Thermo-hydro-mechanical modeling of unsaturated soils using isogeometric analysis: Model development and application to strain localization simulation

Shahriar Shahrokhabadi1,2 | Toan Duc Cao1,3 | Farshid Vahedifard1

1 Department of Civil and Environmental Engineering, Mississippi State University, Mississippi State, MS 39762
2 Intertek-PSI, Fairfax, VA 22031, U.S.A
3 Center for Advanced Vehicular Systems (CAVS), Mississippi State University, Mississippi State, MS 39762, U.S.A

Summary
This study presents a thermo-hydro-mechanical (THM) model of unsaturated soils using isogeometric analysis (IGA). The framework employs Bézier extraction to connect IGA to the conventional finite element analysis (FEA), featuring the current study as one of the first attempts to develop an IGA-FEA framework for solving THM problems in unsaturated soils. IGA offers higher levels of interelement continuity making it an attractive method for solving highly nonlinear problems. The governing equations of linear momentum, mass, and energy balance are coupled based on the averaging procedure within the hybrid mixture theory. The Drucker-Prager yield surface is used to limit the modified effective stress where the model follows small strain, quasi-static loading conditions. Temperature dependency of the surface tension is implemented in the soil-water retention curve. Nonuniform rational B-splines (NURBS) basis functions are used in the standard Galerkin method and weak formulations of the balance equations. Displacement, capillary pressure, gas pressure, and temperature are four independent quantities that are approximated by NURBS in spatial discretization. The framework is used to simulate strain localization in an undrained dense sand subjected to plane strain biaxial compression under different temperatures and displacement velocities. Results show that an increase in the displacement rate leads to reduction in the equivalent plastic strain while an increase in the temperature leads to an increase in the equivalent plastic strain. The findings suggest that the proposed IGA-based framework offers a viable alternative for solving THM problems in unsaturated soils.

KEYWORDS
elastoplasticity, isogeometric analysis, strain localization, thermo-hydro-mechanical model, unsaturated soil
Modeling thermo-hydro-mechanical (THM) processes in variably saturated porous materials has been widely investigated in recent years. The emerging interest is due to wide range engineering applications posing THM processes in porous materials such as soil-atmospheric interactions under a changing climate, nuclear waste disposal, seabed pipelines, geothermal structures, petroleum drilling, high-voltage buried cables, and tunneling.1-7 Temperature variation considerably influences the microstructural characteristics8 and hydro-mechanical behavior9,10 of unsaturated geomaterials, and several studies have been performed to accurately consider these effects in engineering problems. For instance, Gens11 introduced a thermo-mechanical model based on a combination of isothermal constitutive equations in unsaturated soils and thermo-plastic models in saturated soils, while Bolzon and Schrefler12 formulated a non-isothermal elasto-plastic model in unsaturated soils. Francois and Laloui13 offered a thermoplasticity model in saturated and unsaturated soils in a highly coupled framework with a unified approach. Masin and Khalili14 introduced a new formulation based on hypoplasticity that represents a thermomechanical model in unsaturated soils.

In addition to the effect of temperature, shear banding may significantly affect the mechanical and hydraulic properties of geomaterials, leading to a reduction in load carrying capacity or transport properties.15 Strain localization results from material instability and poses a challenging problem for numerical analysis because it is mathematically ill-posed unless an appropriate regularization scheme is also introduced. Extensive theoretical, experimental, and numerical studies on shear banding and localized deformation in soils have been presented in the literature,16-21 yet several unanswered questions remain. Borja22 outlined an isothermal framework to track the onset of strain localization in unsaturated soils. Callari et al23 used a finite element model to simulate the development of strain localization in unsaturated soils. Ehlers et al24 used the general porous media theory to formulate a finite element model for strain localization in unsaturated soils. Song25 studied the transient bifurcation in unsaturated porous media with the finite strain approach. Sanavia et al26 introduced a finite element analysis (FEA) of nonisothermal elasto-plastic model based on mixture theory to analyze strain localization induced by the thermal load.27-29 Cao et al30 extended the Sanavia et al26 model to dynamics using the generalized Newmark scheme for time discretization. Despite the progress made by previous works, more studies are needed for the improvement of both fully coupled THM models and numerical techniques to simulate the strain localization in deforming porous media. For instance, regularization techniques such as gradient dependent models19 should be implemented in the models to avoid numerical pathologies such as mesh dependency.

In recent years, isogeometric analysis (IGA) has been introduced as a new numerical method in computational mechanics31 and has been increasingly used in different fields of engineering including poromechanics.32-35 IGA provides features that are especially useful in geomechanical simulations. These features include the improved continuity of field variables due to the smoothness of the basis functions and the ability to perform simulations with high continuity and regularity in mesh.31 Shahrokhabadi et al35 examined the application of IGA in highly nonlinear flow problems in unsaturated soil and compared the results with those attained from the conventional FEA. They demonstrated the advantages of IGA for modeling unsaturated flow problems that result from IGA’s higher interelement continuity and regularity in the simulation of water front propagation. Shahrokhabadi et al36 employed IGA coupled with FEA to simulate the elastic behavior of saturated soils subjected to THM conditions. Bekele et al37 presented a fully coupled IGA-based THM model for ground freezing simulation and obtained improvement in the accuracy of derived quantities (stress, strain, or fluxes) by using higher continuity in basis functions. Remij et al38 showed that IGA is more accurate than the conventional FEA in the simulation of hydro-thermo-chemo-mechanical concrete problems.

In the present study, (a) an IGA-FEA framework is developed for THM modeling of unsaturated soils and (b) the framework is then used to study the strain localization problem in unsaturated soils. To the best of the authors’ knowledge, neither of these two was done in the literature. The proposed IGA-FEA framework employs the Bézier extraction connecting IGA with the conventional FEA. IGA offers higher level of interelement continuity making it an attractive method for solving highly nonlinear problems,35 whereas the conventional FEA benefits from well-established numerical solutions available in the COMES-GEO code.39 The weak form of governing equations is formulated by using a linear combination of the Bézier extraction operator and Bernstein polynomials to derive nonuniform rational B-splines (NURBS) basis functions for spatial integration.

The rest of the paper is outlined as follows. Section 2 presents a conceptual description of the THM model in unsaturated porous media. In addition, we briefly review NURBS, the Bézier extraction operator in IGA, THM formulations, including regularization procedures, and discretization of governing equations in time and space.
Section 3 introduces the biaxial compression test, along with the corresponding boundary conditions, which are then used to illustrate these methods. The comparison between strain localization simulations, reported by for FEA, and IGA is presented in Section 4. Section 4 presents the results of three loading conditions and discusses the effects of mechanical, thermal, and mechanical-thermal loads on strain localization and shear band propagation. In Section 6, a general discussion on three modes of loading (Section 4) in the simulations is presented, and the conclusion are presented in Section 7.

2 | ISOGEOMETRIC ANALYSIS OF THERMO-HYDRO-MECHANICAL PROCESSES IN UNSATURATED SOILS

Unsaturated porous media is a multiphase system where the voids of solid skeleton(s) are filled with water (w) and gas (g) constituents. Three constituents \( (\pi = s,w,g) \) are generally treated as immiscible. The gas phase is assumed to interact as ideal mixtures for both dry air (g\(\text{a} \)) and water vapor (g\(\text{w} \)), which are miscible. In addition, the solid skeleton and water components are considered incompressible whereas gas components are compressible.

The mathematical representation of the transient THM analysis in Section 2.1 for saturated-unsaturated porous media is developed based on the averaging theories introduced by Hassanizadeh and Gray. Macroscopic balance equations were derived by integrating microscopic equations on a representative elementary volume (dv in Figure 1 A) using spatial averaging operators. The macroscopic balance equations are then assumed to describe a porous media continuum in which all the constituents \( (\pi = s,w,g) \) fill the entire domain simultaneously (see Figure 1B).

In general, the THM analysis is performed in a quasi-static and geometrically linear framework where the constituents are assumed to be isotropic, homogenous, chemically nonreacting, and immiscible (except for gw and ga). Local thermal equilibrium between the phases is valid, which represents the same temperature for all phases. The state of the medium is designated by the displacement of solid particles \( \mathbf{U} \), the gas pressure \( P^g \), the capillary pressure \( P^c \) (where \( P^c = P^g - P^w \)), and the absolute temperature \( T \). The pore pressure is compressive-positive for the fluid components, and stress is tension-positive for the solid phase.

The macroscale equations are implemented within an IGA-FEA framework. Figure 2 outlines the conceptual model that is used in this study for THM modeling of unsaturated soils. The proposed framework includes three main modules including IGA, FEA, and the IGA-FEA interface components. In the IGA module, preprocessing and postprocessing steps are performed using the Computer Aided Design (CAD) technology where we define the geometry (control points), the IGA mesh (control mesh), and the corresponding connectivity array based on CAD. We also use NURBS basis functions to approximate the secondary variables and visualize the results. The coupled conservation equations for linear momentum, energy, and mass in the FEA module are written in terms of solid motion, temperature, and pressures in the fluid phases in light of the constitutive relationships. The IGA-FEA interface module includes the Bézier extraction operator and Bernstein polynomials to derive NURBS basis functions for spatial integration. The weak form of the governing equations is formulated by using a linear combination of the new interpolation functions based on NURBS and the Bézier extraction operator. Finally, the Backward Euler time integration scheme and linearization of the system of equations along with the NURBS-based interpolation function, and the IGA-FEA interface module are incorporated into COMES-GEO, a FEA code developed specifically for THM modeling of porous materials. The following sections provide further details about this framework including the underlying theory, governing equations, IGA-FEA formulation, solution steps, and verification and comparison against the FEA. It is noted that this study builds on the work by Cao et al., who used FEA (via COMES-GEO) for modeling strain localization in unsaturated soils.
completeness, some of the equations and discussion in Sections 2.1 and 2.2 are recapitulated from the pertinent sections from Cao et al.30

2.1 | Governing equations

The macroscopic governing equations for linear momentum, mass, and energy balance equations that mathematically describe the THM coupling in unsaturated porous media are derived based on the following assumptions39:

• The solid phase follows rate-independent elasto-plasticity with small strain.
• The water phase follows Darcy’s law in which water flow is proportional to the total pressure gradient.
• The heat conduction and convection are accounted for by assuming the total conductive heat flux follows Fick’s law assuming an isotropic thermal conductivity.

2.1.1 | Linear momentum balance equation

Total Cauchy stress (\(\sigma\)) that is embedded in the linear momentum balance equation follows:

\[
div\sigma + \rho g = 0
\]  

(1)

where \(g\) is the gravitational acceleration and \(\rho\) is the density of mixture defined as

\[
\rho = (1 - n)\rho^s + nS_w\rho^w + n(1 - S_w)\rho^g
\]  

(2)

with \(\rho^s\), \(\rho^w\), and \(\rho^g\) the density of solid particles, liquid water, and gas, respectively; \(n\) is porosity; and \(S_w\) is the water degree of saturation. One can decompose \(\sigma\) based on the effective stress definition as follows:

\[
\sigma = \sigma' - \lambda\alpha[A^e - S_w P^e]
\]  

(3)
where \( \sigma \) is the effective stress, \( \mathbf{I} \) is the second-order identity tensor, and \( \alpha \) is Biot’s coefficient. Since the solid particles are nearly incompressible \( \alpha = 1 \) is assumed in this study.

### 2.1.2 Mass balance equations

The sum of mass balance equation for water species and solid skeleton is expressed as

\[
\begin{align*}
\text{div} \left( \rho \frac{k_{w}^{\text{rw}} K_w^w}{\mu_w} [-\nabla (P^w - P^c) + \rho^w g] \right) + \text{div} \left( \rho \frac{k_{w}^{\text{rw}} K_g^{\text{rg}}}{\mu_g} [-\nabla P^{\text{rg}} + \rho^w g] \right) - \text{div} \left( \rho \frac{M_w M_w^{\text{rw}}}{M_g^2} D_g^{\text{rg}} \nabla \left( \frac{P^w g}{P^c} \right) \right) \\
+ [\rho^w S_w + \rho^w g [1 - S_w]] \text{div} \mathbf{U} + n [\rho^w - \rho^w g] S_w - [\rho^w \beta g S_w + \rho^w \beta_g [1 - n] [1 - S_w]] T + n [1 - S_w] \rho^g + \rho^w S_w \left[ \frac{P_g}{K_w} [P^g - P^c] \right] = 0
\end{align*}
\]

(4)

where \( k_{w}^{\text{rw}} \) and \( k_{g}^{\text{rg}} \) are relative permeability of liquid water and gas, \( K_w^w \) and \( K_g^g \) are the intrinsic permeability tensors for liquid water and gas, respectively, and \( \mu_w, \mu_g \) are liquid water and gas viscosity, respectively, \( \rho^w, \rho^g \), and \( D_g^{\text{rg}} \) are density, pressure, and effective diffusivity tensor of water vapor in the gas phase, respectively; \( M_a, M_w, \) and \( M_g \) are the molar mass of dry air, liquid water, and gas mixture, respectively; \( K_w \) is water bulk modulus \( (K_w = 2.2 e_0 ^3 \text{ Pa}) \) and \( \beta_g \) is the thermal expansion coefficient of mixture.

Similarly, the sum of dry air constituent and solid particles in term of the mass balance equation leads to

\[
\begin{align*}
\text{div} \left( \rho^g \frac{k_{g}^{\text{rg}} K_g^{\text{rg}}}{\mu_g} [-\nabla P^g + \rho^g g] \right) + \text{div} \left( \rho^g \frac{M_w M_w^{\text{rw}}}{M_g^2} D_g^{\text{rg}} \nabla \left( \frac{P^g}{P^c} \right) \right) \\
+ [\rho^g [1 - S_w]] \text{div} \mathbf{U} + n [1 - S_w] \rho^g - n \rho^g S_w - \rho^g \beta_g [1 - n] [1 - S_w] T \\
= 0
\end{align*}
\]

(5)

where \( \rho^g \) is the dry air density and \( D_g^{\text{rg}} \) is the diffusivity tensor of dry air in the gas phase.

### 2.1.3 Energy balance equation

The energy balance equation in the system is defined as

\[
\begin{align*}
-d \text{div} \left( \rho \frac{k_{w}^{\text{rw}} K_w^w}{\mu_w} [-\nabla (P^w - P^c) + \rho^w g] \right) \Delta H_vap - \text{div} \left( \chi_{\text{eff}} \nabla T \right) - \rho^w S_w (\text{div} \mathbf{U}) \Delta H_vap \\
+ \left[ C_p^w \frac{k_{w}^{\text{rw}} K_w^w}{\mu_w} [-\nabla (P^w - P^c) + \rho^w g] + C_p^{\text{rg}} \frac{k_{g}^{\text{rg}} K_g^{\text{rg}}}{\mu_g} [-\nabla P^g + \rho^g g] \right] \nabla T + \left( \rho C_p \right)_{\text{eff}} T - \frac{\rho^w n S_w}{K_w} [P^g - P^c] \Delta H_vap \\
+ \beta_w T \Delta H_vap - n (\rho^w - \rho^w g) S_w \Delta H_vap \\
= 0
\end{align*}
\]

(6)

where \( \Delta H_vap \) is the latent heat, \( \chi_{\text{eff}} \) is the effective thermal conductivity of porous media, and \( C_p^w, C_p^{\text{rg}}, \) and \( (\rho C_p)_{\text{eff}} \) are specific heat of liquid water, gas, and the effective heat capacity of the mixture, respectively.

### 2.2 Constitutive equations

Darcy’s and Fick’s laws\textsuperscript{39,40} are the two main constitutive equations that control the fluid (water and gas) flow in the mixture. In addition, Fourier’s law\textsuperscript{39} describes the heat flux in the system, and stress-strain relationship for the solid phase is defined based on a rate-independent elasto-plastic model.\textsuperscript{41}
2.2.1 Constitutive models for fluids flow (water and gas)

Water and gas flows follow Darcy’s law based on

$$q_{\pi} = \frac{k_{\pi} \pi \mathbf{K}_{\pi}}{\mu_{\pi}} [-\nabla (P_{\pi}) + \rho_{\pi} \mathbf{g}] \text{ with } \pi = g, w$$  \hspace{1cm} (7)

where $q_{\pi}$ is the fluid flux with respect to constituent $\pi$. Fick’s law represents the diffusion process in the gas phase, which is a miscible mixture of dry air and water vapor:

$$J_{g}^{\pi} = -D_{g}^{\pi} \frac{p_{g}}{P_{g}} \nabla p_{g} = -J_{g}^{\pi}$$ \hspace{1cm} (8a)

$$M_{g} = \left(\frac{p_{g}^{\omega}}{p_{g}} \frac{1}{M_{w}} + \frac{p_{g}^{\alpha}}{p_{g}} \frac{1}{M_{a}}\right)^{-1}$$ \hspace{1cm} (8b)

where $J_{g}^{\pi}$ is the diffusive-dispersive mass flux of constituent $\pi$ in the gas phase. The gas phase is a perfect mixture of water vapor and dry air that is assumed to fulfill the ideal gas law. Accordingly, following the equation of state for a perfect gas and implementing Dalton’s law to moist air ($g$), vapor ($gw$), and dry air ($ga$), the following equations can be derived:

$$p_{gw} = \frac{p_{gw} R T}{M_{w}}$$ \hspace{1cm} (9a)

$$p_{ga} = \frac{p_{ga} R T}{M_{a}}$$ \hspace{1cm} (9b)

$$p_{g} = p_{gw} + p_{ga}$$ \hspace{1cm} (9c)

$$\rho_{g} = \rho_{gw} + \rho_{ga}$$ \hspace{1cm} (9d)

where $R$ is the universal gas constant.

In unsaturated soils, the equilibrium water vapor pressure ($p_{gw}$) can be introduced using the Kelvin-Laplace equation:

$$p_{gw} = p_{gws} (T) \exp \left(-\frac{P_{c} M_{w}}{\rho_{gw} RT}\right)$$ \hspace{1cm} (10)

where $p_{gws}(T)$ is the water vapor saturation pressure depending on the temperature $T$ and one can use the Hyland-Wexler equation to define $p_{gws}$. The degree of saturation $S_{\pi}(P_{c}, T)$ and relative permeability $k_{\pi}(P_{c}, T)$ are either predicted by models based on realistic capillary assumptions or determined experimentally. Appendix A includes the supplementary equations needed to describe a full THM phenomenon along with the principal constitutive equations that are used in this study.

2.2.2 Constitutive model for heat transfer

Heat flux in the porous media is described using the constitutive equation in the generalized form of Fourier’s law:

$$q_{T} = -\chi_{eff} \nabla (T)$$ \hspace{1cm} (11)

where $q_{T}$ is heat flux and $\chi_{eff}$ is the effective thermal conductivity.
Constitutive model for solid deformation (stress-strain)

The stress-strain formulation for the mixture defines the effective stress based on general strain rate tensor as

\[ \sigma' = D^e(\dot{\varepsilon} - m^T \dot{\varepsilon}_s^e - m^T \dot{\varepsilon}_T^e - \dot{\varepsilon}_p) \]  

(12)

where \( D^e \) is the elastic stiffness matrix, \( \dot{\varepsilon}_s^e \) is the elastic strain rate related to the matric suction change, \( \dot{\varepsilon}_T^e \) is the elastic strain rate due to thermal effects, and \( \dot{\varepsilon}_p \) is the plastic strain rate determined by the flow rule.

The Drucker-Prager (D-P) rate-independent elasto-plasticity model is used in this work, which is restricted to geometrically linear problems. The yield criterion is expressed in terms of effective stress \( \sigma' \). In general, the flow rule accounts for the dilation/contraction in dense or loose sands, although in this study an associated flow law is used, which restricts plastic volume change to dilation. The soil model choice was designed to restrict the instability source to strain softening and avoid the numerical inconvenience of the nonsymmetric tangent stiffness created by a nonassociated flow law. The concept of multisurface plasticity, introduced by Hofstetter and Taylor, is implemented to solve the singular behavior of D-P yield surface in the apex zone by developing the return mapping and consistent tangent operator.

The Helmholtz free energy function \( \psi \) governs the mechanical behavior of solid phase:

\[ \psi = \psi(\varepsilon^e, \zeta) \]  

(13)

where \( \varepsilon^e \) is the small elastic strain tensor and \( \zeta \) is the internal strain-like scalar hardening variable that can be identified as the plastic strain. The second law of thermodynamics leads to the following relations in Equation (14a) and dissipation inequality in Equation 14b:

\[ \sigma = \frac{\partial \psi}{\partial \varepsilon^e}, \quad q_p = -\frac{\partial \psi}{\partial \zeta} \]  

(14a)

\[ \sigma' : \varepsilon^e - q_p \zeta \geq 0 \]  

(14b)

where \( q_p \) is the stress-like internal variable that is thermodynamically conjugate to \( \zeta \) and is associated with the energy dissipation as the yield locus evolves. The evolution equations for \( \varepsilon^e \) and \( \zeta \) are obtained based on the maximum plastic dissipation:

\[ \dot{\varepsilon}^e = \dot{\varepsilon} - \dot{\varepsilon}_p = \dot{\varepsilon} - \dot{\gamma} \frac{\partial F}{\partial \sigma'} \]  

(15a)

\[ \dot{\zeta} = \dot{\gamma} \frac{\partial F}{\partial q_p} \]  

(15b)

Accuracy of the model largely depends on adequate evaluation of the parameters that determine the yield criterion, hardening/softening, and flow rule in the D-P plasticity model. When the associative flow rule is used with the D-P cone dilatancy is greatly over estimated. Equation (15) is derived in light of Kuhn-Tucker form in the classical loading-unloading conditions:

\[ \dot{\gamma} \geq 0, \quad F(\sigma', q_p) \leq 0, \quad \dot{\gamma} F = 0 \]

(16)

where \( \dot{\gamma} \) is the consistency parameter rate of change and \( F(\sigma', q_p) \) is the isotropic yield function. The classical D-P yield function with linear isotropic hardening is given as:

\[ F(p, s, \eta) = 3 \alpha_p p + \| s \| - \beta_p \sqrt{\frac{2}{3} (c_0 + h \zeta)} \]

(17)

where \( p \) is the mean effective stress \( p = \frac{1}{3} (\sigma' : I) \), \( \| s \| \) is the \( l_2 \) norm for the deviatoric effective stress tensor, \( c_0 \) is the
initial apparent cohesion, $h$ is the hardening/softening modulus, and $\alpha_{F}, \beta_{F}$ are material parameters that are defined based on the soil frictional angle ($\phi$):

$$\alpha_{F} = 2 \sqrt{\frac{\frac{2}{3} \sin \phi}{3 - \sin \phi}}$$  \hspace{1cm} (18a)$$

$$\beta_{F} = \frac{6 \cos \phi}{3 - \sin \phi}$$  \hspace{1cm} (18b)$$

### 2.2.4 | Internal length scale in regularization procedures

Strain localization is the result of material instability that creates numerical pathologies, such as mesh dependency and localization zones that tend to surfaces of zero thickness upon mesh refinement.\textsuperscript{48,49} From a mathematical point of view, the differential equation of motion (Equation 1) ceases to be hyperbolic as soon as softening occurs and disturbances will not propagate throughout the domain. These mathematical difficulties can be overcome by introducing a so-called regularization scheme. In the current study, two regularization procedures, readily implemented in COMES-GEO, are used to address this issue. Further details about these regularization procedures are provided in the following paragraphs.

To avoid mesh dependency in strain localization modeling, various regularization procedures based on the standard continuum plasticity, such as gradient dependent models, have been proposed in the literature.\textsuperscript{16} For multiphase problems, the gradient term in the mass balance equation of fluid constituent (Equation 4) that arise from Darcy’s law seem to reduce mesh dependency in strain localization simulations making the problem in multiphase media less severe compared with single-phase models.\textsuperscript{50,51} However, despite contribution of the Laplacian term in Equation (4), strain localization in multiphase media remains a challenging problem, since it is simultaneously influenced by both material behavior and fluid-solid interaction.\textsuperscript{52} In all cases, the key to regularization is to introduce internal length scales into the equations for both solid and flow phases. Zhang et al.\textsuperscript{52} derived an internal length scale in dynamic strain localization of multiphase porous media by performing a dispersion analysis for a one-dimensional saturated soil bar by considering single harmonic wave propagation through the domain. Their derivation was built around the cubic characteristic equation in terms of the eigenvalues ($\zeta$) as follows:

$$\zeta^3 + a^* \zeta^2 + b^* \zeta + c^* = 0$$  \hspace{1cm} (19a)$$

$$a^* = Q^* K_y$$  \hspace{1cm} (19b)$$

$$b^* = (h + \alpha^2 S_{w} Q^*) \rho^{-1} K^2$$  \hspace{1cm} (19c)$$

$$c^* = Q^* h \rho^{-1}$$  \hspace{1cm} (19d)$$

$$y = \frac{k_{rw} K_{rw}}{\mu_{rw} K}$$  \hspace{1cm} (19e)$$

$$Q^* = \left[ n \frac{\partial S_{w}}{\partial P_{w}} + n \frac{S_{w}}{K_{w}} + \frac{S_{w}(\alpha - n)}{K_{s}} \left( S_{w} + \frac{\partial S_{w}}{\partial P_{w}} P_{w} \right) \right]^{-1}$$  \hspace{1cm} (19d)$$

where $K$ is the wave number. There exist two types of solution for Equation (19a) when $-\alpha^2 S_{w} Q^* < h < 0$. The first solution (Type I) has one real positive and two conjugate complex roots whereas the second solution (Type II) includes three real roots. The conditions for each case are determined from the sign of the polynomial $Q$ given by

$$Q = \left( \frac{R}{3} \right)^3 + \left( \frac{Q^*}{2} \right)^2$$  \hspace{1cm} (20a)$$
The Type I solution consisting of one real and two complex conjugate roots is characterized by \( Q > 0 \), whereas the Type II solution consisting of three real roots is characterized by \( Q \leq 0 \). For the Type I solution, wave propagation is feasible and hence the governing equations remain hyperbolic even when softening occurs in the solid phase. Consequently, the numerical analysis of Type I problems will not show mesh sensitivity. However, for the Type II solution (\( Q \leq 0 \)), the wave speed will be imaginary, and the governing equations become elliptic. Consequently, the numerical analysis of Type II problems will show mesh dependency unless an internal length scale is introduced. The value of the length scale is chosen such that Equation (19a) has complex roots, which leads to a solution with real wave speed. Zhang et al.\(^{52}\) determined a length scale for multiphase materials by following a similar procedure for rate-dependent single-phase materials.\(^{49}\) The approximate value for the internal length scale for multiphase medium is defined as follows:

\[
l_w = \frac{2c_m \eta}{k K^2 \alpha^2 S_w^2 Q^*} \quad (21a)
\]

\[
c_m = \sqrt{\frac{E_2}{\rho}} \quad (21b)
\]

\[
\eta = \frac{E_2}{Q^*} \quad (21c)
\]

\[
E_2 = h + \alpha^2 S_w^2 Q^* \quad (22c)
\]

\[
k = \frac{k^{nw} K^w}{\mu^{gw}} \quad (22d)
\]

If \( K \) is unknown, one can estimate length scale by taking \( K = 1 \).

It is noted that \( h \) is equal to \(-\alpha^2 S_w^2 Q^*\) when \( E_2 \) is zero. This condition defines a critical value for \( h \) since \( c_m \) is an imaginary number when \( E_2 \) is less than zero. Consequently, Equation (21a) is valid under condition of small permeability and relatively low values of \( Q^* \). Although Equation (21a) suggests a promising approach in the simulation of strain localization in multiphase media, an additional regularization procedure is required to address the following shortcomings:\(^{53}\):

1. If the permeability is very small or large, there would be no internal length scale in the case of \( E_2 \leq 0 \).
2. If the wave number is very small or large, the internal length scale disappears. It is noted that localization occurs for vanishingly small wave lengths.
3. When \( Q^* \) is very large, the internal length scale disappears.

To overcome these shortcomings, Zhang and Schrefler\(^{19}\) introduced a gradient-dependent term as an enhancement of the constitutive model for solid phase of multiphase material. This enhanced model assures the well-posedness of the governing equations during strain localization by allowing the numerical solution to properly converge with mesh refinement. The length scale is determined from a dispersion analysis related to dynamic strain localization whereby the wave speed remains real even under softening conditions. Consequently, a traveling wave is transformed into a
stationary localization wave.\textsuperscript{49} This model has the advantage that the same higher order model remains valid for quasistatic simulations.

The internal length scale that arises from the gradient-dependent model is defined by introducing a gradient parameter ($c^*$):

$$c^* = \frac{\partial F}{\partial \nabla^2 \chi}$$  \hspace{1cm} (23)

where $\chi$ is the plastic strain, $F$ is a yield function, and $c^*$ can be obtained using inverse analysis.\textsuperscript{54} If $h + c^* K^2 \leq 0$, then loss of stability due to softening may occur because the Routh-Hurwitz criterion is violated.\textsuperscript{19} Consequently, the induced instability depends on the wave number. In fact, an unstable zone appears when the wave number $K \leq \sqrt{-\frac{h}{c^*}}$. Thus, by introducing the internal length scale ($l_g$) associated with the gradient effect, one can conclude that

$$l_g = \sqrt{-\frac{h}{c^*}}$$  \hspace{1cm} (24)

The two internal length scales ($l_w$ and $l_g$) have been already implemented in COMES-GEO. The first one, $l_w$, naturally results from Darcy’s law whereas $l_g$ is the result of the gradient-dependent plasticity model for the solid skeleton.\textsuperscript{55}

Zhang and Schrefler\textsuperscript{19} introduced a parametric variational principle for numerical implementation of the aforementioned regularization methods where the original problem is reduced to a standard linear complementary problem in mathematical programming. This approach can be used in solutions where materials do not satisfy Drucker’s postulate of stability (e.g., nonassociated plasticity or softening problems). Here, the variational principle for coupled hydro-mechanical equation is presented while the same procedure can be extended to a THM problem:

$$\Pi_P = \left\langle \Delta u_{i,j}^* D_{ijkl}^e \Delta u_{k,l} \right\rangle_\Omega - 2 \left\langle \Delta u_{i,j}^* D_{ijkl}^e \frac{\partial g}{\partial g_{ij}} \right\rangle_\Omega$$

$$- 2 \left\langle \Delta u_{i,j}^* D_{ijkl}^e \Delta S_w \Delta p \right\rangle_\Omega$$

$$- 2 \left\langle \Delta u_{i,j}^* D_{ijkl}^e \alpha \Delta f_{i,j} \right\rangle_\Gamma$$

$$- 2 \left\langle \Delta u_{i,j}^* \Delta p \Delta f_{i,j} \right\rangle_\Gamma$$

$$- 2 \left\langle \Delta u_{i,j}^* \Delta p \Delta f_{i,j} \right\rangle_\Gamma$$

and the corresponding control equations are

$$\dot{\psi} + n_i \sigma_i = h \dot{\chi} + c^* \eta \nabla \dot{\chi}$$  \hspace{1cm} (26a)

$$\gamma, \dot{\psi} \geq 0, \quad \gamma \dot{\psi} = 0$$  \hspace{1cm} (26b)

where $\eta$ is a constant, $n_i$ is the gradient of yield surface, and $\psi$ is a slack parameter complementing the control parameter $\gamma$, which does not participate as an argument in the presented formula. Interested readers are referred to Sulem and Vardoulakis\textsuperscript{54} for more details.

For spatial discretization purposes, the problem domain can be divided into a finite number of elements, and in each element the continuous displacement, pressure, and plastic multiplier $\gamma$ fields can be interpolated via

$$u_i = N^u_k \Delta u_k \quad (27a)$$

$$p = N^p_k \Delta p_k \quad (27b)$$

$$\gamma = N^\gamma_k \Delta \gamma_k$$  \hspace{1cm} (27c)
Considering the fact that second derivatives of \( \gamma \) enter the yield functions makes it necessary to select \( C^1 \) continuous shape functions for interpolation of \( \gamma \). Consequently, the introduced NURBS basis functions could be used to model strain localization in this study.

2.3 | Isogeometric analysis

Hughes et al.\(^3\) suggested that NURBS not only describe the geometry of a problem, but it can also be used to construct finite approximations for analysis. To establish compatibility between IGA and available FEA code (ie, COMES-GEO), the Bézier extraction operator is introduced. The Bézier extraction operator provides a spline data structure that is easily incorporated into existing FEA codes without any changes to element form, assembly algorithms, and standard data processing array.\(^3\) In the following, we present a brief review of NURBS and the Bézier extraction operator.

2.3.1 | NURBS

The linear combination of NURBS basis functions and control points can generate a given curve \( C(\xi) \) in the one-dimensional space (1D):\(^3\)

\[
C(\xi) = \sum_{i}^{nc} R_{i,p}(\xi) P_i
\]

where \( nc \) is the number of control points, \( P_i \) is the \( i \)th control point coordinate, \( R_{i,p}(\xi) \) is the \( i \)th NURBS basis function, \( p \geq 0 \) is the order of approximation, and \( \xi \) shows a given coordinate in the parametric space. To define NURBS basis functions, it is fundamental to define a knot vector \( \Theta(\xi) \). The knot vector is a set of nondecreasing numbers in the parametric space:

\[
\Theta(\xi) = \{\xi_1, \xi_2, ..., \xi_i, ..., \xi_{nc+p+1}\}, \quad \xi \in [0,1].
\]

NURBS basis functions \( R_{i,p}(\xi) \) in Equation 25 can be introduced over the \( \Theta \) by

\[
R_{i,p}(\xi) = \frac{N_{i,p}(\xi)w_i}{\sum_{j=1}^{n} N_{j,p}(\xi)w_j}
\]

where \( N_{i,p}(\xi) \) is the \( i \)th B-spline basis function of order \( p \), and \( w_i \) is the corresponding weight in conjunction with \( i \)th control point \( (P_i) \). Finally, the B-spline basis functions \( (N_{i,p}) \) based on the recursive Cox-de Boor algorithm\(^5\) can be defined as

\[
N_{i,0}(\xi) = \begin{cases} 
1 & \xi_i \leq \xi < \xi_{i+1} \quad \text{for } p = 0 \\
0 & \text{otherwise}
\end{cases} 
\]

\[
N_{i,p}(\xi) = \frac{\xi - \xi_{i+p}}{\xi_{i+p+1} - \xi_i} N_{i,p-1}(\xi) + \frac{\xi_{i+p+1} - \xi}{\xi_{i+p+1} - \xi_{i+1}} N_{i+1,p-1}(\xi) \quad \text{for } p \geq 1
\]

Using the tensors product, Equation (25) can be extended to higher spatial dimensions (ie, 2D and 3D). For a 2D problem, a NURBS surface, \( Z(\xi, \eta) \) of order \( p \) and \( q \) with respect to \( \xi \) and \( \eta \) directions, can be formed as

\[
Z(\xi, \eta) = \sum_{i}^{mc} \sum_{j}^{mc} R_{i,j}^{p,q}(\xi, \eta)P_{i,j}
\]

where \( P_{i,j} \) are the coordinates of control points in 2D, and \( R_{i,j}^{p,q}(\xi, \eta) \) is the bivariate NURBS basis function in parametric coordinates of \( \xi \) and \( \eta \). The formation of bivariate basis function follows:

\[
R_{i,j}^{p,q}(\xi, \eta) = \frac{N_{i,p}(\xi)M_{j,q}(\eta)w_{i,j}}{\sum_{k=1}^{nc} \sum_{l=1}^{mc} N_{k,p}(\xi)N_{l,q}(\eta)w_{k,l}}
\]

where \( w \) is the 2D weights, and \( M_{j,q}(\eta) \) is the basis function of order \( q \) for \( j \)th knot in the \( \eta \)-direction.
2.3.2 | Bézier extraction operator

Since IGA follows the isoparametric concept, the elements in the parametric space can be mapped into the elements in the physical space and, consequently, the elements in the physical space form a partitioning of the computational domain. Irzal et al.\textsuperscript{32,33} implemented this idea into poroelasticity by which the canonical element functions were mapped onto the element-specific B-spline basis functions via the extraction operator $\mathbf{C}_{\text{ext}}$:

$$
\mathbf{N}^e = \mathbf{C}_{\text{ext}}^e \mathbf{B}^e
$$

where $\mathbf{B}^e$ represents Bernstein polynomial basis functions.\textsuperscript{57}

The Bézier extraction procedure is the result of an algorithm that defines the element extraction operator. This is a commonly used method that is based on standard knot insertions whereby the original B-spline basis continuity is reduced to $C^0$ by repeating all internal knots $p$ times and assembling the smoothness information in the extraction operator.\textsuperscript{58} Similar to NURBS properties, the Bézier extraction operator can be easily extended to a bivariate case using tensor products, resulting in a finite element compatible data structure that is called the Bézier mesh.\textsuperscript{58} The Bézier mesh includes the following properties:

- Control points play the same role as nodes in a FEA because a set of control points, and corresponding weights, are used to map the parametric domain with its primary parent elements onto the physical domain.
- The Bézier mesh introduces a connectivity array (similar to FEA) that dictates which global basis functions are supported over every element.
- The $\mathbf{C}_{\text{ext}}^e$ operator is usually a sparse matrix that leads to efficient storage of continuity information.
- The operators are implemented at the same evaluation level as basis function and derivatives; thus, operators need not appear in the model-specific parts of finite element implementation.

Interested readers are referred to Borden et al.\textsuperscript{58} for further details regarding isogeometric finite element data structures based on Bézier extraction of NURBS.

2.4 | Initial and boundary conditions

The initial conditions within the domain ($\Omega$) and its boundaries ($\Gamma = \Gamma_D^\vartheta \cup \Gamma_M^\vartheta$) are given as follows:

$$
\mathbf{U} = \mathbf{U}_0, \quad P^e = P^e_0, \quad P^c = P^c_0, \quad T = T_0
$$

In a variably saturated THM problem, four types of boundary conditions (BCs) are defined in terms of the primary variables ($\vartheta = \mathbf{U}, P^e, P^c, T$). The boundary conditions for the primary variables (Dirichlet BCs) are indicated by $\Gamma_D^\vartheta$:

$$
\mathbf{U} = \mathbf{U} \quad \text{on} \quad \Gamma_D^\mathbf{U}
$$

$$
P^e = P^e, \quad \text{on} \quad \Gamma_D^{P^e}
$$

$$
P^c = P^c, \quad \text{on} \quad \Gamma_D^{P^c}
$$

$$
T = T, \quad \text{on} \quad \Gamma_D^T
$$

In addition, mixed BCs ($\Gamma_M^\vartheta$) that include heat, mass exchange, and mechanical equilibrium conditions are specified as

$$
\mathbf{\sigma} \mathbf{n} = \mathbf{f} \quad \text{on} \quad \Gamma_M^\mathbf{U}
$$

$$
[n(1 - S_w) \rho_a v^a] \mathbf{n} = q^{\text{ra}}, \quad \text{on} \quad \Gamma_M^{P^e}
$$
where $\mathbf{i}$ is the traction corresponding to total Cauchy stress, $\mathbf{n}$ is the unit normal vector, $q^{\text{av}}, q^{\text{sw}}, q^{w},$ and $q^{T}$ are the dry air, vapor, liquid water, and heat flux, respectively, $\rho^{\text{av}}$ and $T_{\infty}$ are, respectively, the mass concentration of vapor and far field temperature, $e, \alpha_{0}, \beta_{c},$ and $\alpha_{c}$ are the emissivity of interface, Stefan-Boltzmann constant, convective heat exchange coefficient, and mass exchange coefficient, respectively. In Equation (33), $v^{\text{vn}}$ is the relative velocity of phase $\pi$ with respect to solid phase ($v^{\text{vn}} = v^{T} - v^{\text{v}}$).

### 2.5 Temporal and spatial discretization

The IGA-FEA model is derived from the weak form of balance equations by applying the Galerkin procedure for spatial integration and Backward Euler time integration. These discretization procedures follow that used in the conventional FEA as outlined in Lewis and Schrefler. The primary variables are approximated in terms of NURBS basis functions as

$$ \mathbf{U} \approx \mathbf{R}_{u} \mathbf{U}, \quad \mathbf{P} \approx \mathbf{R}_{p} \mathbf{P}, \quad \mathbf{T} \approx \mathbf{R}_{T} \mathbf{T} $$

(37)

Following FEA, the spatial discretization within the isoparametric formulation leads to the following nonsymmetric, nonlinear, and coupled system of equations:

$$ \begin{bmatrix} 0 & 0 & 0 & 0 \\ C_{gu} & C_{gg} & C_{gc} & -C_{gT} \\ C_{cu} & C_{cg} & C_{cc} & C_{cT} \\ -C_{Tu} & -C_{Tg} & -C_{Tc} & C_{TT} \end{bmatrix} \begin{bmatrix} \frac{\partial}{\partial t} & \mathbf{P} & \mathbf{P} & \mathbf{T} \end{bmatrix} + \begin{bmatrix} \mathbf{K}_{uu} & -\mathbf{K}_{ug} & \mathbf{K}_{uc} & \mathbf{K}_{UT} \\ 0 & \mathbf{K}_{gg} & -\mathbf{K}_{gc} & -\mathbf{K}_{gT} \\ 0 & -\mathbf{K}_{cg} & \mathbf{K}_{cc} & \mathbf{K}_{cT} \\ 0 & -\mathbf{K}_{Tg} & \mathbf{K}_{Tc} & \mathbf{K}_{TT} \end{bmatrix} \begin{bmatrix} \mathbf{U} \\ \mathbf{P} \\ \mathbf{P} \\ \mathbf{T} \end{bmatrix} = \begin{bmatrix} \mathbf{F}_{u} \\ \mathbf{F}_{g} \\ \mathbf{F}_{c} \\ \mathbf{F}_{T} \end{bmatrix} $$

(38)

where submatrices that express the coupling of mass, energy, and linear momentum conservation are presented in Appendix B. In a more concise form, Equation (38) can be expressed as first order finite difference relationship:

$$ \mathbf{G}(\mathbf{X}) = [\mathbf{C}](\mathbf{X}) + [\mathbf{K}](\mathbf{X}) = \{ \mathbf{F} \} $$

(39)

where $\mathbf{X} = \{ \mathbf{U}, \mathbf{P}, \mathbf{P}, \mathbf{T} \}^{T}$ is the solution vector. Finite difference analysis in time is used for time discretization in this study. The finite time step $t = t_{n+1} - t_{n}$ is used in the Backward Euler scheme to rewrite Equation (39) at time $t_{n+1}$:

$$ \frac{\partial \mathbf{X}}{\partial t} \bigg|_{t_{n+\theta}} = \frac{\mathbf{X}_{n+1} - \mathbf{X}_{n}}{t_{n+\theta}} $$

(40a)

$$ \mathbf{X}_{n+\theta} = [1 - \theta] \mathbf{X}_{n} + \theta \mathbf{X}_{n+1} \text{ with } \theta \in [0, 1] $$

(40b)

where $\mathbf{X}_{n}$ and $\mathbf{X}_{n+1}$ are the solution vectors at $n^{th}$ and $(n+1)^{th}$ time steps. Now, Equation (37) suggests

$$ \mathbf{G}([\mathbf{X}_{n+1}]) = [\mathbf{C} + \theta \mathbf{K}](\mathbf{X}_{n+1}) \mathbf{X}_{n+1} - [\mathbf{C} - (1 - \theta) \Delta t \mathbf{K}](\mathbf{X}_{n+1}) \mathbf{X}_{n} - \Delta t \mathbf{F}_{n+\theta} $$

(41)

The above equation is evaluated using implicit one-step time integration with $\theta = 1$. Next, the nonlinear system of equations is linearized, which is solved numerically as

$$ \frac{\partial \mathbf{G}(\mathbf{X})}{\partial \mathbf{X}} \bigg|_{\mathbf{X}_{n+1}}^{\mathbf{X}_{n+1}} = -\mathbf{G}(\mathbf{X}_{n+1}) $$

(42)

where $i,n$ are the iterations and time steps, respectively, and $\frac{\partial \mathbf{G}(\mathbf{X})}{\partial \mathbf{X}}$ is the Jacobian matrix:
\[
\frac{\partial G(X)}{\partial X} \bigg|_{X^n} = \begin{bmatrix}
\frac{\partial G^u}{\partial U} & \frac{\partial G^u}{\partial P} & \frac{\partial G^P}{\partial U} & \frac{\partial G^P}{\partial P} & \frac{\partial G^g}{\partial U} & \frac{\partial G^g}{\partial P} & \frac{\partial G^c}{\partial U} & \frac{\partial G^c}{\partial P} & \frac{\partial G^T}{\partial U} & \frac{\partial G^T}{\partial P} & \frac{\partial G^{Tg}}{\partial U} & \frac{\partial G^{Tg}}{\partial P} & \frac{\partial G^{Tc}}{\partial U} & \frac{\partial G^{Tc}}{\partial P} & \frac{\partial G^T}{\partial T}
\end{bmatrix}
\]

(43)

Applying the Newton-Raphson scheme to Equation (39), the solution vector \( X \) is updated incrementally (ie, \( X_{n+1} = X_n + X_{n+1} \)). Further details about time integrations and linearization scheme can be found in Lewis and Schrefler.39

3 | NUMERICAL MODELING OF STRAIN LOCALIZATION AND SHEAR BANDING

Strain localization is studied in three examples where the simulations deal with a plane strain compression test of dense sand with respect to different thermal and mechanical loading conditions. Following Sanavia et al26 a rectangular domain consisting of homogenous soil with 34 cm high and 10 cm width is simulated (see Figure 3). Table 1 is the material parameters in this study. The material is assumed to be initially saturated (\( S_w = 1 \)) with the initial water pressure distributed hydrostatically. The boundaries are impervious and adiabatic with the top boundary subjected to a constant displacement rate (\( v_d \)), and the bottom boundary is constrained (\( U_x = U_y = 0 \)). In all examples, the domain is subject to a constant gravity acceleration.

The first study deals with the effect of displacement rate on strain localization and shear banding formation in an isothermal framework. Figure 3A shows that the top boundary of the model is subjected to \( v_d \) ranging from 0.8 to 1.4 mm/s while uniform temperature 293 K is applied throughout the domain. The second study (Figure 3B) shows the effect of temperature on the system where the top boundary is subjected to a fixed displacement rate \( v_d = 1.2 \) mm/s, and the entire domain is exposed to temperatures ranging from 278 to 353 K. Figure 3C shows a schematic model used in the third study where the displacement and temperature rates are varied concurrently. The fixed displacement rate of \( v_d = 1.2 \) mm/s is imposed on the top boundary while at domain boundaries temperature rates \( v_T \) vary from 0.05 to 0.5 K/s.

Figure 3D depicts the discretized domain with 512 IGA quadratic elements. The elements possess \( C^1 \) everywhere except at the top, bottom, left, and right boundaries where the corresponding elements are \( C^{-1} \) to generate the exact boundaries. The maximum aspect ratio, defined as element length over width, is commonly defined to be less than three to avoid zero or near zero Jacobian in the mapping process from parametric space to physical domain.59 To keep the aspect ratio smaller than three in the IGA mesh and reduce the computational cost, a \( C^0 \) internal boundary is imposed at the middle of the domain in the vertical direction (see Figure 3D). The \( C^0 \) is imposed by repeating the associated knot
vectors two times. Consequently, the element aspect ratio is close to one near the \( C^0 \) boundary and is approximately two near the top and bottom boundaries. Without imposing this internal boundary, a much larger number of elements would be needed to keep the maximum aspect ratio less than three. In addition, the given aspect ratio should satisfy the Courant-Friedrichs-Lewy (CFL) condition for each element. The CFL condition relates ratio of the time step to element lengths to the maximum speed that the solution can propagate in the physical space. To satisfy the CFL condition yet reduce the computational cost, the maximum value of time step \( (t) \) for time integration is chosen to be smaller than the critical time step defined as

\[
t_{\text{crit}} = \frac{l}{v} \quad (44)
\]

where \( l \) is the minimum required element length as defined by Schrefler et al. to study strain localization in two-phase simulation problems, and \( v \) is the velocity, which is defined as

\[
v = \sqrt{\frac{k_w}{\rho_w}} \quad (45)
\]

However, if the solution algorithm does not meet the convergence criteria in Newton-Raphson iterations, an adaptive time step procedure is automatically implemented in the simulation procedure. Moreover, Point A in the discretized geometry is considered to quantitatively evaluate the strain localization inside the shear band.

The numerical integration over quadratic IGA elements is executed using \( 3 \times 3 \) Gauss points. The acceptable tolerance for the iterative Newton-Raphson is limited to \( 10^{-5} \) in the linearization process while the number of iterations is fixed to 40. The time step \( (t) \) is set to \( 10^{-3} \) seconds in the time integration scheme. However, during the Newton-Raphson iterations, automatic time step reduction is implemented.

### 4 | COMPARISON WITH FEA

Cao et al. used FEA to model the abovementioned problem in a THM framework with application to strain localization using (backward) Euler and Newmark techniques for time integration. Quadratic Lagrange shape functions \( (C^0) \) were used for spatial integration with a total of 5545 of freedom. Here, the results from quadratic NURBS basis functions with \( C^1 \) property and a total of 3150 degrees of freedom are compared with quadratic Lagrange shape functions with \( C^0 \) continuity. The results reflect the shear banding formation and inelastic strain evolution in two models in the case of isothermal conditions \((T = 293 \, \text{K})\) and \( v_e = 1.2 \, \text{mm/s} \). Figure 4A,B shows the equivalent plastic strain and shear banding after approximately 27 seconds at which point the solution diverged and the simulation was stop. Figure 4A shows shear band formation in the domain where quadratic IGA mesh with \( C^1 \) continuity is used in the model. However, shear banding of the FEA model shown in Figure 4B, which is based on \( C^0 \) continuity.

Figure 4A,B also emphasizes on accumulation of inelastic strain in the shear band core where Figure 4A reveals that plastic strain is distributed among adjacent elements while Figure 4B shows accumulation of inelastic strain at just one node. In addition, the time history for both IGA-FEA and FEA models were studied where maximum accumulation of inelastic strain occurs (shear band core in Figure 4). Figure 5 shows the equivalent plastic strain versus time in the FEA

| TABLE 1 | Material parameters representing dense sand in this study |
|----------|------------------|------------------|------------------|
| Solid density | \( \rho_s \) | 2000 | \( \text{kg.m}^{-3} \) |
| Young modulus | \( E \) | \( 3.0 \times 10^7 \) | Pa |
| Poisson's ratio | \( \nu \) | 0.4 | - |
| Initial apparent cohesion | \( c_0 \) | \( 5.0 \times 10^5 \) | Pa |
| Linear softening modulus | \( h \) | \( -1.0 \times 10^6 \) | Pa |
| Angle of internal friction | \( \phi \) | 30 | degrees |
| Angle of dilatancy | \( \varphi \) | 20 | degrees |
| Porosity | \( n \) | 0.2 | - |
| Intrinsic water/gas permeability | \( K_w = K_g \) | \( 5.0 \times 10^{-14} \) | m\(^2\) |
model and the proposed IGA-FEA framework. The models were observed to show the beginning of the dilation around the same time \( t \approx 8 \text{ s} \) where the plastic strain is nonzero. However, by increasing the time, the two models show different trends. The FEA model shows the maximum inelastic strain value is 0.46 after 27 seconds whereas the IGA-FEA model shows the accumulation of inelastic strain is 0.4 after 27.7 seconds. The inelastic strain distribution shown in Figure 4 suggests that higher-order continuity across elements in NURBS basis functions allows distribution of stress and strain to occur over larger support in the domain.64

To study the dependency of shear band thickness on the number of IGA elements, volumetric plastic strain and equivalent plastic strain are analyzed with three IGA meshes corresponding to 128, 256, and 512 elements. Figure 6 shows that the shear band width is similar in the three models and that the peak values of volumetric strain and inelastic strain are sensitive to the mesh refinement. This observation may be explained as the competing effects of these two length scales in water saturated and unsaturated porous phase indicating the need for further improvement in regularization procedures.

FIGURE 4 Equivalent plastic strain and shear banding in dense sand after approximately 27 seconds with two approaches: A, Quadratic IGA mesh with \( C^1 \) NURBS basis function. B, Quadratic FEA mesh with \( C^0 \) Lagrange shape functions [Colour figure can be viewed at wileyonlinelibrary.com]

FIGURE 5 Time history for equivalent plastic strain (inelastic strain) based on FEA and IGA-FEA approach [Colour figure can be viewed at wileyonlinelibrary.com]
Figure 4A shows the strain distribution over the physical domain. Here, a one-dimensional example is illustrated to explain how strain, pore-water pressure, and temperature fields are distributed over the domain and element boundaries in this study. Figure 7 presents quadratic interpolation functions based on NURBS basis functions and Lagrangian shape functions commonly used in IGA and FEA, respectively. Figure 7A shows that parametric space could be assigned to the entire patch, and internal knots partition the patch into elements in IGA. Consequently, a single map is enough to transfer the entire patch from the parametric space to the physical space. Similarly, the entire patch could be interpolated to obtain the solution in the physical domain. However, in the conventional FEA, the parametric space is local to individual elements where each element has its own mapping from the reference element (Figure 7B).

To establish a side-by-side comparison between FEA and IGA, one can extend the concepts of element and discretization to the physical space in IGA. Referring to Figure 7A, the given physical domain consists of two quadratic IGA elements E1 and E2, which are connected via a $C^1$ boundary. This feature enables IGA elements to transfer fields...
not only from the boundaries but also from the intermediate nodes through the adjacent elements. For instance, for a given integration point within E1, nodes 1, 2, 3 along with basis functions N1,2, N2,2, N3,2 contribute to find the solution at the desired integration point. Similarly, for a given integration point with E2, nodes 2, 3, 4 along with N2,2, N2,3 and N2,4 contribute to find the solution at the given integration point. In this scheme, nodes 2 and 3 and the corresponding basis functions N2,2, N2,3 contribute in finding the solution in both elements E1 and E2.

On the other hand, quadratic Lagrangian elements with \(C^0\) boundary are connected only via nodes located on the boundaries. Consequently, for a given integration point inside E1 with Lagrangian properties (Figure 7B), nodes 1, 2, and 5 along with shape functions N1, N2, and N3 contribute to the solution. Comparing the interpolation scheme for the presumptive integration point in E1 shows that IGA uses wider range of data involving adjacent elements to obtain the solution. Assessing the results from elements with \(C^0\) continuity and \(C^1\) shows that midnodes of the elements with \(C^0\) continuity are just connected to the side nodes of a given element. However, the IGA mesh with \(C^1\) continuity maintains the same level of connectivity for each degree of freedom, thereby providing a larger support across multiple nodes in the problem domain. This concept explains how displacement, strain, and stress are fields interpolated over the domain in IGA and FEA. Subsequently, the inelastic core is distributed over the adjacent elements, while the inelastic strain may accumulate in just one element (or node) in conventional FEA analysis eventually leading to a higher level of equivalent plastic strain in a shorter time.

Our results show that the proposed IGA-based framework can offer a robust alternative for modeling THM problems in unsaturated soils. The accuracy of the proposed framework is shown to be similar or better when compared with an alternative FEA solution. Further, the IGA can simulate the specific problem studied in this paper with lower degrees of freedom compared with FEA. Review of internal length scales and regularization procedures is beyond the scope of the current study and interested readers are referred to the literatures\(^\text{19,53,65-70}\) for further details regarding the effectiveness of length scales and regularization procedures. For instance, Jirásek and Rolshoven\(^\text{66}\) present a nonlocal approach to implement the required length scale in the conventional FEA. As noted previously, in this study, we used the same two regularization procedures, which were implemented in the core FEA solver (ie, COMES-GEO). There are numerous studies in the literature that merely focus on regularization techniques.\(^\text{67-70}\) However, the focus of this study is not about introducing new regularization methods. Rather, the study takes advantage of existing regularization methods to simulate the strain localization problem using the proposed IGA-based framework. Further studies are indeed required to improve regularization techniques. The reason that improving regularization is beyond the scope of this study is the often overlooked fact that introducing regularization changes the physical description of the material. Of course, the regularization gained from the Laplacian term in the flow equation is clearly the result of using Darcy’s law, giving it a clear physical meaning. Such is not the case for plasticity. We do not know the physics behind the addition of gradient terms to the equations of plasticity. These terms are added from mathematical reasoning and might or might not have sound support in material physics.

**FIGURE 8** Shear banding in dense sand after 27 seconds at \(T = 293\) K and constant \(v_d = 1.2\) mm/s: A, Equivalent plastic strain. B, Volumetric strain. C, Capillary pressure (kPa). D, Degree of saturation. E, Water vapor pressure (kPa) [Colour figure can be viewed at wileyonlinelibrary.com]
5 | SIMULATION RESULTS

5.1 | Effect of mechanical loading on strain localization (isothermal)

The numerical results in Figure 8 show the formation of inelastic strain (A), volumetric plastic strain (B), capillary pressure (C), degree of saturation (D), and vapor pressure (E) in the domain when the displacement rate \( v_d = 1.2 \text{ mm/s} \) is applied on the top boundary and the temperature is fixed to 293 K. Figure 8A indicates the formation of equivalent plastic strain in narrow zones after 27.7 seconds. Gravity loading combined with constraint conditions at the bottom boundary lead to higher stress state in this region causing the shear bands to develop toward the top boundary. The maximum inelastic strain (0.4) occurs at \( x = 5 \text{ mm} \) and \( y = 10.94 \text{ mm} \) (Point A in Figure 3D). The positive values inside the shear bands are the result of the plastic dilation of sand (Figure 8B), while the negative values result for elastic compression elsewhere in the domain. Dilation in the shear bands causes water pressure decreases leading to a transition from saturated to unsaturated phase as observed in Figure 8C \( (P_c = 250 \text{ kPa} \text{ at Point A}) \). Subsequently, the degree of saturation decreases in shear bands (Figure 8D), and the phase change from liquid water to gas phase is observed where the vapor pressure \( (P_{gw}) \) is 2.335 kPa at Point A.

The study was extended by varying the displacement rate \( (v_d = 0.8 \text{–} 1.4 \text{ mm/s}) \) and monitoring the capillary pressure, horizontal and vertical displacement, inelastic and volumetric strain, degree of saturation, vapor pressure, and relative humidity at Point A (Figure 3A). Due to symmetry in the geometry and boundary conditions, the horizontal displacement is zero at Point A. Horizontal displacement on the left (A\(^-\)) and right (A\(^+\)) side of A were considered using a tolerance of ±3 mm. Figure 9 shows the capillary pressure and vertical displacement trends at Point A for the different displacement rates implemented at the top boundary. Since capillary pressure is defined as \( P_c = P_g - P_w \) at equilibrium, the negative values of capillary pressure indicate the water pressure above the gas pressure and identify fully saturated conditions. Figure 9A shows that the capillary pressure increases in the saturated zone \( (P_c < 0) \) to −600 kPa regardless the implemented displacement rates. However, the displacement rates affect the time when \( P_c \) reaches −600 kPa leading to different trends for capillary pressure evolution. \( P_c = −600 \text{ kPa} \) is a turning point where the negative capillary pressure decreases indicating the beginning of dilation in the medium, a value close to the magnitude reported in the experimental test for shear band nucleation.\(^{71}\) The inspection of capillary trends at \( P_c = 0 \) reveals that by increasing the displacement rate, the transition from saturated \( (−P_c) \) to unsaturated phase \( (+P_c) \) occurs in a shorter time. For instance, the transition occurs at approximately 35 seconds when the displacement rate is 0.8 mm/s as compared with the transition at 20 seconds when the displacement rate is 1.4 mm/s. Figure 8B emphasizes the symmetric behavior in horizontal displacement while showing the decrease in ultimate horizontal displacement as the displacement rate increases from 0.8 to 1.4 mm/s. Inspection in Figure 9B also reveals that the changes in the slope of displacement trends are observable when the transition occurs from saturated to unsaturated conditions. Figure 9C indicates steeper slopes for vertical displacement trends by increasing in displacement rate at the top boundary. The changes in the slope of displacement trends are compatible with the time when dilation occurs in the medium. As shown, the horizontal displacement is affected by the phase change in the system whereas the vertical displacement is influenced by the dilation in the system. In addition, the ultimate vertical displacement at Point A slightly increases as the displacement rate increases.

FIGURE 9  The effect of displacement rate variation and constant temperature \( (T = 293 \text{ K}) \) at Point A: A, Capillary pressure. B, Horizontal displacement. C, Vertical displacement [Colour figure can be viewed at wileyonlinelibrary.com]
Figure 10A presents the results for plastic strain resulting from different displacement rates. In general, the plastic strain begins in shorter time when the rate of displacement is higher. For instance, the accumulation of plastic strain at Point A begins at $t = 12$ and $6$ seconds where the displacement rates are $0.8$ and $1.4$ mm/s, respectively. In contrast, the ultimate value in plastic strain decreases when the displacement rate increases. For instance, the ultimate plastic strain is close to $0.5$, $0.45$, $0.4$, and $0.38$ where the displacement rate is $0.8$, $1.0$, $1.2$, and $1.4$ mm/s, respectively. The plastic strain trend changes slope when the saturated phase changes to unsaturated phase, as well as developing toward the ultimate plastic strain with a steeper approach. However, the changes in the trends are less pronounced as the rate of displacement increases. In Figure 10B, the volumetric plastic strain shows trends similar to the equivalent plastic strain inside the shear band.

Figure 10C,D,E quantitatively represents the results for fluid constituents in the coupled THM simulation. These figures indicate that the water pressure decreases inside the shear band, a trend that continues until the capillary pressure builds up. Subsequently, cavitation occurs in the medium and the capillary pressure develops above the air entry value where the material shows unsaturated behavior inside the plastic zone. Figure 10C shows the degree of saturation in time series for Point A, and it reveals that the desaturation process rapidly occurs in the system. For instance, the desaturation process begins swiftly at $t = 20$ seconds in the case of $v_d = 1.4$ mm/s and reduces from $100\%$ (saturated) to approximately $40\%$ (unsaturated) in less than $5$ seconds. Figure 10D shows the vapor pressure variations caused by desaturation in the model as the phase changes from liquid to water vapor. The maximum water vapor is limited to $2.338$ kPa based on the surrounding temperature of $T = 293$ K. However, the vapor pressure decreases to $2.333$ kPa when desaturation occurs in the system. Vapor pressure changes affect the gas phase where $P^{ca}$ and $P^{ev}$ show the effects of miscible water vapor interacting with dry air. Figure 10E shows the influence of water vapor variations on the gas phase by determining the relative humidity at Point A where it falls from $100\%$ to approximately $99.8\%$. 

FIGURE 10  The effect of displacement rate on the time history analysis inside the shear band at Point A in isothermal conditions ($T = 293$ K): A, Equivalent plastic strain. B, Volumetric strain. C, Degree of saturation. D, Vapor pressure (kPa). E, Relative humidity [Colour figure can be viewed at wileyonlinelibrary.com]
5.2 Effect of mechanical loading on strain localization (nonisothermal)

The surrounding temperature affects the constitutive models and defines the soil behavior because the temperature directly affects the hydraulic properties and the deformation of soil skeleton. Thus, the temperature effects can lead to considerable loss of load carrying capability. Figure 11A-11E shows the equivalent plastic strain, volumetric plastic strain, capillary pressure, degree of saturation, and water vapor pressure while the surrounding temperature is maintained at 353 K as a constant displacement rate \( v_d = 1.2 \text{ mm/s} \) is applied on the top boundary. Figure 10A,B shows shear banding and volumetric plastic strain in the medium after 24 seconds as 0.6 and 0.35, respectively. Figure 11A,B shows the influence of temperature on inelastic strain and dilation where the inelastic core in the shear band is bigger and covers more elements. In addition, Figure 11C,D,E shows capillary pressure, degree of saturation, and water vapor pressure. Figure 11C shows that most parts of the domain are close to transition from saturated to unsaturated conditions (\( P_c = 0 \)). Nevertheless, the capillary pressure in the shear band is positive with its maximum value of 250 kPa in the inelastic core. Similarly, the degree of saturation in Figure 11D follows the same scenario in Figure 11C but with an elevated degree of saturation in the shear band where the surrounding temperature is \( T = 353 \text{ K} \). The minimum degree of saturation is 40% at Point A and the surrounding plastic core. On the other hand, Figure 11E shows the vapor pressure in the shear band where it drops from 47.41 to 47.34 kPa, corresponding to unsaturated zones. The previously mentioned patterns in the capillary pressure, degree of saturation, and vapor pressure are compatible with the locations where volumetric strain is positive and emphasizes the role of dilation in the analysis of porous media.

In the second study, the effect of temperature on strain localization and shear banding in dense sand is investigated where the temperature varies from \( T = 278 \) to 353 K in the domain, but the constant displacement rate \( v_d \)
= 1.2 mm/s is implemented on the top boundary (see Figure 3B). Figure 12A shows the capillary pressure trends versus time where they linearly decrease due to $v_d = 1.2$ mm/s. However, the trends change after the dilation occurs in the dense sand from negative to positive slopes. The values for capillary pressure and time corresponding to initial dilation become smaller as the values for temperature increase. For instance, dilation occurs at $t \approx 7.5$ seconds and $P_c \approx -545$ kPa for $T = 278$ K while it begins at $t \approx 5.4$ seconds and $P_c \approx -660$ kPa for $T = 353$ K. Moreover, the increase in temperature leads to a decrease in transition time from saturated to unsaturated phase where it shows transition times of 25 and 20 seconds for $T = 278$ and $353$ K, respectively. Figure 12B shows the time history for horizontal displacement at different temperature levels. Increase in temperature leads to escalation in horizontal displacement, whereas it reduces the time for obtaining the ultimate horizontal displacement. For instance, the maximum horizontal displacements, $U_x \approx \pm 2$ mm and $U_x \approx \pm 4$ mm, are shown at 30 and 24 seconds in, respectively, corresponding to temperatures of $T = 278$ and $353$.

Figure 12C depicts the influence of temperature on vertical displacement evolution at Point A where it shows the temperature does not affect the overall trend. However, the increase in temperature reduces the time for ultimate vertical displacement as well as its magnitude. For instance, the time for obtaining $U_y \approx -11$ and $-8.5$ mm is 30 and 24 seconds for $T = 278$ and $353$ K, respectively.

The parametric study was extended to equivalent plastic strain (Figure 13A), volumetric strain (Figure 13B), degree of saturation (Figure 13C), and relative humidity (Figure 13D) while considering different temperature values over the domain. The effect of temperature on equivalent plastic strain is noticeable in Figure 13A where the rise in temperature leads to an increase in equivalent plastic strain as well. In contrast, the temperature increase leads to a reduction in time for attaining the ultimate plastic strain. For instance, the plastic strain magnitude at Point A is approximately 0.6 at $t \approx$...
23 seconds while $T = 353$ K. On the other hand, the ultimate plastic strain is 0.32 at $t = 30$ seconds while $T = 278$ K. Moreover, the plot shows that decreasing the temperature causes a more pronounced transition in equivalent plastic strain and saturated to unsaturated phase evolution.

Dilation in dense sand (corresponding to positive volumetric strain values) also depends on the temperature, wherein Figure 13B shows that dilation begins sooner when temperature increases in the coupled system. In addition, the ultimate volumetric strain also increases with the increase in temperature. The volumetric strain trend is consistent with plastic strain evolution for a given temperature. The ultimate volumetric strain is approximately 0.17, 0.19, 0.27, 0.32, and 0.37 with respect to temperature variations as 278, 293, 308, 323, and 353 K, respectively.

Figure 13C shows the effect of surrounding temperature on degree of saturation. The trends reveal that the rise in temperature reduces the time when desaturation occurs in the medium. Desaturation in the shear bands intersection at Point A occurs at $t \approx 26, 24, 23,$ and 21 seconds considering $T = 278, 293, 308,$ and 323 K, respectively. Note that desaturation occurs at the same time for both $T = 323$ and 353 K. Similarly, Figure 13D shows the time history for relative humidity where it is consistent with desaturation analysis. Whereas the temperature variation affects the time history for degree of saturation and relative humidity, the ultimate values in all trends are almost the same. For instance, the degree of saturation and relative humidity drop from 100% to the averages 40% and 99.8%, respectively.

Unlike the degree of saturation and relative humidity, the temperature variation considerably affects both vapor pressure and time history. Figure 14 shows the effect of surrounding temperature on vapor pressure for $T = 278, 293,$ and 353 K where it shows that the saturated vapor pressure is 0.8725, 2.3388, and 47.412 kPa, respectively. Since the overall trend is similar for all cases, we do not present the vapor pressure trends for $T = 308$ and 323 K in Figure 14. The vapor pressure falls below the saturated vapor pressure at $t = 24, 23,$ and 21 seconds corresponding to $T = 278, 293,$ and 353 K. Figure 14 also shows that the ultimate vapor pressure under unsaturated conditions is 0.8709, 2.3347, and 47.337 kPa, respectively, at $t = 30, 27.7,$ and 24 seconds for $T = 278, 293,$ and 353 K.

![Figure 14](wileyonlinelibrary.com) The effect of temperature on vapor pressure and time history. [Colour figure can be viewed at wileyonlinelibrary.com]

![Figure 15](wileyonlinelibrary.com) Shear banding in dense sand after 3.82 seconds at $v_T = 0.1$ K/s and $v_s = 1.2$ mm/s: A, Equivalent plastic strain. B, Volumetric strain. C, Capillary pressure (kPa). D, Degree of saturation. E, Water vapor pressure (kPa)
5.3 | Effect of thermo-mechanical loading on strain localization

Heat supply leads to expansion of the mixture, which contributes to mechanical loading for the solid skeleton because of the imposed boundary conditions on the top and constrained bottom boundaries. Here, our study is extended over a nonisothermal model where a constant rate displacement \((v_d = 1.2 \text{ mm/s})\) is imposed on the top boundary whereas the entire model is subjected to temperature rate varying from 0.05 to 0.5 K/s (Figure 3C). Figure 15 shows the contour plots for inelastic strain (A), volumetric strain (B), capillary pressure (C), degree of saturation (D), and vapor pressure while the temperature rate \(v_T = 0.1 \text{ K/s}\).

Figure 15A shows the distribution of inelastic strain over the domain where a shear band forms after 3.82 seconds. Two symmetric plastic zones form and develop toward the upper parts of the domain. Due to stress intensity induced by the combination of \(v_T\) and \(v_d\), the unsaturated zone forms abruptly at Point A and corners of the model while the minimum degree of saturation is limited to 98.3%. Figure 16A shows the effect of displacement and thermal rates on capillary pressure evolution at Point A. Time history analysis shows that the increase in temperature rate leads to a decrease in the maximum pore-water pressure \((-P_c)\) where it decreases from \(-411\) to \(-267 \text{ kPa}\) with respect to temperature rate variation from 0.05 to 0.5 K/s. In addition, the increase in temperature rate also shows that the time for dilation occurrence reduces from 4 to 1.15 seconds. The analysis shows that the unsaturated zone negligibly develops in simulation before divergence occurs in the model representing failure in the system. Figure 16B,C highlights the effect of temperature rate on displacement evolution; the vertical and horizontal displacements reduce significantly as the temperature rate increases in the system. The slope for vertical displacements is constant for the all cases while the vertical displacement magnitudes reduce significantly with respect to \(v_T = 0.05, 0.1, 0.2, 0.3, \text{ and } 0.5 \text{ K/s}\).

Figure 17 shows the inelastic strain (A), volumetric strain (B), and vapor pressure (C) in a time history analysis at Point A. Figure 17A shows that the plastic strain is reduced significantly as the temperature rate increases. The equivalent plastic strain abruptly begins at t = 4.1, 3, 2.1, 1.7, and 1.1 seconds corresponding to \(v_T = 0.05, 0.1, 0.2, 0.3, \text{ and } 0.5 \text{ K/s}\).

**FIGURE 16** The effect of temperature \((v_T)\) and displacement rate \((v_d)\) at Point A: A, Capillary pressure. B, Horizontal displacement. C, Vertical displacement [Colour figure can be viewed at wileyonlinelibrary.com]

**FIGURE 17** The effect of displacement and temperature rates on the time history analysis inside the shear band at Point A: A, Equivalent plastic strain. B, Volumetric strain. C, Vapor pressure (kPa) [Colour figure can be viewed at wileyonlinelibrary.com]
0.3, and 0.5 K/s, respectively. The volumetric plastic strain shown in Figure 17B is consistent with equivalent plastic strain, except that the changes in the time history in volumetric plastic strain appear smoother compared with equivalent plastic strain in Figure 17A. Figure 17C depicts the effect of temperature rate on vapor pressure where the increase in temperature rate leads to exponential variation in vapor pressure trends. The transition from saturated to unsaturated conditions instantly occurs when the temperature and displacement rate are simultaneously imposed in this model. The changes in degree of saturation and relative humidity were negligible, thus are not shown in Figure 17.

6 | DISCUSSION

Comparing the results from the analyses demonstrates the impact of mechanical load, temperature, and thermo-mechanical loads on porous media. From the mechanical point of view, comparing the results for horizontal deformation in three studies (Sections 5.1, 5.2, and 5.3) shows how the temperature and mechanical loading affect the soil behavior. The lateral displacement increases as the surrounding temperature increases whereas the mechanical loading rate decreases. The thermo-mechanical loading considerably affects the horizontal displacement. The results in Section 5.3 show that the soil reaches the state of failure in a very short time when the maximum thermo-mechanical load is applied on the soil ($v_T = 1.2 \text{ mm/s}$ and $v_T = 0.5 \text{ K/s}$). The inspection in vertical displacement shows that despite the lateral deformation, the vertical displacement decreases as the surrounding temperature increase. In contrast to the variations in the slope of vertical displacement trend in Section 5.1, the temperature and temperature rate variations do not affect the rate of vertical deformation in the soil. The plastic strain is reduced as mechanical load increases and surrounding temperature decrease, which indicates that the soil reaches the state of failure in low temperatures and intensified mechanical loading conditions.

For the fluid analysis, the variation in mechanical loading reduces the time for the capillary pressure to obtain its maximum value, but it does not affect the maximum value. However, the maximum capillary pressure increases as the surrounding temperature increases whereas it also reduces the corresponding time. The imposed thermo-mechanical loading significantly reduces both maximum capillary pressure and corresponding time. The dilation in shear bands leads to desaturation of soil in this region. However, the unsaturated zone has no significant role when a thermo-displacement rate is imposed on the model. The minimum degree of saturation is observed as 40% in Sections 5.1 and 5.2 where the variation in mechanical loading and surrounding temperature is implemented. The increase in the surrounding temperature and displacement rate reduces the time when desaturation occurs in the system. Moreover, the effect of displacement rate variation on transition time is more evident than the rise in the surrounding temperature. The rise in surrounding temperature only increases the saturated vapor saturation level, and it drops when unsaturated zone forms. On the other hand, the vapor pressure exponentially increases when the thermo-displacement rate is imposed.

7 | CONCLUSIONS

In this research an alternative numerical framework is introduced to model THM problems in unsaturated soils with application in strain localization. We use NURBS basis functions in an IGA framework in the simulation process. We implemented the IGA-FEA interface using Bézier-extraction operator to derive NURBS from the THM finite element code (COMES-GEO). The proposed method introduces higher orders of approximation functions and interelement connectivity along the element's boundaries. Interelement connectivity and uniform basis functions in a coupled THM model enable IGA to properly capture strain localization features. The results of this study demonstrate that the combination of the second order of approximation functions along with $C^1$ continuity helps to distribute smoothly the inelastic strain over the domain (elements).

Using IGA with higher order basis functions and interelement connectivity over the IGA elements provides a larger support across multiple nodes in the problem domain. Implementing the aforementioned continuity across the IGA elements mitigates deleterious effects of possible oscillations in the results and provides larger support for strain distribution over the domain. Instabilities in the results can be observed when the orders of approximation are not selected appropriately for different fields (i.e., solid, fluid, and gas phases) in THM problems. Accordingly, mixed elements are commonly used in numerical methods such as FEA, with each field having a different order of approximation. Although it is well understood that equal order of approximations is not prone to inf-sup instabilities, the IGA-FEA
framework proposed in this study is not faced with such problems. Comparing the results with those attained from the conventional FEA reveals that the proposed IGA-FEA framework is able to simulate strain localization and shear banding using fewer degrees of freedoms. The results suggest that the proposed IGA-FEA framework offers a robust alternative for numerical modeling of THM problems in unsaturated soils.

The studies of shear banding on dense sand under different compressional displacement rates, surrounding temperatures, and thermo-mechanical loads emphasize the importance of temperature effects on shear band formation. Dense sand reaches the state of failure in shorter time when exposed to higher mechanical loads while the surrounding temperature is low and vice versa. In addition, applied thermo-mechanical rates on the model show that expansion due to dilation occurs in considerably shorter time and vapor pressure exponentially increases in the domain with respect to growth in temperature magnitudes. The results show that the surrounding temperature governs the dense sand behavior with respect to inelastic strain, volumetric strain, and vapor pressure variation.

ACKNOWLEDGEMENT

This material is based upon work supported in part by the National Science Foundation under Grant No. CMMI-1634748. Any opinions, findings, and conclusions or recommendations expressed in this material are those of the authors and do not necessarily reflect the views of the National Science Foundation. The authors would like to thank Prof. Thomas JR Hughes and his team in the Institute for Computational Engineering and Sciences (ICES), the University of Texas at Austin for their helpful comments in developing numerical formulations. The authors greatly appreciate Dr. John Peters for his assistance for the revision of this paper.

ORCID

Farshid Vahedifard https://orcid.org/0000-0001-8883-4533

REFERENCES

1. Schrefler BA. Computer modelling in environmental geomechanics. Computers & Structures. 2001; 79(22-25): 2209-2223.
2. Vahedifard F, AghaKouchak A, Robinson JD. Drought threatens California’s levees. Science. 2015; 349(6250): 799. https://doi.org/10.1126/science.349.6250.799-a
3. Laloui L, Nuth M, Vulliet L. Experimental and numerical investigations of the behaviour of a heat exchanger pile. International Journal for Numerical and Analytical Methods in Geomechanics. 2006; 30(8): 763-781.
4. Robinson JD, Vahedifard F. Weakening mechanisms Impose on California’s levees under multiyear extreme drought. Climatic Change. 2016; 137(1): 1-14. https://doi.org/10.1007/s10584-016-1649-6
5. McCartney, J.S., Jafari, N.H., Hueckel, T., Sanchez, M., Vahedifard, F. (2019). Thermal energy issues in geotechnical engineering. Geotechnical Fundamentals for Addressing New World Challenges. N. Lu and J.K. Mitchell, Eds. Springer. 275-317, ISBN: 978-3-030-06249-1, https://doi.org/10.1007/978-3-030-06249-1_10
6. Leshchinsky B, Vahedifard F, Koo HB, Kim SH. Yumokjeong Landslide: an investigation of progressive failure of a hillslope using the finite element method. Landslides. 2015; 12(5):997-1005. https://doi.org/10.1007/s10346-015-0610-5
7. Shahrokhabadi S, Cao TD, Vahedifard F. Thermal effects on hydro-mechanical response of seabed supporting hydrocarbon pipelines. Int J Geomechanics. 2019. https://doi.org/10.1061/(ASCE)GM.1943-5622.0001534
8. Goodman CC, Vahedifard F. Microstructural evaluation of clay at elevated temperatures. Geotechnique Letters. 2019; 9(3): 225-230. https://doi.org/10.1680/jgele.19.00026
9. Vahedifard F, Cao TC, Ghazanfari E, Thota SK. Closed-form models for nonisothermal effective stress of unsaturated soils. Journal of Geotechnical and Geoenvironmental Engineering, ASCE. 2019; 145(9): 04019053. https://doi.org/10.1061/(ASCE)GT.1943-5606.0002094
10. Vahedifard F, Cao TC, Thota SK, Ghazanfari E. Nonisothermal models for soil water retention curve. Journal of Geotechnical and Geoenvironmental Engineering, ASCE. 2018; 144(9): 04018061. https://doi.org/10.1061/(ASCE)GT.1943-5606.0001939
11. Gens A. Constitutive Laws. New York: Springer; 1995.
12. Bolzon G, Schrefler BA. Thermal effects in partially saturated soils: a constitutive model. International journal for numerical and analytical methods in geomechanics. 2005; 29(9): 861-877.
13. François B, Laloui L. Unsaturated soils under non-isothermal conditions: framework of a new constitutive model. In: GeoCongress 2008: Characterization, Monitoring, and Modeling of GeoSystems; 2008:1077-1083.
14. Mašín D, Khalili N. A thermo-mechanical model for variably saturated soils based on hypoplasticity. International Journal for Numerical and Analytical Methods in Geomechanics. 2012; 36(12): 1461-1485.
15. Song X, Wang K, Ye M. Localized failure in unsaturated soils under non-isothermal conditions. Acta Geotechnica. 2017;1-13.
16. De Borst R, Sluys LJ, Muhlhaus HB, Pamin J. Fundamental issues in finite element analyses of localization of deformation. Engineering Computations. 1993;10(2):99-121.
17. Rice JR, Rudnicki JW. A note on some features of the theory of localization of deformation. International Journal of Solids and Structures. 1980;16(7):597-605.
18. Vardoulakis I. Deformation of water-saturated sand: I. uniform undrained deformation and shear banding. Géotechnique. 1996;46(3):441-456.
19. Zhang HW, Schrefler BA. Gradient-dependent plasticity model and dynamic strain localization analysis of saturated and partially saturated porous media: one dimensional model. European Journal of Mechanics-A/Solids. 2000;19(3):503-524.
20. Jiang M, Chen H, Tapias M, Arroyo M, Fang R. Study of mechanical behavior and strain localization of methane hydrate bearing sediments with different saturations by a new DEM model. Computers and Geotechnics. 2014;57:122-138.
21. Zhu H, Zhou WH, Yin ZY. Deformation mechanism of strain localization in 2D numerical interface tests. Acta Geotechnica. 2017;1-17.
22. Borja RI. Cam-Clay plasticity. Part V: A mathematical framework for three-phase deformation and strain localization analyses of partially saturated porous media. Computer methods in applied mechanics and engineering. 2004;193(48-51):5301-5338.
23. Callari C, Armero F, Abati A. Strong discontinuities in partially saturated poroplastic solids. Computer Methods in Applied Mechanics and Engineering. 2010;199(23-24):1513-1535.
24. Ehlers W, Graf T, Ammann M. Deformation and localization analysis of partially saturated soil. Computer methods in applied mechanics and engineering. 2004;193(27-29):2885-2910.
25. Song X. Transient bifurcation condition of partially saturated porous media at finite strain. International Journal for Numerical and Analytical Methods in Geomechanics. 2017;41(1):135-156.
26. Sanavia L, Pesavento F, Schrefler BA. Finite element analysis of non-isothermal multiphase geomaterials with application to strain localization simulation. Computational Mechanics. 2006;37(4):331.
27. Hassanizadeh M, Gray WG. General conservation equations for multi-phase systems: 1. Averaging procedure. Advances in Water Resources. 1979;2:131-144.
28. Hassanizadeh M, Gray WG. General conservation equations for multi-phase systems: 2. Mass, momenta, energy, and entropy equations. Advances in Water Resources. 1979;2:191-203.
29. Hassanizadeh M, Gray WG. General conservation equations for multi-phase systems: 3. Constitutive theory for porous media flow. Advances in Water Resources. 1980;3(1):25-40.
30. Cao TD, Sanavia L, Schrefler BA. A thermo-hydro-mechanical model for multiphase geomaterials in dynamics with application to strain localization simulation. International Journal for Numerical Methods in Engineering. 2016;107(4):312-337.
31. Hughes TJ, Cottrell JA, Bazilevs Y. Isogeometric analysis: CAD, finite elements, NURBS, exact geometry and mesh refinement. Computer methods in applied mechanics and engineering. 2005;194(39):4155-4195.
32. Irzal F, Remmers JJ, Verhoosel CV, Borst R. Isogeometric finite element analysis of poroelasticity. International Journal for Numerical and Analytical Methods in Geomechanics. 2013;37(12):1891-1907.
33. Irzal F, Remmers JJ, Verhoosel CV, Borst R. An isogeometric analysis Bézier interface element for mechanical and poromechanical fracture problems. International Journal for Numerical Methods in Engineering. 2014;97(8):608-628.
34. Nguyen MN, Bui TQ, Yu T, Hirose S. Isogeometric analysis for unsaturated flow problems. Computers and Geotechnics. 2014;62:257-267.
35. Shahrokhabadi S, Vaheedifard F, Bhatia M. Head-based isogeometric analysis of transient flow in unsaturated soils. Computers and Geotechnics. 2017;84:183-197.
36. Shahrokhabadi S, Cao TD, Vaheedifard F. Isogeometric analysis through Bézier extraction for thermo-hydro-mechanical modeling of saturated porous media. Computers and Geotechnics. 2019;107. https://doi.org/10.1016/j.compgeo.2018.11.012
37. Bekele YW, Kyokawa H, Kvarving AM, Kvamsdal T, Nordal S. Isogeometric analysis of THM coupled processes in ground freezing. Computers and Geotechnics. 2017;88:129-145.
38. Remij EW, Pesavento F, Bazilevs Y, Smeulders DMJ, Schrefler BA, Huyghe JM. Isogeometric analysis of a multiphase porous media model for concrete. Journal of Engineering Mechanics. 2017;144(2):04017169.
39. Lewis RW, Schrefler BA. The Finite Element Method in the Static and Dynamic Deformation and Consolidation of Porous Media. John Wiley; 1998.
40. Zienkiewicz OC, Chan AHC, Pastor M, Schrefler BA, Shomi T. Computational Geomechanics. Chichester: Wiley; 1999.
41. Drucker DC, Prager W. Soil mechanics and plastic analysis for limit design. Quarterly of Applied Mathematics. 1952;10(2):157-165.
42. Hyland RW, Weder A. Formulations for the thermodynamic properties of dry air from 173.15 K to 473.15 K, and of saturated moist air from 173.15 K to 372.15 K, at pressures to 5 MPa. ASHRAE Transactions. 1983;89(2A):520-535.
43. Hyland RW, Weder A. Formulations for the thermodynamic properties of the saturated phases of H₂O from 173.15 K to 473.15 K. ASHRAE Transactions. 1983;89(2A):500-519.
44. Hofstetter G, Taylor RL. Treatment of the corner region for Drucker-Prager type plasticity. *Zeitschrift für angewandte Mathematik und Mechanik*. 1991;71(6):TS89-TS91.
45. Sanavia L, Schrefler BA, Steinmann P. A formulation for an unsaturated porous medium undergoing large inelastic strains. *Computational Mechanics*. 2002;28(2):137-151.
46. Szabó L, Kossa A. A new exact integration method for the Drucker-Prager elastoplastic model with linear isotropic hardening. *International Journal of solids and structures*. 2012;49(1):170-190.
47. Simo JC. Numerical analysis and simulation of plasticity. *Handbook of Numerical Analysis*. 1998;6:183-499.
48. Lasry D, Belytschko T. Localization limiters in transient problems. *International Journal of Solids and Structures*. 1988;24(6):581-597.
49. Sluys L. J., & Wave propagation, localisation and dispersion in softening solids, Ph.D. thesis, Department of Civil Engineering, Delft University of Civil Engineering, Netherlands.
50. Schrefler BA, Majorana CE, Sanavia L. Shear band localization in saturated porous media. *Arch. Mech*. 1995;47(3):577-599.
51. Schrefler BA, Sanavia L, Majorana CE. A multiphase medium model for localisation and postlocalisation simulation in geomaterials. *Mechanics of Cohesive-frictional Materials: An International Journal on Experiments, Modelling and Computation of Materials and Structures*. 1996;1(1):95-114.
52. Zhang HW, Sanavia L, Schrefler BA. An internal length scale in dynamic strain localization of multiphase porous media. *Mechanics of Cohesive-frictional Materials: An International Journal on Experiments, Modelling and Computation of Materials and Structures*. 1999;4(5):443-460.
53. Sanavia L, Pesavento F, Schrefler BA. Finite element analysis of strain localization in multiphase materials. *Revue européenne de genie civil*. 2005;9(5-6):767-778.
54. Sulem J, Vardoulakis IG. *Bifurcation Analysis in Geomechanics*. CRC Press; 2014.
55. Schrefler BA, Zhang HW, Sanavia L. Interaction between different internal length scales in strain localization analysis of fully and partially saturated porous media—the 1-D case. *International journal for numerical and analytical methods in geomechanics*. 2006;30(1):45-70.
56. De Boor C. On calculating with B-splines. *Journal of Approximation theory*. 1972;6(1):50-62.
57. Farouki RT, Rajan VT. Algorithms for polynomials in Bernstein form. *Computer Aided Geometric Design*. 1988;5(1):1-26.
58. Borden MJ, Scott MA, Evans JA, Hughes TJ. Isogeometric finite element data structures based on Bézier extraction of NURBS. *International Journal for Numerical Methods in Engineering*. 2011;87(1-5):15-47.
59. Bhatti MA. *Fundamental Finite Element Analysis and Applications: With Mathematica and Matlab Computations* (p. 720). Hoboken, NJ: John Wiley; 2005.
60. Schrefler BA, Majorana CE, Sanavia L. Shear band localization in saturated porous media. *Archives of Mechanics*. 1995;47(3):577-599.
61. Biot MA. Theory of propagation of elastic waves in a fluid-saturated porous solid, part I-low-frequency range. *The Journal of the Acoustical Society of America*. 1956;28(2):168-178.
62. Biot MA. Theory of propagation of elastic waves in a fluid-saturated porous solid, part II-low-frequency range. *The Journal of the Acoustical Society of America*. 1956;28(2):179-191.
63. Gawin D, Schrefler BA. Thermo-hydro-mechanical analysis of partially saturated porous materials. *Engineering Computations*. 1996;13(7):113-143.
64. Plúa C, Tamagnini C, Bésuelle P. Isogeometric analysis of hydro-mechanical problems in saturated soils with second gradient regularization. In: *Poromechanics VI*. 304-311.
65. Diebels S, Ehlers W, Ellsiepen P, Volk W. On the regularization of shear band phenomena in liquid-saturated and empty soils. In: Brillard A, Ganghoffer JF, eds. *Proceedings of the Euromech Colloquium 378 on Nonlocal Aspects in Solid Mechanics*, University of Mulhouse; 1998:58-63.
66. Jirásek M, Rohlshoven S. Comparison of integral-type nonlocal plasticity models for strain-softening materials. *International Journal of Engineering Science*. 2003;41(13-14):1553-1602.
67. Simone A, Askes H, Sluys LJ. Incorrect initiation and propagation of failure in non-local and gradient-enhanced media. *International journal of solids and structures*. 2004;41(2):351-363.
68. Chen JS, Zhang X, Belytschko T. An implicit gradient model by a reproducing kernel strain regularization in strain localization problems. *Computer methods in applied mechanics and engineering*. 2004;193(27-29):2827-2844.
69. Jirásek M. Objective modeling of strain localization. *Revue française de génie civil*. 2002;6(6):1119-1132.
70. Wells GN, Sluys LJ, de Borst R. Simulating the propagation of displacement discontinuities in a regularized strain-softening medium. *International Journal for Numerical Methods in Engineering*. 2002;53(5):1235-1256.
APPENDIX A.

SUPPLEMENTARY EQUATIONS

In conjunction with linear momentum, mass, energy balance, and constitutive equations, the following supplementary equations and parameters in Table A.1 are used in this study30:

\[
\beta_{sw} = \beta_s [1 - n] + n \beta_w S_w
\]

\[
(\rho C_p)_{eff} = (1 - n)\rho_s C_s^p + n \rho_w C_w^p + n \rho_s [1 - S_w] C_s^p
\]

\[
\chi_{eff} = \chi_{dry} \left[ 1 + \frac{4 n S_w \rho_w}{[1 - n] \rho_s} \right]^{\cdot}
\]

where \( \beta_s \) and \( \beta_w \) are the thermal expansion coefficient for solid and water constituents, \( C_s^p \) is the specific heat of solid, and \( \chi_{dry} \) is thermal conductivities in isotropic constituents, respectively.

Hyland-Wexler equation expresses the water vapor saturation pressure depending on the temperature \( T \) as42,43

\[
P_{gw}(T) = \exp \left( \frac{c_8}{T} + c_9 T + c_{10} T^2 + c_{11} T^3 + c_{12} T^4 + c_{13} \ln(T) \right)
\]

(A.2)

where \( T \) is absolute temperature and the rest of coefficients are \( c_8 = -5.80 e^3 \), \( c_9 = 1.39 \), \( c_{10} = -4.86 e^{-2} \), \( c_{11} = -4.18 e^{-5} \), \( c_{12} = -1.44 e^{-8} \), and \( c_{13} = 6.54 \).

The degree of saturation and relative permeability in the liquid phase are defined as30

\[
S_w = S_r + (1 - S_r) \left( \frac{P^b}{P^c} \right) \lambda \left\{ \begin{array}{ll}
S_w = 1 & \text{if } P^c \leq P^b \\
S_w = S_r & \text{if } P^c \geq 1 e^8
\end{array} \right.
\]

(A.3a)

| TABLE A.1 Parameters used in this study |
|---------------------------------------|
| **Molar mass of dry air** | \( M_a \) | \( 2.89 e^{-5} \text{ (m}^3 \text{.mol}^{-1}) \) |
| **Molar mass of liquid water** | \( M_{w} \) | \( 1.8 e^{-5} \text{ (m}^3 \text{.mol}^{-1}) \) |
| **Universal gas constant** | \( R \) | \( 8.314 \text{ (J.mol}^{-1}.K^{-1}) \) |
| **Thermal expansion coefficient of water** | \( \beta_w \) | \( 3.42 e^{-4} \text{ (K}^{-1}) \) |
| **Thermal expansion coefficient of solid** | \( \beta_s \) | \( 0.9 e^{-4} \text{ (K}^{-1}) \) |
| **Specific heat of solid** | \( C_s^p \) | \( 16760 \text{ (J.Kg}^{-1}.K^{-1}) \) |
| **Specific heat of water** | \( C_w^p \) | \( 4181 \text{ (J.Kg}^{-1}.K^{-1}) \) |
| **Specific heat of gas** | \( C_g^p \) | \( 1005.7 \text{ (J.Kg}^{-1}.K^{-1}) \) |
| **Thermal conductivities in soli constituent** | \( \chi_{dry} \) | \( 0.84 \text{ W.M}^{-1}.K^{-1} \) |
| **Residual saturation** | \( S_r \) | \( 0.2 \) |
| **Bubbling pressure** | \( P^b \) | \( 1680 \text{ (Pa)} \) |
| **Pore size distribution** | \( \lambda \) | \( 3 \) |
| **Effective diffusivity tensor** | \( D_{gw}^{pg} = D_{gw}^{pa} \) | \( 2.5 e^{-5} \) |
\[ S_e = \frac{S_w - S_r}{1 - S_r} \] (A.3b)

\[ k^{\text{rw}} = \frac{S_e}{\lambda} \begin{cases} k^{\text{rw}} = 0 & \text{if } S_w \leq S_r \\ k^{\text{rw}} = 1 & \text{if } S_w = 1 \end{cases} \] (A.3c)

where \( S_r \) is the residual saturation, \( P_b \) is the bubbling pressure, \( \lambda \) is pore size distribution, and \( S_e \) is effective degree of saturation. The relative permeability in the gas phase is defined based on Brooks and Corey as\(^{44}\)

\[ k^{\text{rw}} = (1-S_e)^2 \left( 1 - S_e \left( \frac{h}{h_e} \right)^{1.59} \right) \] (A.4)

Water properties (\( \mu_w, \rho_w \)) are dependent on the temperature, and the following supplementary equations define\(^{45,46}\)

\[ \mu_w = 0.6612(T-229)^{-1.562} \] (A.5a)

\[ \rho_w = (b_0 + b_1T + b_2T^2 + b_3T^3 + b_4T^4 + b_5T^5) + (a_0 + a_1T + a_2T + a_3T^3 + a_4T^4 + a_5T^5) \left( \rho_{w1} - \rho_{wrf} \right) \] (A.5b)

where \( T \) is temperature in Celsius (\( T_c = T - 273.15 \)), and the rest of coefficients are \( b_0 = 1.02e^3, b_1 = -7.74e^{-1}, b_2 = 8.77e^{-3}, b_3 = 9.21e^{-5}, b_4 = 3.35e^{-7}, b_5 = -4.40e^{-10}, a_0 = 4.89e^{-7}, a_1 = -1.65e^{-9}, a_2 = 1.86e^{-12}, a_3 = 2.43e^{-13}, a_4 = -1.59e^{-15}, a_5 = 3.37e^{-18}. \)

The latent heat is approximated by Watson formula as\(^{45,47}\)

\[ \Delta H_{\text{vap}} = 2.672[T_{\text{crit}} - T]^{0.38} \times 1.0e^5 \] (A.7)

where \( T_{\text{crit}} = 647.3 \text{ K} \) is the critical temperature of water.

**APPENDIX B.**

**SUBMATRICES IN THM FORMULATION**

The matrices that show the discretized form of linear momentum, mass, and energy balance equations:

\[ \mathbf{K}_{\text{ug}} = \int \mathbf{B}^T \mathbf{m} \mathbf{R}_g d\Omega \] (B.1)

\[ \mathbf{K}_{\text{uc}} = \int \mathbf{B}^T \mathbf{m} S_w \mathbf{R}_c d\Omega \] (B.2)

\[ \mathbf{F}_u = \int \mathbf{R}_u^T \rho g d\Omega + \int \mathbf{R}_u^T \mathbf{f} d\Gamma \] (B.3)

\[ \mathbf{C}_{\text{gg}} = \int \mathbf{R}_g^T \left[ n_g S_g \left( \frac{\partial \rho}{\partial P} \right) \right] \mathbf{R}_g d\Omega \] (B.4)

\[ \mathbf{C}_{\text{gc}} = \int \mathbf{R}_g^T \left[ n_g S_g \left( \frac{\partial \rho}{\partial P} \right) - n P \frac{\partial S_w}{\partial P} \right] \mathbf{R}_c d\Omega \] (B.5)
\[ C_{gt} = \int R_T \left[ \rho \frac{\partial S_w}{\partial T} - n[1 - S_w] \frac{\partial \rho_{sw}}{\partial T} + \rho_{sw}[1 - n][1 - S_w] \right] R_T d\Omega \] (B.6)

\[ C_{gu} = \int R_T [\rho_{sw}[1 - S_w]] m^T B d\Omega \] (B.7)

\[ K_{gg} = \int \nabla R_T \left[ \rho \frac{k^g K^g}{\mu^g} + \frac{\rho \theta M_a M_w D^{e_w} p^{e_w}}{M^g} \right] \nabla R_g d\Omega \] (B.8)

\[ K_{gc} = \int \nabla R_T \left[ \frac{\rho \theta M_a M_w D^{e_w} 1}{p^w} \frac{\partial p^{e_w}}{\partial P^w} \right] \nabla R_c d\Omega \] (B.9)

\[ K_{cT} = \int \nabla R_T \left[ \frac{\rho \theta M_a M_w D^{e_w} 1}{p^w} \frac{\partial p^{e_w}}{\partial P^w} \right] \nabla R_T d\Omega \] (B.10)

\[ F_g = \int \nabla R_T \left[ \rho \frac{k^g K^g}{\mu^g} \rho^w \right] gd\Omega - \int R_T [q^w] q^w d\Omega \] (B.11)

\[ C_{cg} = \int R_T \left[ \frac{\rho n S_w}{K_w} \right] R_g d\Omega \] (B.12)

\[ C_{cc} = \int R_T \left[ \rho w S_w + \frac{\partial S_w}{\partial P^w} + n[1 - S_w] \frac{\partial \rho_{sw}}{\partial P^w} - \rho_{sw} \frac{n S_w}{K_w} \right] R_c d\Omega \] (B.13)

\[ C_{ct} = \int R_T \left[ -\rho w [1 - n][1 - S_w] + n[1 - S_w] \frac{\partial \rho_{sw}}{\partial T} + \rho w \frac{n S_w}{K_w} \right] R_T d\Omega \] (B.14)

\[ C_{cu} = \int R_T [\rho w S_w + \rho_{sw}[1 - S_w]] m^T B d\Omega \] (B.15)

\[ K_{cg} = \int \nabla R_T \left[ \frac{\rho \theta M_a M_w D^{e_w} p^{e_w}}{M^g} \right] \nabla R_c d\Omega \] (B.16)

\[ K_{cc} = \int \nabla R_T \left[ \frac{\rho \theta M_a M_w D^{e_w} 1}{p^w} \frac{\partial p^{e_w}}{\partial P^w} - \rho w \frac{k^{e_w} K^w}{\mu^w} \right] \nabla R_c d\Omega \] (B.17)

\[ K_{cT} = \int \nabla R_T \left[ \frac{\rho \theta M_a M_w D^{e_w} 1}{p^w} \frac{\partial p^{e_w}}{\partial P^w} \right] \nabla R_T d\Omega \] (B.18)

\[ F_c = -\int \nabla R_T \left[ -\rho w \frac{k^{e_w} K^w}{\mu^w} \right] gd\Omega - \int R_T [q^w + q^{e_w} + \beta_c [\rho_{sw} - \rho_{sw}]] d\Omega \] (B.19)

\[ C_{Tg} = \int R_T \left[ \frac{\rho n S_w}{K_w} \Delta H_{vap} \right] R_g d\Omega \] (B.20)
\[
\begin{align*}
C_{Tc} &= \int R_T^T \left[ \Delta H_{vap} \left[ n \left( \rho^w - \rho^n \right) - nS_w \frac{\partial S_w}{\partial P} - \rho^w \frac{\partial \rho^w}{\partial T} \right] \right] R_T d\Omega \\
C_{TT} &= \int R_T^T \left[ (\rho C_p)_\text{eff} + \beta_{sw} H_{vap} - H_{vap} n \left( \rho^w - \rho^n \right) \frac{\partial S_w}{\partial T} \right] R_T d\Omega \\
C_{Tu} &= \int R_T^T \left[ \rho^w S_w H_{vap} \left[ \kappa^w \right] \right] \nabla R_T d\Omega \\
K_{Tg} &= \int \nabla R_T^T \left[ \rho^w H_{vap} \frac{k^w \kappa^w}{\mu^w} \right] \nabla R_g d\Omega \\
K_{Tc} &= \int \nabla R_T^T \left[ \rho^w H_{vap} \frac{k^w \kappa^w}{\mu^w} \right] \nabla R_c d\Omega \\
K_{TT} &= \int R_T^T \left[ \rho^w C_p \frac{k^w \kappa^w}{\mu^w} \left[ - \nabla R_g \tilde{B}^{\tilde{g}} + \nabla R_g \tilde{P}^{\tilde{c}} + \rho^w \tilde{g} \right] + \rho^w C_p \frac{k^w \kappa^w}{\mu^w} \left[ - \nabla R_g \tilde{B}^{\tilde{g}} + \rho^w \tilde{g} \right] \right] \nabla R_T d\Omega \\
F_T &= \int R_T^T \left[ \left( q^T + \alpha_c \left[ T - T_\infty \right] \right) dT - \int \nabla R_T^T \left[ \Delta H_{vap} \left( \rho^w \right) \frac{k^w \kappa^w}{\mu^w} \right] \nabla R_T d\Omega \right]
\end{align*}
\]

where:

\[
B = \nabla R_u = \begin{bmatrix}
\frac{\partial R_1}{\partial x} & 0 & \frac{\partial R_2}{\partial x} & 0 & \ldots & \frac{\partial R_{nR}}{\partial x} & 0 \\
0 & \frac{\partial R_1}{\partial y} & 0 & \frac{\partial R_2}{\partial y} & \ldots & 0 & \frac{\partial R_{nR}}{\partial y} \\
\frac{\partial R_1}{\partial y} & \frac{\partial R_2}{\partial y} & \ldots & \frac{\partial R_{nR}}{\partial y} & \frac{\partial R_1}{\partial x} & 0 & \ldots & \frac{\partial R_{nR}}{\partial x} \\
\end{bmatrix}
\]

\[
m = \{1, 1, 1, 0, 0, 0\}^T
\]