n}^+ &= K_n \llbracket d\mathbf{u}_n \rrbracket + K_\tau \llbracket d\mathbf{u}_\tau \rrbracket - \alpha_f dp_f \mathbf{n}^+ \\ &= K_n \llbracket (d\mathbf{u} \cdot \mathbf{n}^+) \mathbf{n}^+ \rrbracket + K_\tau \llbracket d\mathbf{u} - (d\mathbf{u} \cdot \mathbf{n}^+) \mathbf{n}^+ \rrbracket - \alpha_f dp_f \mathbf{n}^+ \end{aligned} \quad (114)$$

518 where $\llbracket d\mathbf{u}_n \rrbracket$ and $\llbracket d\mathbf{u}_\tau \rrbracket$ represent the jump of the displacement in normal and tangential directions
519 through the cleat, α_f the Biot coefficient of the cleat, K_n and K_τ the normal and shear stiffness, which
520 are given by the Bandis and Barton relation

$$\begin{aligned} K_n &= \frac{K_{ni} V_m^2}{(V_m + \llbracket u_n \rrbracket)^2} \\ K_\tau &= \frac{K_{\tau i} V_m^2}{(V_m + \llbracket u_n \rrbracket)^2} \end{aligned} \quad (115)$$

521 with K_{ni} , $K_{\tau i}$ and V_m being the initial normal and shear stiffness and the maximum closure of the cleat
522 when $\sigma_n \rightarrow -\infty$.

523 To determine the Biot coefficient α_f of the cleat, the normal charge P perpendicular to the cleat
524 plane is increased by dP whereas the fluid pressure in the cleat p_f is increased by dp_f . Since
525 an incremental procedure is performed, the loading can be considered as linear and is split into two
526 distinct steps. In the first step, the fluid remains at pressure p_f and the charge is increased by $dP - dp_f$.
527 In the second one, the charge and the fluid pressure are increased both by dp_f . Here, only normal
528 displacement are considered. During the first step according to Bandis-Barton relation, we have

$$-d(P - p_f) = K_n d\llbracket u_n^I \rrbracket \quad (116)$$

529 During the second step, the stress tensor is uniform both inside the solid and fluid phases and is equal

530 to $-dp_f \mathbf{I}$. Therefore the fluid can be replaced by the solid phase. The solid strain tensor is $-\frac{dp_f}{3k_s} \mathbf{I}$
 531 where k_s is the solid bulk modulus. Therefore, the deformation is given by

$$\frac{d[[u_n^{\text{II}}]]}{V_m + [[u_n]]} = \frac{-dp_f}{3k_s} \quad (117)$$

532 The total displacement is the sum of the displacements of the two steps

$$d[[u_n]] = d[[u_n^{\text{I}}]] + d[[u_n^{\text{II}}]] \quad (118)$$

533 Combining the preceding relations leads to

$$-dP = K_n \left(d[[u_n]] + dp_f \frac{V_m + [[u_n]]}{3k_s} \right) - dp_f \quad (119)$$

$$= K_n d[[u_n]] - \underbrace{\left[1 - \frac{K_n}{3k_s} (V_m + [[u_n]]) \right]}_{\alpha_f} dp_f \quad (120)$$

534 The Biot coefficient of the cleat is given by

$$\alpha_f = 1 - \frac{K_n}{3k_s} (V_m + [[u_n]]) = 1 - \frac{K_{ni} V_m - \bar{\sigma}_n^{\text{BB}}}{3k_s} \quad (121)$$

535 Since $K_{ni} V_m - \bar{\sigma}_n^{\text{BB}} \ll k_s$ for the coal material, it is suitable to assign $\alpha_f = 1$ in numerical simulations.

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618 Notation

Ω_s : solid domain of the matrix

Ω_n : nanopore domain

Γ_{ns} : nanopore-solid interface

Z : representative unit cell of the matrix

Z_s : solid domain in the unit cell Z

Z_n : nanopore domain in the unit cell Z

∂Z_{ns} : nanopore-solid interface in the unit cell Z

Y : unit cell at microscale

Y_m : matrix domain in the unit cell Y

∂Y_{mf} : matrix-fracture interface in the unit cell Y

$\mathbf{\Pi}$: solvation force vector

p_m : bulk pressure in the matrix

619

p_f : bulk pressure in the fractures

\mathbf{F}_s : swelling stress

\mathbf{u} : displacement vector

\mathbf{u}_s : solid displacement in Z_s

\mathbf{u}_n : fluid displacement in Z_n

\mathbf{u}_m : matrix displacement in Z_m

\mathbf{u}_f : fluid displacement in Z_f

\mathbb{I} : fourth-order identity tensor

ϕ_m : porosity of matrix

ϕ_{cleat} : cleats porosity

$\boldsymbol{\alpha}_m$: microscopic Biot-Willis tensor

$\boldsymbol{\alpha}_{m,i}^*$: modified microscopic Biot-Willis tensor

620

σ_s : solid stress tensor in the solid phase

σ_n : fluid stress tensor in nanopores

σ_m : stress tensor in the matrix

σ_f : stress tensor in the fracture

621

\mathbf{c}_s : elastic stiffness tensor of the solid

\mathbf{C}_m : effective elastic stiffness tensor of matrix

\mathbf{C}_m^* : modified effective elastic stiffness tensor of matrix

\mathbb{C}^{eff} : effective elastic stiffness tensor of macroscopic domain