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Three-invariant model and bifurcation analysis of deformation bands for a sandstone subjected to true triaxial loading paths

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Abstract

This paper presents a general three-invariant model to evaluate the theoretical prediction of strain localization against laboratory measurements performed during mechanical loading experiments, for a high-porosity Vosges sandstone (North-Eastern France). The model is based on a mean stress and Lode angle-dependent yield surface, calibrated using extensive experimental data from mechanical tests in triaxial, biaxial and true triaxial loading conditions. The general expression of a three-invariant and non-associated constitutive relation is then developed for 10 true triaxial loading paths, performed at constant mean stresses and prescribed Lode angles. The Rice's criterion by bifurcation analysis enables the theoretical prediction of deformation bands (onset, orientation and volumetric strain). The qualitative evolution of predicted band kinematics, as well as quantitative values obtained for the 10 loading paths, proves to be in good agreement with experimental observations from full-field characterization of localized zones. The relevance and predictiveness of the presented three-invariant model are further evidence by comparisons with simplified, associated and two-invariant models using the same initial dataset.

Keywords Bifurcation · Constitutive modeling · Deformation band · Experimental mechanics · Localization · Sandstone · Shear band · Stress invariants · True triaxial · Yield surface

1 Introduction

Deformation processes in mechanically stressed geomaterials often lead to the development of planar kinematic zones of highly localized strain at failure, known as deformation or shear bands. The occurrence of this pervasive structural mode of deformation has been widely observed both in the field [2, 15, 20] and in laboratory settings [7, 10, 47, 53, 59].

In cohesive granular material such as porous sandstone, well-developed mature deformation bands are often indicative of a degenerative failure mode, resulting in a non-reversible transition in the global mechanical response near and beyond the peak stress. The emergence of these

localized structures is generally concurrent with the culmination of a global weakening of the material through the accumulation of inelastic deformations, leading to a transition into the softening and permanent regimes. A theoretical study of these modes of localized deformation, in relation to rarely studied true triaxial stress states representative of underground rock formations, is of clear interest to better understand and predict mechanical conditions leading to transition failure modes of confined porous rocks.

The study of material bifurcation aims to evaluate the existence of constitutive limit states in the material, for which, in addition to further homogeneous deformation, a non-uniform kinematic solution is admissible. In particular, localized bifurcation modes, as opposed to diffuse bifurcation (*e.g.*, bulging and buckling modes), are highly relevant to the field of geomechanics, since they can be related to the emergence of material instabilities and abrupt transitions in deformation mechanisms. This type of analysis helps to further investigate geometrical aspects of kinematic structures at failure and therefore provides

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valuable predictions of dominant deformation modes controlling the mechanical response during the post-peak regime.

A particular case of localized bifurcation can be studied within the Thomas–Hill–Mandel deformation band model [25, 37, 56]. This formalism provides a set of theoretical conditions for the emergence of deformation bands in the material continuum. The deformation band is therefore conceptualized as a material layer of infinite length in a plane and of finite thickness, bounded by two parallel surfaces, characterized by a weak discontinuity in the incremental displacement gradient [25]. This form of an idealized deformation band considers the compatibility of one or multiple planar localized zone with an equilibrium constitutive bifurcation state in the material and a set of prescribed boundary conditions at the interface [5, 50, 58].

To the authors' knowledge, few scientific works have systematically examined and compared with experiments the effect of true triaxial conditions on the prediction of deformation localization (e.g., [11, 17, 23, 27, 43]). This is probably due to the scarcity of such experimental data, especially for porous rocks, where laboratory-scale experimental tests are generally carried out on axisymmetric loading paths, very often in compression (e.g., [48]), sometimes in extension [6, 24], or more rarely in plane stress [38] and plane strain compression [29, 32, 46]. In a limited number of studies, experiments have also been performed under true triaxial conditions, allowing the effect of the intermediate principal stress or Lode angle to be fully studied [1, 13, 19, 22, 26, 35, 40, 42, 52, 55].

The effect of the Lode angle on the theoretical localization conditions is twofold. On the one hand, the anisotropy of the stress tensor is sufficient to induce a dependence with the Lode angle. On the other hand, the constitutive law can itself include a dependence on the Lode angle, which adds an effect on the localization conditions. This dependence of the constitutive law can be introduced by a non-circular shape of the yield or limit surfaces, as well as the plastic potential, in the octahedral (deviatoric) plane. Examples of such surfaces can be found in the literature, such as the Mohr–Coulomb surface or other smooth surfaces [8, 31, 39, 57, 60].

In the scope of the present study, the bifurcation analysis follows on the seminal development for geomaterials proposed in [51]. For this type of material, the constitutive behavior is expressed using a non-associated, pressure-dependent elasto-plastic relation. The specific model presented in this paper is extended to a three-invariant-dependent high-porosity sandstone from the Vosges region in France. The analysis considers the constitutive state of this material at the peak stress, where the initiation conditions for the emergence of fully developed deformation bands

are met in the brittle and brittle–ductile transition regimes of the studied sandstone.

Using experimental data for the Vosges sandstone reported in [13], the deformation bands kinematics, their orientation and dilatancy angle, are theoretically predicted for different loading paths. The model parameters, *i.e.*, the normal to the yield surface, the direction of plastic strain and the elastic moduli, are first retrieved from the macroscopic response of the material. The deformation band kinematics at the peak stress predicted from the bifurcation analysis using this model are then compared to full-field experimental measurements, as well as alternative and simplified models using the same dataset.

Hereafter, the index summation convention is used and δ_{ij} is the Kronecker delta.

2 Constitutive model

This section describes a constitutive model, with isotropic and no time dependence assumptions, which is used for the later presented bifurcation analysis. The model is inspired by several series of experimental test results on a Vosges sandstone, including tests under true triaxial conditions. For the present analysis, the constitutive model is based on a classical development in elasto-plasticity with an additive decomposition of the total strain rate, $d\epsilon_{ij} = d\epsilon_{ij}^e + d\epsilon_{ij}^p$, where $d\epsilon^e$ and $d\epsilon^p$ denote the elastic and plastic strain rates, respectively. The constitutive tensor, defining the relation between incremental stress and strain ($d\sigma_{ij} = L_{ijkl} d\epsilon_{kl}$), is established according to the development of an isotropic work-hardening material. It can therefore be expressed as

$$L_{ijkl} = E_{ijkl} - \frac{1}{h} E_{ijuv} P_{uv} Q_{mn} E_{mnkl}, \quad (1)$$

with $h = H + Q_{ij} E_{ijkl} P_{kl}$ where H is a plastic coefficient, \mathbf{E} is the elastic stiffness tensor, \mathbf{Q} is the unit normal to the yield surface F and \mathbf{P} is the direction of plastic strain increment, theoretically defined as the unit normal to a plastic potential surface G . The classical development of the constitutive relation is briefly presented in Appendix 1 for completeness. The yield surface F is described hereafter, based on experimental observations.

2.1 Yield surface description

In the current model, the three invariants of the stress tensor are introduced in the formulation of the yield surface. Compressive stresses are considered positive. The octahedral-Lode invariants are selected as a reference frame in a cylindrical coordinate system with the three invariants as

$$\begin{aligned}\sigma_m &= \frac{1}{3}I_1 = \frac{1}{3}[\sigma_1 + \sigma_2 + \sigma_3], \\ \tau_{oct} &= \sqrt{\frac{2}{3}J_2} \\ &= \frac{1}{3}[(\sigma_1 - \sigma_2)^2 + (\sigma_1 - \sigma_3)^2 + (\sigma_2 - \sigma_3)^2]^{1/2}, \\ \theta_\sigma &= \frac{1}{3}\arccos\left[\frac{3\sqrt{3}J_3}{2J_2^{3/2}}\right] \\ &= \arctan\left[\sqrt{3}\frac{\sigma_2 - \sigma_3}{(\sigma_1 - \sigma_2) + (\sigma_1 - \sigma_3)}\right],\end{aligned}\quad (2)$$

154 where I and J are, respectively, the principal invariants of
155 the second-order stress tensor and the deviatoric part of its
156 additive decomposition, and σ_i are the three principal
157 stresses (eigenvalues of the stress tensor). For consistency
158 with loading paths from experiments considered in the
159 calibration of the model, a single sextant of the octahedral
160 plane is considered, where σ_1 and σ_3 are defined as the
161 major (most compressive) and minor principal stresses,
162 respectively. In this sector of the octahedral plane, and for
163 the selected invariants in Eq. (2), $\theta_\sigma = 0^\circ$ and $\theta_\sigma = 60^\circ$
164 correspond, respectively, to an axisymmetric compression
165 and axisymmetric extension stress state. An extrapolation
166 of the model to the other five sectors of the octahedral
167 plane is possible and requires the assumption that the
168 studied rock is mechanically isotropic.

169 A suitable function for the yield surface of the modeled
170 sandstone, with a dependency on the three invariants of the
171 stress tensor, is selected based on restrictions on the con-
172 vexity of the elastic domain and the continuity of its
173 derivatives in the compressive stress regime. To this effect,
174 a single continuous yield surface is deemed compatible
175 with the observations of a progressive evolution in the
176 deformation modes with both the mean stress and Lode
177 angle. From a microstructural point of view, it implies that
178 the change in deformation mechanisms from a brittle to a
179 ductile regime, known to occur around the stationary point
180 of the yield surface in the $\sigma_m - \tau_{oct}$ plane, is characterized
181 by a smooth transition. Thus, the single yield surface for
182 the present model is developed from a combination of two
183 complementary functions, acting in both the $\sigma_m - \tau_{oct}$
184 (meridian) plane and the $\theta - \tau_{oct}$ (octahedral) plane in the
185 compressive section of the stress space.

186 The first function is a mean stress-dependent linear-
187 exponential (Linex) function

$$F^a(\sigma_m) = A[e^{a_1(\sigma_m - a_2)} - a_1(\sigma_m - a_2) - a_3], \quad (3)$$

189 where a_i are fitting parameters influencing the shape (a_1)
190 and the position (a_2 and a_3) of the function, and A is a
191 scaling parameter. The single shape parameter, a_1 , controls

192 the steepness and asymmetry of the curve around the sta-
193 tionary point, where τ_{oct} reaches a maximum value. At
194 limit values of the mean stress, the Linex function is
195 dominated either by its linear term, at $a_1\sigma_m \rightarrow -\infty$, or by
196 its exponential term, at $a_1\sigma_m \rightarrow +\infty$. Around the station-
197 ary point, the exponential and linear terms are of the same
198 order of magnitude, resulting in a smooth transition in the
199 curve. The choice of a Linex function is particularly well
200 suited due to the ease of its differentiation, its convexity
201 and the control it provides over the asymmetry of the
202 curve, providing a good fit for experimental data in both
203 the brittle and ductile regimes.

204 The second function is based on the van Eekelen [57]
205 surface which is a relatively flexible function that can be
206 adapted to various Lode angle-dependent forms and for
207 which the friction angles in axisymmetric stress states
208 ($\theta_\sigma = 0^\circ$ and 60°) can be expressed independently. It is
209 written as

$$F^b(\theta) = B(1 - \xi \sin 3\theta)^n, \quad (4)$$

211 where ξ and n are both shape parameters, and B is a scaling
212 parameter. These parameters are bounded in a specific
213 range to ensure the convexity of the fitted function. [57]
214 has shown that a value for the exponent $n = -0.229$ pro-
215 vides an optimal range for the parameterization of ξ , over
216 which the function remains convex. Selecting this value for
217 n , the convexity limit of the function is $|\xi| \leq 0.793$ (In [57]
218 β is used instead of ξ for the same parameter). A constant
219 value of ξ implies a constant shape of the surface in all
220 octahedral planes. Experimental observations on the dis-
221 tribution of peak stresses for mechanical experiments on
222 porous rocks, including the Vosges sandstone studied here,
223 have demonstrated a clear evolution of the shape with the
224 mean stress. Consequently, a function taking into account
225 this dependency should be evaluated according to the
226 modeled material. Accordingly, a second-order
227 polynomial,

$$\xi(\sigma_m) = b_1 + b_2\sigma_m^2, \quad (5)$$

229 is selected to take into account this mean stress depen-
230 dency. The upward open-endedness of the function guar-
231 anties the convexity limit is respected over the range of
232 mean stresses. The suitability of the function to represent
233 the shape parameter evolution is contingent on the exper-
234 imental data and alternative functions for (5) can be
235 selected without any difficulty.

236 Combining Eqs. (3), (4) and (5), the three-invariant
237 yield surface in the Octahedral-Lode space can be formally
238 written as

$$F = \tau_{oct} - C \{ e^{a_1(\sigma_m - a_2)} - a_1(\sigma_m - a_2) - a_3 \} \{ 1 - (b_1 + b_2 \sigma_m^2) \sin(3\theta) \}^n, \quad (6)$$

240 where C is a general scaling parameter. The outward normal
241 to the yield surface, \mathbf{Q} , is simply defined in terms of
242 the derivative of the yield surface with respect to the stress
243 invariants and the Cauchy stress tensor using the flow rule.
244 It can be written as

$$Q_{ij} = \frac{\partial F}{\partial \sigma_{ij}} = F_\sigma \frac{\partial \sigma_m}{\partial \sigma_{ij}} + F_\tau \frac{\partial \tau_{oct}}{\partial \sigma_{ij}} + F_\theta \frac{\partial \theta}{\partial \sigma_{ij}}, \quad (7)$$

246 where the subscript in F denotes the direction of the partial
247 derivative with respect to each of the three octahedral-Lode
248 invariants. The expansion of each derivative, while
249 straightforward, can be quite extensive and is therefore
250 provided in full in Appendix 2.

251 2.2 Yield surface calibration

252 The objective of this study is to determine the conditions
253 for the existence of a localized solution, in the spirit of a
254 bifurcation analysis similar to [51]. For this purpose, a
255 complete description of the model, including the strain
256 hardening law, is not necessary. Only the description of the
257 yield surface, the plastic strain rate directions and the
258 elastic moduli are required. The assumption will be made
259 that when the bifurcation criterion is about to be satisfied,
260 the yield surface shape approximates the experimentally
261 obtained failure envelope [4, 45], this envelope being
262 defined by the octahedral stress peaks of the different tests.
263 The set of parameters in Eq. (6) is defined using the
264 experimental measurements available for the Vosges
265 sandstone. The different datasets used for this purpose
266 consist of mechanical tests performed over a wide range of
267 loading paths in axisymmetric triaxial compression [6],
268 plane strain compression [32] and true triaxial compression
269 [13]. The sandstone samples used in these three experi-
270 mental campaigns were extracted from the same homoge-
271 neous block and therefore have similar initial mechanical
272 properties. Additionally, the samples were all tested at a
273 comparable laboratory scale, and under similar quasi-static
274 and monotonic loading conditions.

275 The suitability of the second-order polynomial function
276 in Eq. (5), taking into account the mean stress dependence
277 of the parameter ζ in the octahedral plane, is first evaluated
278 using the series of true triaxial experiments in [13]. For
279 these experiments, the stress peaks are constrained by the
280 selected loading paths to remain in specific octahedral
281 planes, corresponding to two constant mean stresses of 60
282 MPa and 90 MPa. In each plane, where experiments at five
283 different Lode angles are performed, the van Eekelen part
284 of the yield surface in Eq. (4) is fitted to a single value of ζ ,

285 where a least square regression results in $\zeta = -0.587$ and
286 $\zeta = -0.430$, at 60 MPa and 90 MPa, respectively. This
287 increase in the value ζ reflects a clear evolution in the
288 shape of the van Eekelen surface with increasing mean
289 stress, as shown by the two data points represented in
290 Fig. 1. These values can be compared to the continuous
291 curve in Fig. 1, representing the evolution of ζ for the
292 selected second-order polynomial function with parameters
293 b_1 and b_2 . The value of these two parameters is obtained by
294 regression of Eq. (6), concurrently to other parameters in
295 Table 1, and for the full dataset in triaxial, biaxial and true
296 triaxial loading. This comparison confirms that the choice
297 of the function for ζ , defining the shape evolution in the
298 octahedral plane, is compatible with the yield surface
299 optimization with the complete dataset of available peak
300 stress values for the studied Vosges sandstone. Note that in
301 Fig. 1, ζ tends toward the convexity limit as the mean
302 stress approaches zero. The choice of a second-order
303 polynomial ensures that the function remains above this
304 limit for positive mean stresses. However, another choice
305 of function could be made depending on the experimental
306 data and different shape evolution of the surface for other
307 rocks.

308 The six parameters defining the yield surface (Eq. 6) are
309 fitted to the peak stress from the three datasets using a least
310 square optimization scheme. The optimized parameters for
311 the represented surface are provided in Table 1. A graphi-
312 cal representation of the yield surface for this set of
313 parameters, along with the peak stress values retrieved
314 from the different datasets, is shown in Fig. 2 for isovalues

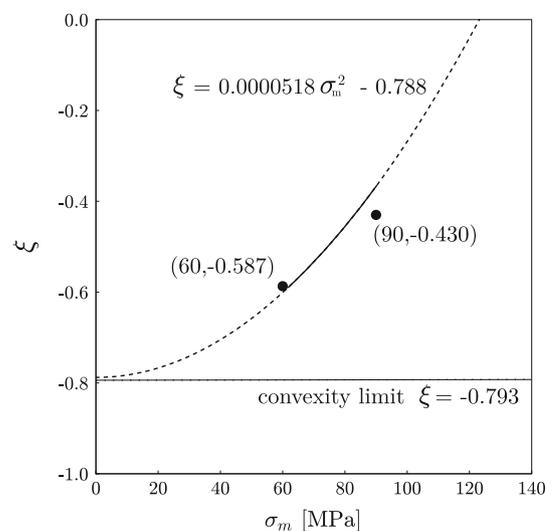


Fig. 1 Evolution of ζ with σ_m for a second-order polynomial function. The labeled points denote the value obtained from an independent regression at 60 MPa and 90 MPa using Eq. (4). The parameters b_1 and b_2 for the continuous curve are obtained from the least square regression on the combined formulation of the yield surface, in Eq. (6)

Table 1 Yield surface parameters for the Vosges sandstone

Parameter	Value	Unit
n^1	-0.229	1
C	-42.5	MPa
a_1	0.0185	MPa ⁻¹
a_2	108	MPa
a_3	2.22	1
b_1	-0.788	1
b_2	5.18×10^{-5}	MPa ⁻²

¹ The parameter n is prescribed and not optimized in the fitted function

angle, as evidenced by the triangular shape of the yield surface in the octahedral plane. The mean stresses dependence of ξ influences the shape of the yield surface to evolve from an upward triangular shape, at low mean stress, toward a circular shape, at $\sigma_m = 123$ MPa corresponding to $\xi = 0$. Above this threshold, which occurs in the domain $F_\sigma < 0$, ξ becomes positive, showing a possibility for the deviatoric stress peaks at a high Lode angle to be higher than the peak at a low Lode angle. Evidently, this failure regime falls outside of the available data points for the studied set of experiments and the choices are rather arbitrary and could have been different. Nonetheless, the continuous evolution of the yield surface, for $\sigma_m > 123$

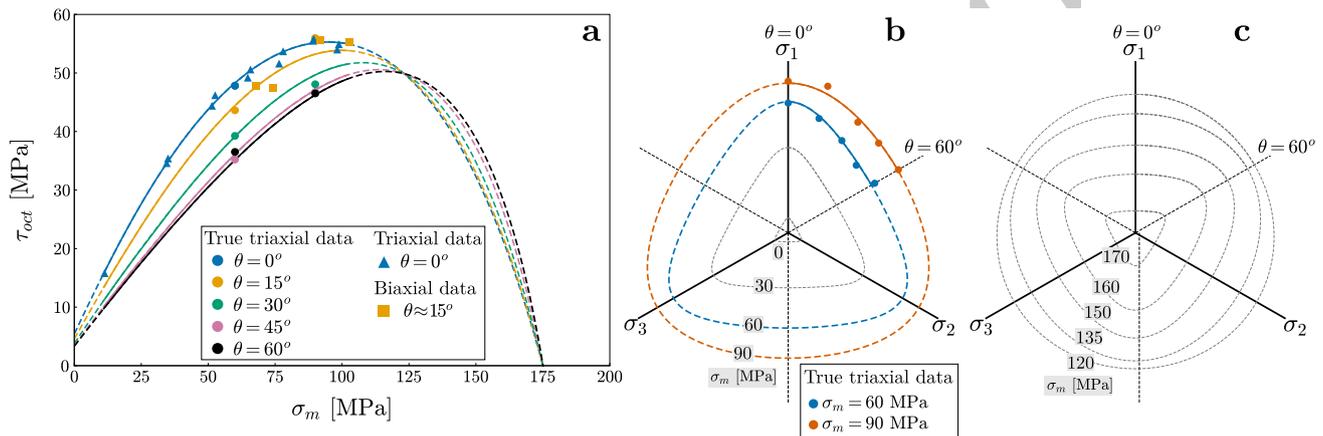


Fig. 2 Representation of the peak octahedral stresses for different stress paths from three experimental datasets on the studied Vosges sandstone. The curves represent the yield surface from Eq. (6) with fitted parameters from Table 1. The shape evolution of the yield surface is clearly visible for both isovalues of Lode angles in the meridian plane (a), and isovalues of mean stresses in the octahedral planes, for low σ_m in (b) and high σ_m in (c)

of θ , in the meridian planes, and isovalues of σ_m , in the octahedral planes. Note that both sets of isovalue curves are convex, which is a necessary condition for the convexity of the 3D surface.

In these cross-sectional plane representations, the complementarity of the different datasets to generate a well-defined yield surface in the 3D stress space is apparent. In the meridian plane, the shape of the yield surface is mostly influenced by experiments performed in triaxial axisymmetric compression ($\theta = 0^\circ$) for a large range of mean stresses up to the stationary point (*i.e.*, at the change in the sign of F_σ). Additionally, the true triaxial dataset, spanning the entire sextant of the octahedral plane at two mean stress levels, captures effectively the influence of the Lode angle. It is complemented by biaxial (plane strain) experiments, with peak stresses situated where the shape of the yield surface varies more significantly with respect to the Lode angle, around $\theta = 15^\circ$.

In the range of available peak stress data where $F_\sigma > 0$, the peak stress consistently decreases with increasing Lode

MPa, into a downward triangular shape, shown in Fig. 2c, has been observed in analog high-porosity sandstone and carbonate rocks [16, 36].

2.3 Elastic moduli from experiments

The elastic stiffness tensor \mathbf{E} is evaluated from the stress-strain measurements during isotropic and deviatoric loading of true triaxial mechanical tests reported in [13]. Therefore, in this section and onward, the specific method is presented to determine the elastic moduli for the Vosges sandstone, in the context of loading paths with prescribed invariants of the stress tensor.

Under the assumption of isotropic linear elasticity, with applicable symmetries in the constitutive tensor, the elastic part of the stress-strain relation is

$$d\sigma_{ij} = 3K \left(\frac{1}{3} d\epsilon_{kk}^e \delta_{ij} \right) + 2S \left(d\epsilon_{ij}^e - \frac{1}{3} d\epsilon_{kk}^e \delta_{ij} \right), \quad (8)$$

with the elastic properties of the material determined by the

364 bulk modulus (K) and shear modulus (S). For an initially
 365 isotropic loading phase, the deviatoric part of the elastic
 366 strain tensor theoretically vanishes, resulting in
 367 $d\sigma_{ij} = Kd\epsilon_{kk}\delta_{ij}$. Similarly, during the subsequent purely
 368 deviatoric loading phase, at constant mean stress, the
 369 elastic part of the volumetric strain vanishes, resulting in
 370 $d\sigma_{ij} = 2Sd\epsilon_{ij}^e$. Consequently, the two elastic moduli can be
 371 retrieved individually from the isotropic and deviatoric
 372 loading phases as

$$K = \frac{\Delta\sigma_m}{\Delta\epsilon_v^e}, \text{ and } S = \frac{\Delta\tau_{oct}}{2\Delta\gamma_{oct}^e}, \quad (9)$$

374 in terms of the first and second invariants, respectively. The
 375 constitutive fourth-order elastic tensor can be expressed
 376 using the Lamé parameters, $\lambda = K - \frac{2}{3}S$, $\mu = S$, as

$$E_{ijkl} = \lambda\delta_{ij}\delta_{kl} + \mu(\delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk}). \quad (10)$$

378 In the scope of this analysis, elastic moduli are defined
 379 from the ten loading paths in the range of mean stresses
 380 from 60 MPa to 90 MPa. Therefore, K and S , and the
 381 related Lamé duals, are, respectively, estimated from (i) the
 382 linear range of the isotropic and volumetric stress–strain
 383 curve between 60 and 90 MPa, and (ii) the average initial
 384 slope of the octahedral stress–strain curve. These estimated
 385 values are reported in Table 2.

386 It should be noted that elastic parameters are known to
 387 evolve according to the loading history [54], and an aver-
 388 age scalar representation does not fully take into account
 389 this evolution of the material behavior during loading. For
 390 the studied Vosges sandstone, inelastic volumetric defor-
 391 mation present from the beginning of the deviatoric loading
 392 phase of the experiments suggests that the initial slope of
 393 the stress–strain octahedral curve does not correspond to a
 394 purely elastic behavior. Nonetheless, isotropic loading–
 395 unloading tests on a similar porous sandstone, studied by
 396 [41], have shown a decrease in the inelastic part of the
 397 volumetric deformations with increasing mean stress,
 398 accounting for less than 20% of the total volumetric strain
 399 above $\sigma_m = 40$ MPa. The importance of elasticity in the
 400 model will be assessed through a sensitivity analysis of the
 401 elastic moduli, in comparison with the influence of the
 402 plastic parameters (the outward normal \mathbf{Q} and plastic strain
 403 increment \mathbf{P}) evaluated at the stress peak.

Table 2 Elastic moduli

Parameter	Value (GPa)
K	10
S, μ	6.0
λ	6.0

2.4 Incremental plastic strain from experiments

404

In the following calculation of the incremental plastic
 strain direction \mathbf{P} , the octahedral-Lode invariants of the
 plastic strain tensor ϵ_{ij}^p , are analog to the invariants
 expressed for the stress tensor in Eq. (2). For a coaxial
 model, the direction of plastic strain increment can be
 represented in the stress space where it is normalized for a
 unit increment of stress. For a non-associated model, \mathbf{P}
 is normally assumed as the derivative of a plastic potential G ,
 as

$$P_{ij} = \frac{\partial G}{\partial \sigma_{ij}} = G_\sigma \frac{\partial \sigma_m}{\partial \sigma_{ij}} + G_\tau \frac{\partial \tau_{oct}}{\partial \sigma_{ij}} + G_\theta \frac{\partial \theta_\sigma}{\partial \sigma_{ij}}, \quad (11)$$

where the subscripts in G denote the derivatives in the
 direction of each octahedral-Lode invariant. However, in
 the present analysis the plastic strain increments are eval-
 uated directly from experimental measurements close to
 the peak octahedral stress. Therefore, its derivation from a
 generating function is only theoretical and the plastic
 potential does not need to be explicitly evaluated.

From the imposed constraints on σ_m and θ during the
 deviatoric loading phase, the elastic part of the strain
 increment vanishes in the direction of those invariants (*i.e.*,
 $\epsilon_{vol}^e = 0$ and θ_ϵ^e). Therefore, the shear modulus is taken into
 account only in the direction of deformation increments
 following the octahedral direction (*i.e.*, the radial direction
 in the octahedral plane). The strain invariants $\epsilon_{vol}, \gamma_{oct}$ and
 θ_ϵ are therefore obtained from the principal strain mea-
 surements using a combination of strain gauges and aver-
 aged displacement from digital image correlation for the
 reported experiments in [13]. The incremental plastic strain
 are

$$\begin{aligned} G_\sigma &= \Delta(\epsilon_{vol} - \epsilon_{vol}^e) = \Delta\epsilon_{vol}, \\ G_\tau &= \Delta(\gamma_{oct} - \gamma_{oct}^e) = \Delta\gamma_{oct} - \frac{\Delta\tau_{oct}}{2S}, \\ G_\theta &= \Delta(\theta_\epsilon - \theta_\epsilon^e) = \Delta\theta_\epsilon, \end{aligned} \quad (12)$$

where S is the elastic shear modulus defined in Eq. (9). For
 all measurements, Δ represents a fixed time interval of 60
 measurement points (at 1 Hz acquisition rate) before the
 peak octahedral stress. This time interval is selected in
 order to minimize errors in the measurement noise,
 acquisition synchronicity and stick-slip frictional behavior
 in the loading piston.

The orientations of the normalized \mathbf{P} in the meridian and
 octahedral planes are represented in Fig. 3 for the ten true
 triaxial experiments. The origin of the arrows coincides
 with the yield surface, at the prescribed mean stress and
 Lode angle for each loading path, and where the normal \mathbf{Q}
 is also represented. In the meridian plane representation,
 the orientation of \mathbf{Q} is seen to be systematically lower than

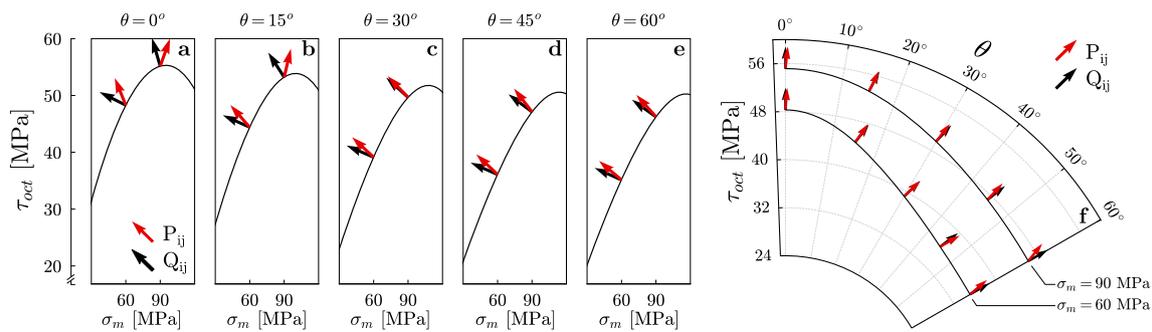


Fig. 3 Direction of the outward normal \mathbf{Q} and plastic deformation direction, \mathbf{P} , at the intersection of the yield surface and the respective loading paths in the meridian plane (a–e) and octahedral plane (f). In each plane, the orientations for each true triaxial experiment are represented at the two mean stresses of 60 MPa and 90 MPa, and the five Lode angles. In the meridian plane, non-associativity of the model is stronger at low Lode angle and weaker at high Lode angle. In the octahedral plane, deviatoric associativity is observed for all loading paths

449 \mathbf{P} , where a significant difference in their orientation is most
 450 notable at lower Lode angles. This difference is less pro-
 451 nounced at Lode angles above 30° , where fewer dissimi-
 452 larities are observed between loading paths at both mean
 453 stresses. The orientation of both \mathbf{P} and \mathbf{Q} in the meridian
 454 planes tends to decrease as the Lode angle increases. The
 455 difference in the orientation of \mathbf{P} and \mathbf{Q} denotes a strong
 456 non-associativity for the Vosges sandstone in the meridian
 457 plane, *i.e.*, with respect to the effect of the mean stress.
 458 This type of non-associativity of the Vosges sandstone is
 459 consistent with reported observations from previous stud-
 460 ies, which identified similar behavior in the meridian plane
 461 for high-porosity rocks [4, 28, 45]. Conversely, in the
 462 octahedral plane represented in Fig. 3f, \mathbf{P} and \mathbf{Q} are seen to
 463 have comparable outward orientations, suggesting a deviatoric
 464 associativity of the material. This characteristic of the model
 465 was also observed in non-cohesive geomaterials
 466 [30, 49, 61] and is often postulated in theoretical studies for
 467 the type of instabilities studied herein [34].

468 3 Bifurcation analysis

469 The following bifurcation analysis consists in seeking
 470 admissible localized kinematic solutions for the inception
 471 of strain localization. This bifurcation from initially
 472 homogeneous deformation is characterized by a loss of
 473 ellipticity in the material constitutive tensor, where multi-
 474 ple solutions to further deformation become possible. The
 475 material response is then contingent to the theoretical
 476 constraints on the nature of the localization structure, in the
 477 form of a planar deformation band of finite thickness.
 478 Based on the bifurcation framework proposed by [50],
 479 these constraints are imposed in the form of a kinematic
 480 condition, relating the rate of deformation inside and out-
 481 side the deformation band, and an equilibrium condition,

prescribing continuity in the traction rate at the band
 interfaces. As such, the surface boundaries of the localized
 region are defined by two parallel weak planar disconti-
 nuities, which orientation is described by the normal to the
 plane n , with a vanishing intermediate principal value [5].
 The localization conditions appear to be strongly depen-
 dent on both the constitutive model and the nature of the
 loading.

Regarding the 3D planar orientation of the band, post-
 mortem X-ray scans of the sandstone samples revealed that
 the out-of-plane orientation of an average plane passing
 through the deformation band was generally well aligned
 with the intermediate principal stress direction [12]. Con-
 sequently, the initial assumption of a vanishing interme-
 diate principal value of the deformation band can be
 confirmed and its orientation is represented only in the
 major–minor plane.

499 3.1 Deformation band angle prediction

From the set of prescribed conditions, a general criterion
 for continuous bifurcation is classically established as
 $\det[L_{ijkl}n_jn_l] = 0$ [51]. For the model presented above,
 the constitutive tensor \mathbf{L} is given by the elasto-plastic for-
 mulation expressed in Eq. (8). Solving the equation in terms of
 the plastic coefficient leads to

$$H = - (Q_{ij}E_{ijkl}P_{kl}) + (Q_{ij}E_{ijkl}n_l)(n_jn_lE_{ijkl})^{-1} (n_jE_{ijkl}P_{kl}) . \quad (13)$$

From this expansion of the bifurcation criteria, with known
 material plastic and elastic parameters (\mathbf{Q} , \mathbf{P} and \mathbf{E}) at the
 onset of strain localization, Eq. (13) relates the value of the
 plastic coefficient H to a direction of the deformation band
 unit normal n . The relation between H and β , the angle
 between n and the maximum principal stress direction in

513 the localization plane, which satisfies the bifurcation
 514 criteria is shown in Fig. 4 for the 10 true triaxial loading
 515 paths. It is seen in this representation that a unique maxi-
 516 mum for H can be identified for β in the range of 0° to 90° .
 517 The criteria for the angle of conjugated bands, at an angle
 518 symmetrical to the maximum principal stress axis, are also
 519 symmetrical. Conjugated band orientation duals are there-
 520 fore associated with the same value of H and equally
 521 probable.

522 For a hardening solid, the tangent modulus of the con-
 523 stitutive relation continuously decreases during the accu-
 524 mulation of plastic strain. Therefore, [51] have argued that
 525 the critical orientation (n_c) for localization to occur is at the
 526 maximum, or critical, value of the plastic coefficient (H_c).
 527 It follows that the orientation n_c provides a prediction for
 528 the most likely band orientation in the minor-major prin-
 529 cipal plane. Figure 4 shows the maximum value of H/S to
 530 occur near the transition between the hardening and soft-
 531 ening regime (stress peak) for $\theta > 0^\circ$ and well in the
 532 softening regime for $\theta = 0^\circ$.

533 Figure 5 shows the critical angle (β_c) predicted by the
 534 model for the different loading paths. It is seen to sys-
 535 tematically increase with an increase in the Lode angle and
 536 a decrease in the mean stress. The change in angle is also
 537 more pronounced at lower Lode angles. These results can
 538 be compared to the deformation band angle measured
 539 experimentally at the peak octahedral stress, as reported in
 540 [13]. The model provides a good prediction of the general
 541 trend in the evolution of the band orientation, with
 542 increasing Lode angle. For most loading paths, the quan-
 543 titative prediction of the deformation band angle is also in
 544 good agreement with observations. A discrepancy is
 545 noticeable for $\sigma_m = 90$ MPa and $\theta = 0^\circ$ and 15° , where
 546 the deformation band angle is predicted at a lower angle
 547 than experimentally measured. This discrepancy can be attrib-
 548 uted to the pronounced change in the normal to the yield

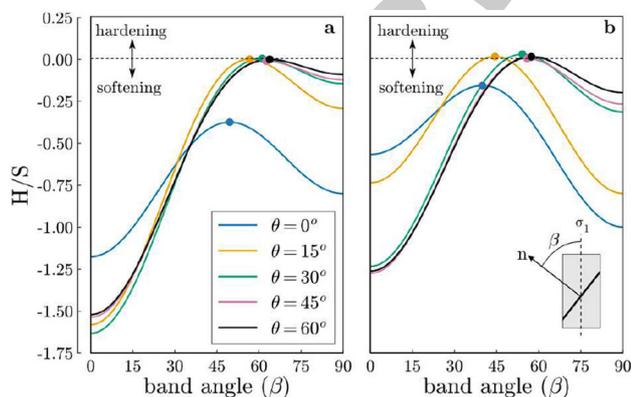


Fig. 4 Evolution of the normalized plastic coefficient (H/S) with respect to the deformation band angles satisfying the bifurcation criteria, for loading paths at 60 MPa (a) and 90 MPa (b) mean stress

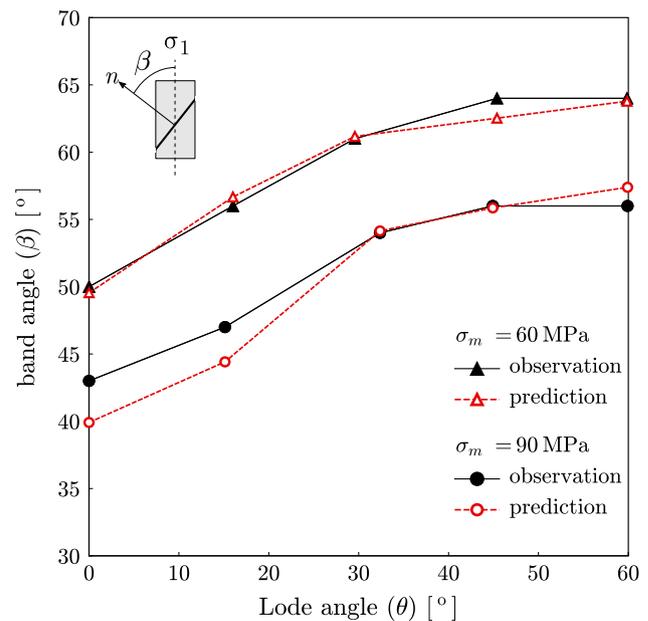


Fig. 5 Deformation band angle (β) with increasing Lode angle at the two mean stresses of 60 MPa and 90 MPa. The three-invariant model predictions are plotted against experimental observations

549 surface in the meridian plane around $\sigma_m = 90$ MPa (see
 550 Fig. 2). With fewer data points available in this region of
 551 the plane, there is a higher uncertainty in the calibration of
 552 the yield surface.

3.2 Dilatancy angle prediction

554 The dilatancy angle (ϕ) of the deformation band is defined,
 555 according to [4], as the ratio of volumetric and shear
 556 components of the deformation jump measured parallel to
 557 the band,

$$\tan \phi = \frac{\Delta D^{vol}}{\Delta D^{shear}} \quad (14)$$

559 For the unit normal associated with the critical band angle,
 560 n^c ,

$$\begin{aligned} \Delta D^{vol} &= g_s n_s^c, \\ \Delta D^{shear} &= \left\| \frac{1}{2} (g_k n_s^c + g_s n_k^c) n_k^c - D^{vol} n_s^c \right\| \end{aligned} \quad (15)$$

562 are the change in volumetric and shear deformation in the
 563 normal and tangential directions of the deformation band.
 564 The directional vector g is derived from the bifurcation
 565 condition as

$$g_k = \gamma (n_j^c n_l^c E_{ijkl})^{-1} (n_j^c E_{ijmn} P_{mn}), \quad (16)$$

567 where γ is an arbitrary constant multiplier.

568 For the two investigated mean stresses, the predicted
 569 dilatancy angle over the range of Lode angles is shown in

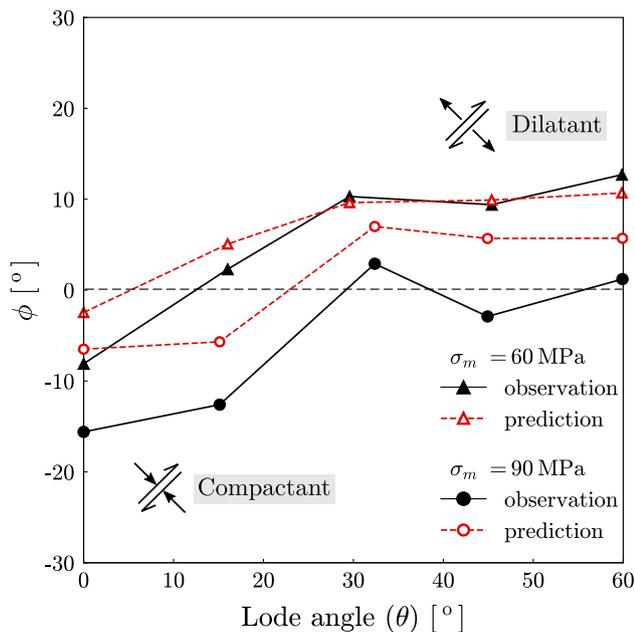


Fig. 6 Dilatancy angle (ϕ) across the deformation band with increasing Lode angle, at the two mean stresses of 60 MPa and 90 MPa. The three-invariant model predictions are plotted against experimental observations. A negative value of the angle denotes compaction and a positive value denotes a dilation associated to the shearing

570 Fig. 6. Similarly to the deformation band angle, the dilata-
 571 tancy angle can be compared to an experimental value at
 572 the peak stress. The experimental dilatancy angles were
 573 determined from respective displacement fields obtained
 574 by digital image correlation over strain increments where
 575 the deformation band is seen to emerge on the surface of
 576 the sample [13]. Since this value of the dilatancy angle is
 577 assessed from an average measurement of the propagating
 578 band, it is not constant over the length of the deformation
 579 band and is thus sensitive to some variability in the band
 580 inclination. Considering these uncertainties in the mea-
 581 surement of ϕ from the displacement field, the trend in the
 582 evolution of observed and predicted dilatancy angle is
 583 reasonably well matched. At the low mean stress of
 584 60 MPa, where strain localization initially concentrates
 585 into narrow and straight mature deformation bands,
 586 experimental measurements of the band angles are also in
 587 good quantitative agreement with the model prediction. At
 588 the higher mean stress of 90 MPa, the predicted dilatancy
 589 angle is more dilatant than for experimental observations.
 590 Nonetheless, the evolution of the dilatancy angle with the
 591 Lode angle is generally well represented in the model, with
 592 the correct tendency for dilatancy or compaction associated
 593 to the shearing through the deformation band.

3.3 Alternative models and elastic sensitivity

594

595 The development of the constitutive model introduced
 596 above is made possible thanks to extensive experimental
 597 data available for the studied Vosges sandstone. The
 598 experimental methods to retrieve the model parameters
 599 further rely on an advanced true triaxial loading apparatus
 600 and sophisticated approaches to the acquisition of local
 601 strain measurements. Alternatively, most analyses in
 602 bifurcation reported in the literature are conducted using
 603 simplified models, for which some important mechanical
 604 behavior identified for porous rocks are not fully accounted
 605 for. It is the case for models dependent on two invariants of
 606 the stress tensor (Lode angle independent), and models
 607 assuming associated plasticity ($\mathbf{P} = \mathbf{Q}$). These model
 608 simplifications can be highly valuable, and sometimes
 609 necessary, when the shape of the yield surface in the
 610 octahedral plane cannot be defined, or when the directions
 611 of plastic strain at failure are not available or unreliable. In
 612 the same spirit as in the previous analysis, the deformation
 613 band kinematic can be predicted for these alternative
 614 models. In this section, their comparison with the initially
 615 presented model in terms of prediction accuracy enables us
 616 to assess the merit of added complexities in a more general
 617 approach.

618 The inclination of the deformation band and the band
 619 dilatancy angle are first predicted for a two-invariant model
 620 where the yield surface is optimized for the Linex function
 621 in the meridian plane, with a constant circular shape in the
 622 octahedral plane, *i.e.*, imposing $b_1 = b_2 = 0$ in Eq. (6). It
 623 results that the solution to the bifurcation criteria is not
 624 influenced by $F_\theta = 1$, but the effect of the Lode angle for
 625 the different stress paths is still accounted for in $\frac{\partial \theta}{\partial \sigma}$. For this
 626 two-invariant model, the direction of plastic strain incre-
 627 ment \mathbf{P} remains unchanged compared to the initial three-
 628 invariant model.

629 The comparison of band angle, in Fig. 7a, shows that a
 630 two-invariant model leads to a systematic underestimation
 631 of β compared to the three-invariant model. This effect is
 632 most pronounced at higher Lode angles and lower mean
 633 stresses, where the outward normal to the van Eekelen
 634 surface in the initial model is most divergent from the
 635 radial direction. Concurrently, the predicted band dilata-
 636 tancy angle for this model, as seen in Fig. 7d, is higher than for
 637 the initial model, providing a less accurate prediction
 638 against experimental measurements.

639 A second predictive model comparison is made for an
 640 associated model, where directions of plastic strain rate
 641 would be a priori unknown and therefore assumed equal to
 642 the outward normal to the yield surface (*i.e.*, $\mathbf{P} = \mathbf{Q} = \frac{\partial F}{\partial \sigma}$).
 643 Since the initial model is close to deviatoric associativity,
 644 the main effect of this simplified model lies in the imposed

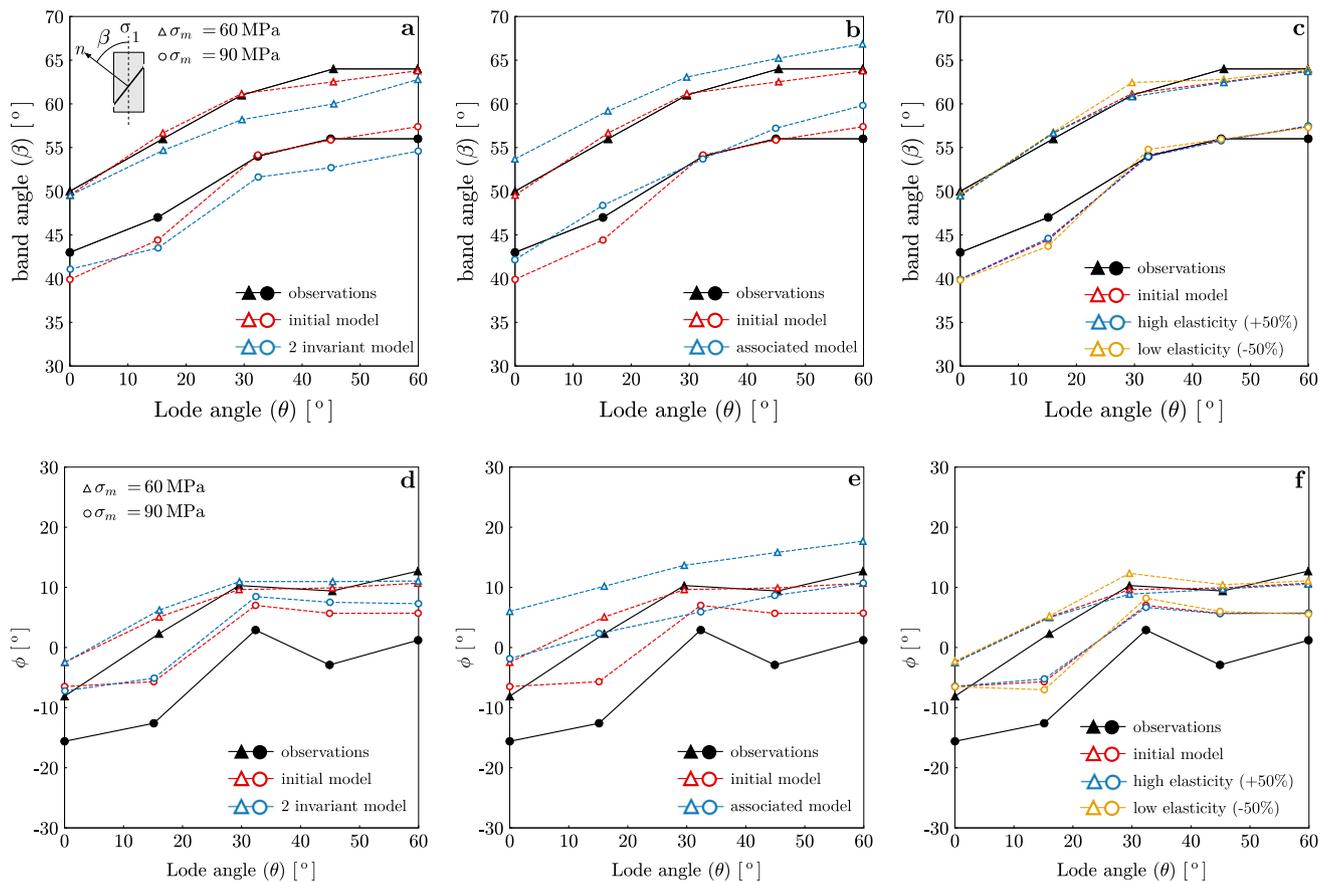


Fig. 7 Comparison of the deformation band angle (a, b, c) and band dilatancy angle prediction (d, e, f) between experimental observations (black), the initially presented three-invariant and non-associated model (red) and alternative models (blue, green): two-invariant model (a, d), associated model (b, e) and elastic moduli sensitivity (c, f)

645 associativity in the meridian plane. Therefore, imposing the
 646 direction of \mathbf{P} for an intrinsically non-associated sandstone
 647 overestimates the dilatancy of the material and leads to an
 648 increase in both the deformation band angle (Fig. 7b) and
 649 band dilatancy angle (Fig. 7e) predicted by the bifurcation
 650 analysis. This results in a poorer prediction at 60 MPa, as
 651 well as for the high Lode angles at 90 MPa. At low Lode
 652 angle and a mean stress of 90 MPa, this model improves
 653 the prediction of the band angle β . However, this is due to a
 654 volume behavior that is considered to be dilating, whereas
 655 it is measured as contracting (Fig. 7e).

656 The sensitivity of the initial model to variations in the
 657 elastic parameters extracted from the stress–strain relations
 658 is evaluated by prescribing, in two different cases, a 50%
 659 increase and decrease in both the bulk and shear elastic
 660 moduli. Figure 7c and f shows that, even for such large
 661 variations in the elastic parameters, the predicted band
 662 angle and dilatancy angle remain mostly unaffected. These
 663 results demonstrate the marginal effect of possibly large
 664 uncertainties in the values for the elastic parameters
 665 selected in this analysis. The observation of such a small
 666 effect is consistent with the loading of a rock material

667 since, under the present conditions, elastic strains remain
 668 small compared to plastic strains at the onset of bifurcation.
 669 In fact, higher moduli, or a stiffer elastic response, would
 670 not change the prediction. However, for lower elastic
 671 moduli of the material, in the order of the hardening
 672 modulus, the elastic contribution would have a significant
 673 influence on the deformation response and thus on the
 674 resulting kinematic predictions.

675 4 Discussion

676 Some considerations in the bifurcation criteria and consti-
 677 tutive relation considered previously are hereafter contex-
 678 tualized and compared to recent experimental observations,
 679 as well as known deformation mechanisms occurring in
 680 porous rocks.

681 In the previous section, the kinematics predictions from
 682 the bifurcation analysis were compared to laboratory
 683 experimental data for a porous sandstone, obtained by full-
 684 field measurements and digital image correlation [13]. The
 685 authors of the experimental study described different

686 localized deformation modes and their evolution, from the
687 beginning of the deviatoric loading phase to a post-peak
688 state after substantial and well-developed strain
689 localization.

690 The authors introduced a distinction between early
691 deformation bands, appearing well before the stress peak,
692 and mature deformation bands, emerging near the stress
693 peak and initiating a softening response of the material. In
694 the presented bifurcation analysis, as well as in previous
695 studies where bifurcation theory is used to evaluate the
696 localization behavior of rocks, it is the kinematics of
697 mature deformation bands that are predicted by the theo-
698 retical results. Therefore, the presented analysis is based on
699 a model for the constitutive state of the material at their
700 inception, considering a diffuse deformation prior to the
701 development of mature strain localization. However, if the
702 onset of mature strain localization bands can be considered
703 as a matter of non-uniqueness of solution, as introduced by
704 bifurcation analysis, what about early localization bands?

705 In contrast to mature localization, the early localization
706 regions are characterized by numerous parallel and conju-
707 gate bands, where shear deformation is concentrated. These
708 bands also exhibit a dilatant behavior which induces a
709 relative dilatancy at the sample scale. Similarly, they are
710 concomitant with a loss of linearity in the octahedral stress
711 vs. strain response. As the loading progresses, the number
712 of active early bands decreases, and as the peak is
713 approached, a localization zone associated with a loss of
714 sample strength (initiation of softening) appears. The ori-
715 entation of the early and mature bands is close but differs
716 by a few degrees.

717 This mode of early localization has also been observed
718 in a clayey rock under specific loading conditions (for
719 sufficiently high mean stresses) [3]. One may also wonder
720 whether the secondary localization bands in a carbonate
721 rock observed *postmortem* by Mogi ([42], fig. 3.78) are not
722 evidence of an early localization? Furthermore, early
723 localization has also been observed in granular materials
724 [18, 33].

725 On the numerical modeling side, a few studies have
726 reported this pre-peak localization. In the context of
727 modeling in a continuous medium, it is generally observed
728 if a slight material heterogeneity has been introduced into
729 the medium [21, 44]. It is also observed in the context of
730 discrete medium modeling [14].

731 Thus, it appears that the localization process in sand-
732 stone occurs in two stages. A first early stage (before the
733 peak stress) is characterized by a large number of short
734 bands inducing a change in the tangential stiffness and
735 dilatancy of the sample, without inducing a softening of the
736 sample. It is followed by a second stage which sees the
737 appearance of mature bands, which may be dilating or
738 contracting depending on the level of mean stress and Lode

739 angle, and induces a softening of the sample. Microstruc-
740 tural observations of early and mature shear bands have
741 been done on the same Vosges sandstone loaded under
742 plane strain compression [32]. The early bands appear to be
743 marked by low damage (intragranular and intergranular
744 cracking), while the mature bands are characterized by
745 high damage (grain crushing).

746 This second phase of localization, inducing a strong
747 microstructural change of the material, and in the loading
748 conditions studied here, a softening of the material, is
749 consistent with the predictions of the bifurcation analysis.
750 Let us recall that the Rice's bifurcation criterion can be
751 interpreted as a state linked to the existence of a direction n
752 and a kinetic g for which the mechanical response in the
753 band corresponds to the condition $(L_{ijkl} g_k n_l) n_j = \dot{\sigma}_{ij} n_j =$
754 0 due to the predominance of the in-band kinetic compared
755 to the out-of-band kinetic (infinite ratio) [9]. In other
756 words, considering the incipient band as a layer undergoing
757 a homogeneous deformation over its thickness, described
758 by $1/2 (g_k n_l + g_l n_k)$, the traction vector rate applied to
759 this layer is vanishing at the onset of localization. This kind
760 of material response needs a substantial microstructural
761 evolution that could be met only during the mature local-
762 ization process. Clearly, further work will be needed to
763 clarify the theoretical conditions for the early localization.

764 Another interesting aspect is the brittle–ductile transi-
765 tion in the mechanical behavior of porous rocks. This has
766 been discussed in [13], in terms of the different views one
767 can have on this transition, in terms of the pre-peak
768 response, the post-peak response, the orientations of the
769 localization bands, the volume strain within the bands and
770 finally the more or less complex pattern of localization. A
771 relevant prism to consider in this paper is the orientation of
772 the bands and the nature of the deformation. It is now well
773 understood that the orientation of the bands (angle between
774 the band and the most compressive stress direction)
775 increases during this transition and that also the volume
776 strain associated with the shear deformation (slip parallel to
777 the band) evolves from expansion to compaction, with the
778 extreme cases being dilation and compaction bands (no
779 slip). This transition is generally attributed to an increase in
780 the mean stress, and our study is a further confirmation of
781 this. While the effect of the Lode angle is less well docu-
782 mented, the experimental and theoretical results clearly
783 show here that, at a given mean stress, the response is more
784 brittle for high Lode angles and more ductile for low angles
785 (state close to the axisymmetric compression state), this in
786 quite noticeable proportions.

787 **5 Conclusion**

788 In the scope of this study, an original three-invariant con-
789 stitutive model was first presented for a well-studied
790 Vosges sandstone. In the context of bifurcation theory, this
791 general model was used to evaluate theoretical predictions
792 of strain localization for unconventional loading paths, in
793 the form of deformation bands. These predictions have
794 been further evaluated in comparison with full-field
795 experimental observations and alternative models.

796 The proposed yield surface, with both mean stress and
797 Lode angle dependency, has been derived from a large
798 number of mechanical loading experiments, including tri-
799 axial, biaxial and true triaxial invariant controlled loading
800 paths. With the flexibility of a combined linear–exponen-
801 tial and van Eekelen function, the yield surface showed a
802 good fit with experimental peak stresses over the wide
803 range of axisymmetric and non-axisymmetric loading
804 paths, in both the brittle and brittle–ductile transition
805 regimes.

806 Using this model, a bifurcation analysis was conducted
807 for a series of 10 laboratory loading tests in true triaxial
808 conditions. For these experiments, local deformation
809 measurements revealed a marked variation in the normals
810 to the yield surface and direction of plastic strain at the
811 peak stress, in both the octahedral (deviatoric) and merid-
812 ian planes. This tendency results in a continuous evolution
813 of the band kinematic predictions, where the orientation
814 and dilatancy angles of the bands increase nonlinearly with
815 an increase in the Lode angle and a decrease in the mean
816 stress. This prediction is both consistent with the expected
817 decrease in the ductility of the material and with full-field
818 experimental measurements of the localized regions. It was
819 also evidenced that the proposed non-associated three-in-
820 variant model performs better than simplified alternative
821 models in predicting the band kinematics.

822 The findings presented herein demonstrate the validity
823 and potential for this general bifurcation framework to
824 corroborate observations in terms of the kinematics of so-
825 called mature deformation bands, i.e., instigating a soft-
826 ening response, in porous rocks. The complementary role
827 of early localization, i.e., emerging prior to the peak stress,
828 and its relation to a later bifurcation state still needs to be
829 investigated, perhaps from a different perspective.

830 **Appendix 1: Elasto-plastic formulation**

831 For an elasto-plastic material with additive incremental
832 strain decomposition, $d\epsilon_{ij} = d\epsilon_{ij}^e + d\epsilon_{ij}^p$, the elastic and
833 plastic strains are, respectively, defined as

$$d\epsilon_{ij}^e = C_{ijkl} d\sigma_{kl}, \quad d\epsilon_{ij}^p = d\lambda P_{ij}, \quad (17)$$

where \mathbf{C} is the elastic compliance tensor and $\mathbf{P} = \frac{\partial \mathbf{G}}{\partial \boldsymbol{\sigma}}$ is the 835
direction of plastic strain. The magnitude of plastic 836
deformation is determined by the plastic multiplier $d\lambda$, 837
according to the flow rule. The incremental stress tensor, 838
 $d\sigma(d\epsilon)$, is therefore written as 839

$$d\sigma_{ij} = E_{ijkl}(d\epsilon_{kl} - d\lambda P_{kl}), \quad (18)$$

where \mathbf{E} is the elastic stiffness tensor, i.e., the inverse of \mathbf{C} . 841
Considering isotropic hardening in the material, the con- 842
sistency condition, $F = 0$ and $dF = 0$, is expressed in the 843
form of 844

$$Q_{ij} d\sigma_{ij} - Hd\lambda = 0, \quad (19)$$

where $\mathbf{Q} = \frac{\partial F}{\partial \boldsymbol{\sigma}}$ is the normal to the yield surface and H is a 846
plastic coefficient. Combining Eqs. (18) and (19), the 847
plastic multiplier can be written as 848

$$d\lambda = \frac{1}{h} Q_{uv} E_{uvrs} d\epsilon_{rs}, \quad (20)$$

with $h = H + Q_{ij} E_{ijkl} P_{kl}$. 850

This equation for the plastic multiplier is inserted back 851
into the stress–strain relation in Eq. (18), resulting in 852

$$d\sigma_{ij} = E_{ijkl}(d\epsilon_{kl} - \frac{1}{h} Q_{uv} E_{uvrs} d\epsilon_{rs} P_{kl}). \quad (21)$$

Alternatively, 854

$$d\sigma_{ij} = L_{ijkl} d\epsilon_{kl}, \quad (22)$$

with the elasto-plastic constitutive tensor \mathbf{L} as in Eq. (1). 856

857 **Appendix 2: Invariants derivatives**

The derivatives of the principal invariants (I_1, J_2, J_3) are first 858
expressed as 859

$$\begin{aligned} \frac{\partial I_1}{\partial \sigma_{ij}} &= \delta_{ij}, \\ \frac{\partial J_2}{\partial \sigma_{ij}} &= s_{ij}, \\ \frac{\partial J_3}{\partial \sigma_{ij}} &= \delta_{pi} \delta_{jq} s_{qr} s_{rp} - \frac{1}{3} \delta_{pq} \delta_{ki} \delta_{jk} s_{qr} s_{rp}, \end{aligned} \quad (23)$$

where s_{ij} is the deviatoric part of the stress tensor resulting 861
from its additive decomposition, $\sigma_{ij} = \frac{1}{3} \sigma_{kk} \delta_{ij} + s_{ij}$. Using 862
these results, the derivatives of the octahedral–Lode 863
invariants can therefore be written as 864

$$\begin{aligned} \frac{\partial \sigma_m}{\partial \sigma_{ij}} &= \frac{1}{3} \delta_{ij}, \\ \frac{\partial \tau_{oct}}{\partial \sigma_{ij}} &= \frac{s_{ij}}{3\tau_{oct}}, \\ \frac{\partial \theta_\sigma}{\partial \sigma_{ij}} &= \frac{-\sqrt{2}}{3 \sin(3\theta_\sigma) \tau_{oct}^3} \\ &\quad \left(s_{jr} s_{ri} - \delta_{ij} \tau_{oct}^2 - \frac{\sqrt{2} \cos(3\theta_\sigma) \tau_{oct}}{2} s_{ij} \right). \end{aligned} \quad (24)$$

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869 **Data availability** The datasets generated during and/or analyzed
870 during the current study are available from the corresponding author
871 upon reasonable request.

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