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Modeling of fault gouges with Cosserat Continuum Mechanics: Influence of thermal pressurization and chemical decomposition as coseismic weakening mechanisms

Emmanuil Veveakis*

*National Technical University of Athens, School of Applied Mathematics and Physics,
Theocharis Bld, Iroon Politechniou 5, Zografou, Athens, 15773, Greece*

Jean Sulem

*UR Navier-CERMES, Ecole des Ponts ParisTech, Université Paris-Est, 6,8 Avenue
Blaise Pascal, Champs-sur-Marne, 77455, Marne-la-Vallée Cedex 2, France*

Ioannis Stefanou

*National Technical University of Athens, School of Applied Mathematics and Physics,
Theocharis Bld, Iroon Politechniou 5, Zografou, Athens, 15773, Greece*

Abstract

In this paper we study the impact of thermal pressurization and mineral decomposition reactions under seismic deformation conditions (e.g., slip rates of about 1 m/s) triggered by shear heating, to the stability of a saturated fault material. By using higher order continuum considerations, allowing for rotational degrees of freedom to the gouge material, we verify that the micro-inertia of the Cosserat continuum may regularize the ill-posed problem of simple shear of a fault and that the thermal effects promote localization of deformation into ultra-thin shear bands. It is shown that the width of these

*Corresponding Author. Email: manolis@mechan.ntua.gr, Tel:+30 210 772 1373

structures depends on the parameters of the decomposition reaction considered, obtaining values as low as $100\text{ }\mu\text{m}$, in agreement with microstructural evidence from natural and artificial faults. .

Key words: *Shear Heating, Cosserat Continuum, Reaction kinetics, Undrained adiabatic shearing, Micro-Inertia*

1. Introduction

Geomaterials exhibit failure in various patterns, like the propagation of single fractures in otherwise intact rock, crack growth in presence of multiple interacting fractures, initiation and percolation of damage zones under quasi-static and dynamic loading, strain localization into shear- or compaction bands.

The theory describing localized failure has been a direct extension of the classic Mohr's strength of materials theory, and is applied for geomaterials using the so-called Thomas - Hill - Mandel shear-band model (Hill (1962); Mandel (1966)), which was introduced in the early 60s and it was widely publicized by the paper of Rudnicki and Rice (1975). More recently, the mathematical formulation of bifurcation and post-bifurcation phenomena and related instabilities was summarized by Vardoulakis and Sulem (1995) to form the basis of a contemporary continuum theory of failure of geomaterials.

Apart from the theoretical point of view of failure, shear banding has been claimed as the primary failure pattern for faults (Rice (2006)) and landslides (Vardoulakis (2002a)). However, field evidence from exhumed faults reveals that seismic events take place in even narrower zones within shear-bands, formed from post-failure evolution (Chester and Chester (1998)), dominated

20 by weakening mechanisms that are considered to be mainly thermal of origin
21 (Rice (2006)). Indeed, field observations suggest that slip in individual events
22 may then be extremely localized, and may occur primarily within a thin shear
23 zone, $< 1 - 5 \text{ mm}$ thick, called the principal slipping zone (PSZ) (Sibson
24 (2003)). This localized shear zone lies within a finely granulated fault core
25 of typically tens to hundreds millimeter thickness, as shown schematically in
26 the idealized description of Fig. 1.

27 Evidence for that morphology can be found in the North Branch San
28 Gabriel fault (Chester et al. (1993)) and Punchbowl (Chester and Chester
29 (1998)) fault of the San Andreas system in southern California, the Median
30 Tectonic Line fault in Japan (Wibberley and Shimamoto (2003)), and in the
31 Hanaore fault in southwest Japan (Noda and Shimamoto (2005)). Note also
32 that from drilling cores in the Aigion system, central Greece, the fault core
33 of clay size particles consisting of finely crushed radiolarites, extended to
34 about 1 m , was found to be intercepted by a “fresh” distinct slip surface of
35 sub-millimeter size (Sulem (2007); Cornet et al. (2004)).

36 As perhaps the best characterized case, a thin principal slipping zone
37 was identified along an exposure of the Punchbowl fault at 2 to 4 km depth,
38 which has accommodated 44 km of slip (Chester and Chester (1998)). Also,
39 a thin central slip zone was identified by Wibberley and Shimamoto (2003)
40 along the Median Tectonic Line fault. The nominal thickness of such a shear
41 zone is usually of the order of sub-millimeter and, as described by Smith et al
42 (2011), it could be met in calcite-bearing fault rocks even in the absence of
43 pressure-solution and precipitation, providing thus field evidence of extreme
44 localization during coseismic slip in natural faults. On the other hand the

Figure 1: Idealized description of a natural fault zone, as presented by Chester et al. (1993) and Wibberley et al. (2008). The fault core, d , is of the order of centimeters, whereas the Principal Slipping Zone (PSZ) D is of the order of millimeter or less.

45 thickness of the cataclastic core may vary up to a few centimeters.

46 In geomechanics there are several studies focusing on the thickness of
47 shear bands in soils. Morgenstern and Tschalenko (1967) calculated that
48 shear bands for a clay, kaolin may have thicknesses of order 10 – 100 times
49 a clay platelet size ($\sim 0.5 \mu m$). For granular materials on the other hand
50 usually use the mean particle diameter, d_{50} , is used as a scaling measure,
51 defined for nonuniform size distributions such that 50 % by weight of the
52 particles have larger size.

53 Under purely mechanical effects, Muhlhaus and Vardoulakis (1987) cal-
54 culated for sands the thickness of the initial shear band (with thickness d
55 in Figure 1) to be around $d \sim 16d_{50}$. In any case, this zone seems to be
56 rather wide to be considered as the primary slip surface (Rice (2006)). In-
57 deed, Chester and Goldsby (2003) showed that the nominal thickness of the
58 Punchbowl’s cataclastic core varies from 0.6 to 1.1 mm. However, as Rice
59 (2006) mentions: “*within this ~ 1 mm thick nominal shear zone, most of the*
60 *shearing seems to have been accommodated within a zone of extreme shear*
61 *localization having an apparent thickness of 100 – 300 μm ”. Rice (2006)*
62 showed that d_{50} is not always a characteristic length scale for cataclastic
63 and ultracataclastic formations, since apparently $d_{20} - d_{30}$ seems to be more
64 appropriate for modeling the PSZ. Thus, in principle the PSZ represents a
65 very fine shear localization, consisting of ultrafine particles that have usually
66 undergone mechano-chemical degradation (gelification, decarbonation and
67 dehydration reactions, melting, as thoroughly discussed by Di Toro et al.
68 (2011)). Therefore, other mechanisms that are responsible for the formation
69 of these structures and the dynamic weakening of faults should be looked

70 after.

71 Since fault zones usually exhibit the presence of fluid interacting with the
72 rock, hence inducing coupled effects including shear heating and pore fluid
73 pressurization, such mechanisms are expected to act as weakening mecha-
74 nisms during fault slip (Sibson (1973); Lachenbruch (1980); Wibberley and
75 Shimamoto (2005)). These mechanisms have also been suggested for weak-
76 ening in catastrophic landslides (Vardoulakis (2002a); Veveakis et al. (2007);
77 Goren and Aharonov (2007); Pinyol and Alonso (2010); Goren et al. (2010)).
78 Thermo-poro-mechanical couplings due to shear heating (Sulem et al. (2005);
79 Rice (2006)) can be also associated to chemical effects such as dehydration
80 of minerals or decomposition of carbonates, theoretically studied recently by
81 Brantut et al. (2010, 2011); Sulem and Famin (2009); Veveakis et al. (2010)
82 and reported to take place in real faults (Hirono et al. (2007)) and experi-
83 ments at laboratory conditions (Han et al. (2007); Ferri et al. (2010); Brantut
84 et al. (2011a); De Paola et al. (2011)).

85 In a recent paper, Sulem et al. (2011) have shown that by resorting to a
86 Cosserat continuum (Vardoulakis and Sulem (1995)) for describing the kinet-
87 ics of a granular material, a preferred wave length for the instability mode
88 of a layer under shear can be selected. They showed that instability can
89 occur even in the hardening regime of the stress-strain curve, due to ther-
90 mal pressurization, confirming the claim that thermal in origin mechanisms
91 play a major role in the formation and evolution of the PSZ. The localizing
92 structures obtained were comparable in thickness with the ones observed in
93 nature, rationalizing thus the viscous and second gradient regularization ini-
94 tially proposed by Vardoulakis (1985, 1986, 1996) for regularizing these type

95 of problems. In this work we extend this analysis by including chemical re-
96 actions that may take place inside a rapidly deformed shear-band and study
97 the impact of certain decomposition reactions to the dynamic weakening and
98 localization of deformation in granular media.

99 **2. Problem Formulation**

100 In classical Continuum mechanics, where the continuum is allowed only
101 for translational degrees of freedom (displacements), one may be able to pre-
102 dict the onset of a shear band (Rudnicki and Rice (1975)). However it can
103 be shown that the instability tends to localize in a strip of zero thickness.
104 Classical theories are thus unable to simulate the localization of the defor-
105 mation in a shear band of finite thickness. This drawback can be traced back
106 to the fact that conventional constitutive models do not contain material pa-
107 rameters with dimension of length which can scale the shear band thickness
108 (internal length).

109 Thus, a fault is usually modelled as a discontinuity surface for the velocity
110 fields. Such an oversimplifying assumption however would overestimate sig-
111 nificantly the heat produced in a fault, and thus the temperature (as shown
112 by Rice (2006)), imposing difficulties in our effort to determine the processes
113 taking place during dynamic weakening of faults. To raise this discrepancy,
114 the introduction of a thin but finite-in-width slipping zone of intense shear is
115 requested. Vardoulakis (1985, 1986, 1996) showed that introducing viscous
116 (rate-dependent) considerations, combined with second gradient plasticity
117 models, may alleviate the ill-posedness of the problem. Later, Veveakis et al.
118 (2010) showed that indeed non-linear viscous responses provide the necessary

119 counterbalancing effect to stabilize the problem of simple shear.

120 Early approaches by Hill (1962) and Mandel (1966) envisioned such a
121 structure with width d , which however could only be artificially imposed,
122 since -as said before- in classical continua d is undetermined. It seemed as if
123 the solutions obtained from classical continua correspond to the limit $d \rightarrow 0$
124 of a corresponding higher grade extension of it (see Vardoulakis and Sulem
125 (1995), p. 268 for a comprehensive discussion). Following this conclusion, as
126 well as experimental observation of the influence of the effect of particle ir-
127 regularities and rotations inside the shear bands, Muhlhaus and Vardoulakis
128 (1987) resorted to concepts from Cosserat Continuum mechanics to naturally
129 determine d . Thus, by allowing both particle displacements and particle ro-
130 tations, they accounted for the angularities of the grains, and enriched the
131 classical continuum with additional kinematic and static fields, and calcu-
132 lated for sands that $d \sim 16d_{50}$. Other mechanisms leading to localization,
133 and initially neglected by Muhlhaus and Vardoulakis (1987), are reported
134 to be flash heating and powder lubrication (Di Toro et al. (2011); De Paola
135 et al. (2011); Han et al. (2010, 2011); Tisato et al. (2011)) or grain breakage
136 (Nguyen and Einav (2010)).

137 In this study we follow Muhlhaus and Vardoulakis (1987) and consider a
138 layer of saturated granular material of thickness D that is sheared in plane
139 strain (Fig. 2) in such a way that there is no extensional strain in the x_1
140 -direction and displacements u_1 and u_2 of material points vary only with x_2
141 (and time t). The additional rotational degree of freedom of the considered
142 2D Cosserat continuum is ω_c . The grains themselves are not allowed for
143 breakage or wear, excluding thus breakage and flash heating, since the scope

Figure 2: Problem formulation. Cosserat stresses, couple stresses and degrees of freedom.

of this study is to provide insights on the thickness of the PSZ at different temperature regimes.

2.1. Constitutive equations of elasto-plasticity

The incremental constitutive equations for the considered 2D Cosserat continuum are derived from the Muhlhaus - Vardoulakis plasticity model (Muhlhaus and Vardoulakis (1987)). The main feature of the model is that a 2D flow theory of plasticity for granular media with Cosserat microstructure can be derived by keeping the same definitions for the yield surface and the plastic potential as in the classical theory and by generalizing appropriately

the stress and strain invariants involved in these definitions. The details of the model for isothermal deformation are given in Vardoulakis and Sulem (1995) and in Sulem et al. (2011). They are briefly recalled in the following.

In a two-dimensional Cosserat Continuum each material point has two translational degree of freedom (v_1, v_2) and one rotational degree of freedom $\dot{\omega}_c$. The four components of the rate of the non-symmetric deformation tensor are given as

$$\begin{aligned}\dot{\epsilon}_{11} &= \frac{\partial v_1}{\partial x_1} ; \dot{\epsilon}_{12} = \frac{\partial v_1}{\partial x_2} + \dot{\omega}_c \\ \dot{\epsilon}_{21} &= \frac{\partial v_2}{\partial x_1} - \dot{\omega}_c ; \dot{\epsilon}_{22} = \frac{\partial v_2}{\partial x_2},\end{aligned}\tag{1}$$

and the two components of the curvature of the deformation rate (gradient of the Cosserat rotation rate)

$$\dot{\kappa}_1 = \frac{\partial \dot{\omega}_c}{\partial x_1} ; \dot{\kappa}_2 = \frac{\partial \dot{\omega}_c}{\partial x_2}.\tag{2}$$

Moreover we decompose the stresses and strain rates into spherical and deviatoric parts, $\sigma_{ij} = s_{ij} + \sigma_{kk}\delta_{ij}/2$ and $\dot{\epsilon}_{ij} = \dot{e}_{ij} + \dot{\epsilon}_{kk}\delta_{ij}/2$, where δ_{ij} is the Kronecker's delta. The following generalized stress and strain invariants are used:

$$\begin{aligned}\sigma &= \frac{\sigma_{ii}}{2} ; \tau = \sqrt{h_1 s_{ij} s_{ij} + h_2 s_{ij} s_{ji} + h_3 m_k m_k / R} \\ \dot{\epsilon}^p &= \dot{\epsilon}_{kk}^p ; \dot{\gamma}^p = \sqrt{g_1 \dot{e}_{ij}^p \dot{e}_{ij}^p + g_2 \dot{e}_{ij}^p \dot{e}_{ji}^p + R^2 g_3 \dot{\kappa}_k \dot{\kappa}_k},\end{aligned}\tag{3}$$

166 where $h_i = [3/4, -1/4, 1]$, $g_i = [3/2, 1/2, 1]$ for the so-called static Cosserat
 167 model, and R is the internal length (Vardoulakis and Sulem (1995)).

168 Besides the four components of the non-symmetric stress-tensor σ_{ij} , there
 169 are two couple stresses m_k ($k = 1, 2$). As in classical small-strain plasticity
 170 theory, the deformation is decomposed into elastic and plastic parts

$$\dot{\epsilon}_{ij} = \dot{\epsilon}_{ij}^e + \dot{\epsilon}_{ij}^p ; \dot{\kappa}_k = \dot{\kappa}_k^e + \dot{\kappa}_k^p. \quad (4)$$

171 Following Sulem et al. (2011) we assume a Terzaghi decomposition of the
 172 stress tensor in effective stress and pore pressure ($\sigma_{ij} = \sigma'_{ij} - p\delta_{ij}$) and assume
 173 a Coulomb yield stress and plastic potential for the effective stresses:

$$\begin{aligned} F &= \tau + \mu(\sigma + p), \\ Q &= \tau + \beta(\sigma + p), \end{aligned} \quad (5)$$

174 where the mobilized friction coefficient μ and the dilatancy coefficient β are
 175 functions only of the accumulated plastic strain γ^p . Under these consid-
 176 erations, the rate thermo-poro-elasto-plastic relationships are expressed as
 177 follows

$$\begin{aligned} \dot{\gamma} &= \frac{\dot{\tau}}{G} + \dot{\gamma}^p \\ \dot{\epsilon} &= \frac{1}{K}(\dot{\sigma} + \dot{p}) + \alpha_s \dot{T} + \dot{\epsilon}^p, \end{aligned} \quad (6)$$

178 where G and K are the elastic shear and bulk modulus respectively, α_s the
 179 thermal dilation coefficient of the solid skeleton and T the temperature. The

180 rate of plastic deformation is written as

$$\dot{\gamma}^p = \frac{1}{H} [\dot{\tau} + \mu(\dot{\sigma} + \dot{p})] ; \dot{\epsilon}^p = \beta \dot{\gamma}^p, \quad (7)$$

181 where $H = H(\gamma^p) = h(\sigma + p)$ (with $h = d\mu/d\gamma^p$) is the plastic hardening
 182 modulus, which is related to the tangent modulus H_{tan} of the τ versus γ curve
 183 through the relationship $H_{tan} = \frac{H}{1+H/G}$ and is either positive or negative ac-
 184 cording to whether the $\tau - \gamma$ curve is increasing (hardening) or decreasing
 185 (softening). Notice that, in principle H_{tan} is varying with strain, as thor-
 186 oughly presented by Rudnicki and Rice (1975). When H_{tan} is non positive
 187 then the material is entering an unstable regime, where softening induces
 188 localization of deformation in a shear band (Holcomb and Rudnicki (2001)).
 189 However, when the material is fluid saturated (Sulem et al. (2011)), ther-
 190 mal pressurization may cause localization of deformation even at hardening
 191 regimes, before reaching $H_{tan} = 0$, where the material is supposed to be
 192 stable. In this work we study the effect of a chemical reaction at high tem-
 193 peratures, near the activation temperature of the reaction, to assess whether
 194 the reaction itself may induce softening and localization at even higher values
 195 of the hardening modulus.

196 *2.2. Stress Equilibrium*

197 For the considered 2D Cosserat continuum and the configuration of Fig.
198 2, the local equilibrium equations are

$$\begin{aligned}\frac{\partial \sigma_{12}}{\partial x_2} &= 0, \\ \frac{\partial \sigma_{22}}{\partial x_2} &= 0, \\ \frac{\partial m}{\partial x_2} + \sigma_{21} - \sigma_{12} &= 0,\end{aligned}\tag{8}$$

199 where $m = m_2$ and $m_1 = 0$. The stresses applied at the boundary are a
200 shear stress τ and a normal stress σ_n in the x_2 direction. It is assumed
201 that no couple stress is imposed at the boundary. Prior to localization, the
202 state of stress and strain is uniform and considering the couple free boundary
203 condition, the couple stress is identically zero in the sheared layer. Therefore
204 the rock behaves as a classical continuum before localization.

205 *2.3. Reaction kinetics*

206 We assume the presence of a decomposition reaction that decomposes the
207 solid skeleton and produces excess pore fluid. In particular, as an example
208 we consider the reaction of calcite decomposition ($\text{CaCO}_3 \rightarrow \text{CaO} + \text{CO}_2$),
209 producing CO_2 which at high pressures and temperatures (conditions similar
210 to the ones met in faults at depth) is at supercritical, liquid state (Sulem and
211 Famin (2009)). Evidence of the presence of this reaction in faults is found
212 in many active crustal faults (Famin et al. (2008)), and experimentally re-
213 produced for example by Han et al. (2007) from experiments on simulated

214 faults in Carrara marble. Other types of chemical reactions such as min-
 215 eral dehydration (Brantut et al. (2011)) could be studied following the same
 216 methodology.

217 Following Sulem and Famin (2009) and Veveakis et al. (2010), we assume
 218 that the reaction is taking place with a rate r , which on its turn can be
 219 expressed from first order reaction kinetics as (Law (2006))

$$r \approx \frac{\rho_s}{M_{\text{CaCO}_3}} A_0 e^{-T_c/T}, \quad (9)$$

220 where $T_c = E/R_a$ the activation temperature of the reaction, E the activation
 221 energy and R_a the universal gas constant. In this expression A_0 is the pre-
 222 exponential factor, a parameter that may vary significantly, obtaining for
 223 calcite decomposition values between $10^2 s^{-1}$ and $10^{20} s^{-1}$ (Lvov et al. (2002)).

224 The Arrhenius model assumed in Eq. (9), is the simplest one, but has
 225 received much criticism for its validity, mainly due to the strongly varying
 226 magnitudes of both A_0 and T_c for a given reaction (Lvov et al. (2002)). In the
 227 pertinent literature there are numerous models suggested to replace it (Law
 228 (2006), pp. 67-72) for evaluating the reaction rate of a decomposition reac-
 229 tion. Lvov et al. (2002) provide a comprehensive literature guide through the
 230 models used, along with experimental data for calcite decomposition. Even
 231 for this well reported reaction, the production rates are measured through
 232 experiments at zero or very low pressures, of the order of *mbar*. Nonetheless
 233 it is known that pressure reduces significantly the rate of a reaction (Lvov
 234 (2007), pp. 79), hence when applying to geomechanical problems, one would
 235 need experimental data of calcite decomposition at pressures of the order of
 236 several tens of *MPa*. To our knowledge, such information is not available in
 237 the literature.

238 Apart from the pressure dependency of the production rates, we need to
 239 emphasize that the activation energy of a reaction also varies with grain size
 240 and the deformation history of a material. In the case of calcite, when the
 241 grain size decreases from 2 – 5 micron to 40 nm (a grain size typically found
 242 in high speed experiments performed on limestones (Tisato et al. (2011);
 243 Han et al. (2007, 2011); De Paola et al. (2011)), the activation energy for the
 244 reaction decreases from 200 kJ/mol to 130 kJ/mol (see Table 1 in Yue et al
 245 (1999)), even without plastic deformation of the particles. Thus, T_c could be
 246 temperature dependent on itself, correlating the nanoparticles produced with
 247 the chemical reaction (due to chemical precipitation, Yue et al (1999)), unlike
 248 the plastically deformed nanoparticles produced in high speed experiments.
 249 The internal plastic deformation induced by milling during frictional sliding
 250 might further reduce the activation energy of the reaction (Fisher. (1988)).
 251 Hence, emphasis should be given on thorough experimental determination of
 252 the reaction parameters at various temperature and pressure regimes.

253 2.4. *Fluid-mass Conservation*

254 Following the decomposition of the plastic strain rates into elastic and
 255 plastic parts (Eq. 4), we consider the volumetric plastic strain rate to consist
 256 of a mechanical part $\dot{\epsilon}_m^p$ subject to the constitutive behavior of Eq. 7 and a
 257 chemical part $\dot{\epsilon}_c^p$, influenced by the reaction rate r

$$\dot{\epsilon}^p = \dot{\epsilon}_m^p + \dot{\epsilon}_c^p. \quad (10)$$

258 Under the above considerations and by assuming that the solid matrix is plas-
 259 tically incompressible, the diffusion-reaction equation for the pore pressure

260 is obtained from the fluid mass equation as (Sulem and Famin (2009))

$$\frac{\partial p}{\partial t} = c_{hy} \frac{\partial^2 p}{\partial x_2^2} + \Lambda \frac{\partial T}{\partial t} - \frac{\beta}{\beta^*} \frac{\partial \dot{\gamma}^p}{\partial t} + \frac{\rho_s - \rho_f \zeta}{\rho_f \beta^*} \frac{A_0}{M_{CaCO_3}} e^{-T_c/T}, \quad (11)$$

261 where $\zeta = \frac{M_{CaCO_3}}{M_{CO_2}} - \frac{\rho_{CaCO_3}}{\rho_{CaO}} \frac{M_{CaO}}{M_{CO_2}}$, ρ_i the density of the i -th constituent and ρ_s
 262 the density of the solid skeleton, c_{hy} the hydraulic diffusivity, β^* the storage
 263 capacity and $\Lambda = (\lambda_f - \lambda_n)/\beta^*$ the pressurization coefficient, expressed as
 264 the difference of the thermal expansion coefficient of the fluid (λ_f)
 265 and the pore volume (λ_n).

266 2.5. Heat Equation

267 By assuming that all the mechanical work input is converted into heat
 268 (Chester et al. (2005); Pittarello et al. (2008)), and that the heat is ex-
 269 pressed through Fourier's law, we may obtain the diffusion-reaction temper-
 270 ature equation (Sulem and Famin (2009); Veveakis et al. (2010))

$$\frac{\partial T}{\partial t} = c_{th} \frac{\partial^2 T}{\partial x_2^2} + \frac{1}{\rho C} \tau \dot{\gamma}^p - \frac{|\Delta H|}{\rho C} \frac{\rho_s}{M_{CaCO_3}} A_0 e^{-T_c/T}, \quad (12)$$

271 where c_{th} is the thermal diffusivity, ρC the specific heat capacity of the
 272 mixture and $|\Delta H| \approx E$ the specific enthalpy of the reaction, expressing the
 273 energy consumed during an endothermic reaction.

274 3. Undrained-adiabatic limit

275 The first approximation in our effort to assess the influence of these weak-
 276 ening mechanisms during earthquake slip is to prohibit drainage and heat flux
 277 at the boundaries of the layer ($q_f = q_h = 0$). This case corresponds to the
 278 well known undrained-adiabatic limit, acknowledged to be established at or

near seismic rates, i.e. when the heat production rate and pore pressure increase in the slipping zone is significantly larger than the heat and pore pressure diffusion times towards the fault core and in the damage zone (Gargash and Rudnicki. (2003a,b)). It provides a first insight on the impact of each mechanism on the dynamic weakening of faults. The actual value of heating rate required for the onset of the weakening mechanisms varies with the material of the fault gouge (Di Toro et al. (2011)).

In addition to the above, we assume that the normal stress σ_n acting on the sheared layer is constant. From Eqs. (7),(11),(12) we may obtain the following relationship between the shear stress rate, the strain rate and the temperature rate:

$$\dot{\tau} = \frac{\bar{H}}{1 + \bar{H}/G} \dot{\gamma} + \frac{\bar{B}}{1 + \bar{H}/G} \dot{T}, \quad (13)$$

where

$$\begin{aligned} \bar{H} &= H + \mu \frac{\beta}{\beta^*} - \mu \tau \left(\frac{1}{\beta^* |\Delta H|} \frac{\rho_s - \zeta \rho_f}{\rho_f} \right), \\ \bar{B} &= \mu \left(\frac{\rho C}{\beta^* |\Delta H|} \frac{\rho_s - \zeta \rho_f}{\rho_f} - \Lambda \right). \end{aligned} \quad (14)$$

Obviously, when the thermal effects are neglected (i.e. in the absence of thermal pressurization and chemical reaction) and incompressible solid and fluid are assumed (so that $\beta^* = 1/K$) the classical expression for dilatant hardening effect, as proposed by Rice (1975) is retrieved

$$\dot{\tau} = \frac{H + \mu \beta K}{1 + (H + \mu \beta K)/G} \dot{\gamma}. \quad (15)$$

For dilatant material ($\beta > 0$) we may recognize in (13) a hardening effect due to dilatancy with the term $\mu \beta / \beta^*$ and a strong softening effect from the

297 reaction due to the term $\frac{\mu\tau}{\beta^*} \left(\frac{\rho_s - \zeta\rho_f}{\rho_f|\Delta H|} \right)$ (positive for calcite decomposition, as
 298 shown by Sulem and Famin (2009)).

299 As shown by Sulem et al. (2011), in the absence of a chemical reaction
 300 instability may occur even in the hardening regime of the $\tau - \gamma$ curve ($H > 0$)
 301 if the dilatancy effect is very weak (as it is the case at great depth) and if
 302 the thermal pressurization effect is significant. Here we verify this claim and
 303 indicate that the presence of a chemical reaction may lead to instability at
 304 even higher hardening regimes.

305 **4. Linear Stability Analysis of undrained adiabatic shearing of a** 306 **Cosserat layer**

307 At any given state, the evolution time of the kinematic quantities, the
 308 pore fluid pressure and the temperature determine the stability of the shear-
 309 ing of the Cosserat layer. The small perturbations considered herein are
 310 defined as follows:

$$\begin{aligned} u_1(x_2, t) &= u_1^0(x_2, t) + \tilde{u}_1(x_2, t), \\ u_2(x_2, t) &= u_2^0(x_2, t) + \tilde{u}_2(x_2, t), \\ \omega_c(x_2, t) &= \omega_c^0(x_2, t) + \tilde{\omega}_c(x_2, t), \\ p(x_2, t) &= p^0(x_2, t) + \tilde{p}(x_2, t), \\ T(x_2, t) &= T^0(x_2, t) + \tilde{T}(x_2, t). \end{aligned} \tag{16}$$

311 The governing equations for the perturbed fields ($\tilde{u}_1$, $\tilde{u}_2$, $\tilde{\omega}_c$, $\tilde{p}$, $\tilde{T}$) are of
 312 the same form as the ones derived in the previous section. Similarly, the fluid

313 and heat fluxes are prevented at the boundaries of the layer. However, the
 314 internal fluid and heat flows are permitted inside the layer.

315 4.1. Normalized equations

316 The system of equations can be brought in a dimensionless form by in-
 317 troducing the dimensionless quantities:

$$\begin{aligned} x &= \frac{x_1}{R}, \quad z = \frac{x_2}{R}, \quad \bar{u}_i = \frac{u_i}{R}, \\ \bar{p} &= \frac{p}{\sigma_n}, \quad \bar{\sigma}_{ij} = \frac{\sigma_{ij}}{\sigma_n}, \quad \bar{t} = \frac{c_{th}}{R^2} t, \quad \bar{T} = \frac{\Lambda}{\sigma_n} T, \end{aligned} \quad (17)$$

318 where R is the internal length of the Cosserat model, which can be related to
 319 the mean grain size $R = d_{50}/2$. The linearized forms of the pore pressure and
 320 heat equation (linearized around $T^0 = T_c$, i.e. at higher temperature regimes,
 321 near the activation temperature of the reaction) may be reduced in their
 322 dimensionless forms as (the superimposed bars are omitted for convenience):

$$\begin{aligned} \frac{\partial p}{\partial t} &= \eta \frac{\partial^2 p}{\partial z^2} + \frac{\partial T}{\partial t} + \delta \frac{\partial \dot{\gamma}^p}{\partial t} + \chi \frac{T - T_c}{T_c}, \\ \frac{\partial T}{\partial t} &= \frac{\partial^2 T}{\partial z^2} + \alpha \frac{\partial \dot{\gamma}^p}{\partial t} - \psi \frac{T - T_c}{T_c}, \end{aligned} \quad (18)$$

323 where

$$\begin{aligned} \eta &= \frac{c_{hy}}{c_{th}}, \quad \delta = \frac{\beta}{\beta^* \sigma_n}, \quad \alpha = \frac{\Lambda \tau_0}{\rho C \sigma_n} \\ \chi &= \frac{\rho_s - \zeta \rho_f}{\rho_f \beta^*} \frac{R^2}{\Lambda c_{th}} A_0 \\ \psi &= \frac{\rho_s \Delta H}{\rho C M_{CaCO_3}} \frac{R^2}{c_{th}} \frac{\Lambda}{\sigma_n} A_0, \end{aligned} \quad (19)$$

324 and

$$\begin{aligned} \frac{\partial \gamma^p}{\partial t} &= \frac{1}{H^*} \left[\frac{\partial \sigma_{12}}{\partial t} + \frac{\sigma_{21}}{\partial t} + \mu \left(\frac{\sigma'_{11}}{\partial t} \right) + \frac{\sigma'_{22}}{\partial t} \right], \\ H^* &= \frac{H}{\sigma_n} = h \frac{\sigma'}{\sigma_n}. \end{aligned} \quad (20)$$

325 The corresponding dimensionless form of the linear and angular momen-
326 tum with inertia and micro-inertia terms is as follows:

$$\begin{aligned} \frac{\partial \sigma_{12}}{\partial z} - I \frac{\partial^2 u_1}{\partial t^2} &= 0, \\ \frac{\partial \sigma'_{22}}{\partial z} - \frac{\partial p}{\partial z} - I \frac{\partial^2 u_2}{\partial t^2} &= 0, \\ \frac{\partial m}{\partial z} + \sigma_{21} - \sigma_{12} - \frac{I}{2} \frac{\partial^2 \omega_c}{\partial t^2} &= 0, \end{aligned} \quad (21)$$

327 where $I = \frac{c_{th}^2 \rho_s}{R^2 \sigma_n}$ and the expressions of the stresses and couple stresses are
328 derived from the elastoplastic model presented in Section 2.1 (Sulem et al.
329 (2011)).

330 Following Vardoulakis and Sulem (1995) and Sulem et al. (2011), we
331 introduce the perturbed fields (16) for a given initial configuration, and the
332 spatial dependency of the perturbations is decomposed into Fourier modes
333 with wavelength λ . Hence we introduce perturbations of the form

$$\begin{aligned} \tilde{u}_1(x_2, t) &= U_1 e^{st} \sin \left(\frac{z}{\lambda} \right), \\ \tilde{u}_2(x_2, t) &= U_2 e^{st} \sin \left(\frac{z}{\lambda} \right), \\ \tilde{\omega}_c(x_2, t) &= \Omega e^{st} \cos \left(\frac{z}{\lambda} \right), \\ \tilde{p}(x_2, t) &= \Pi e^{st} \cos \left(\frac{z}{\lambda} \right), \\ \tilde{T}(x_2, t) &= \Theta e^{st} \cos \left(\frac{z}{\lambda} \right), \end{aligned} \quad (22)$$

334 with $\lambda = D/(\pi NR)$ and N equal to an integer satisfying the zero heat
 335 and fluid flux boundary conditions at $z = \frac{x_2}{R} = 0$. By substituting the
 336 perturbation fields (22) into the linearized governing equations (18, 21), we
 337 obtain a homogeneous algebraic system for the coefficients $U_1, U_2, \Omega, \Pi, \Theta$. A
 338 nonzero solution is possible only when the determinant of the linear system
 339 vanishes. This request results in a characteristic polynomial equation of
 340 degree 8 for the growth coefficient s . If a root has a positive real part, then
 341 the corresponding perturbation grows exponentially in time.

342 *4.2. Numerical example*

343 We consider the case of a 7-*km* deep fault, of a calcite-made gouge ma-
 344 terial having the parameters depicted in Table 4.2. With these values, and
 345 by performing the method presented in the Appendix A, we obtain a critical
 346 value for the hardening modulus $h_{cr} \approx 6$, such that for $h \geq h_{cr}$ all the roots
 347 of the polynomial equation have negative real part, and thus the system is
 348 stable. For $h < h_{cr}$ roots with positive real parts exist, bringing the system
 349 to instability.

350 We observe that the destabilizing effect of the chemical reaction by the
 351 fact that instability can occur in the hardening regime, for values of the hard-
 352 ening modulus significantly larger than in the case of thermal pressurization,
 353 $h'_{cr} = 0.014$ (Sulem et al. (2011)). Hence, as temperature increases reaching
 354 the activation temperature of the reaction, the material becomes unstable
 355 even at regimes mechanically considered as stable in the absence of chemical
 356 reaction.

357 In order to assess the localizing effect of the chemical reaction, we plot in
 358 the Appendix A the greatest root (i.e. the one corresponding to the insta-

Figure 3: (a) Wave length λ corresponding to the fastest growth coefficient of the instability versus the hardening modulus h . (b) The same as in (a), focused in the area $0 < h < 1$, where the selected (minimum) wavelength, λ_m , is located. The results are calculated for $A_0 = 10^6$.

Parameter	Value	Units	Parameter	Value	Units
ϕ_0	0.03	—	c_{hy}	10^{-5}	m^2/s
σ'_n	200	MPa	c_{th}	10^{-6}	m^2/s
M_{CaCO_3}	0.1	kg/mol	R	0.1	mm
M_{CaO}	0.056	kg/mol	G	10^4	MPa
M_{CO_2}	0.044	kg/mol	K	$2 \cdot 10^4$	MPa
ρ_s	$2.5 \cdot 10^3$	kg/m^3	μ	0.5	—
ρ_f	10^3	kg/m^3	β	0	—
ρC	2.8	$MPa/^\circ C$	A_0	10^6	$1/s$
Λ	0.5	$MPa/^\circ C$	$ \Delta H $	200	kJ/mol

Table 1: Indicative material parameters for a fault at 7 km depth, where the initial temperature is about 200°C. For these values of the parameters and for $T_c = 800^\circ C$ the corresponding dimensionless groups are $\zeta = 1.24$, $\alpha = 0.06$, $\delta = 0$, $\eta = 10$, $I = 1.25 \cdot 10^{-9}$, $\bar{\alpha}_s = 10^{-2}$, $\chi \approx 2A_0 = 2 \cdot 10^6$, $\psi \approx 0.01A_0 = 10^4$

bility mode with the fastest growth in time) as a function of the wavelength
 λ (Figure 6b) and select the wavelength number $\lambda = \lambda_m$ corresponding to
 the maximum value of the growth coefficient s , so that a wavelength with
 the fastest growth in time appears. In Figure 3 this selected wavelength
 is plotted against the hardening modulus. As in Sulem et al. (2011) the
 selected wavelength tends to infinity for $h \rightarrow h_{cr}^-$ denoting that at initial
 instability no localization takes place. As the hardening modulus decreases
 the wavelength decreases as well, reaching a minimum at $h \approx 0.16$, where

367 $\lambda_m \approx 3.95$. Muhlhaus and Vardoulakis (1987) similarly obtained that at
 368 the bifurcation state the shear-band thickness for dry granular materials is
 369 infinite and decreases beyond the bifurcation state as the strain localization
 370 process evolves.

371 We notice that the selected wavelength ($\lambda_m \approx 3.95$) in this case is sig-
 372 nificantly smaller than in the absence of the chemical reaction ($\lambda'_m \approx 187$),
 373 revealing the crucial, localizing role of the chemical reaction. Since for this
 374 example we have used indicative values for the reaction parameters, like the
 375 pre-exponential factor and the activation temperature, we proceed with an
 376 analysis of these parameters in order to reveal their influence on the width
 377 of the PSZ and the type of instability.

378 **5. Parametric Analysis. Impact of the chemical reaction and the** 379 **pressurization mechanism**

380 From the parameters appearing in 4.2, those being less constrained in
 381 values are the parameters of the reaction A_0 and T_c . Since they always appear
 382 in the parameter groups as a ratio A_0/T_c , we emphasize on the influence of
 383 this ratio on the stability of the system by treating it as a parameter.

384 *5.1. Effect of the chemical reaction*

385 To assess the influence of the chemical reaction, we plot in Figure 4 the
 386 values of h_{cr} with the ratio of the reaction parameters $\frac{A_0}{T_c}$ varying from 10^{-4}
 387 to 10^{12} . We observe that as $\frac{A_0}{T_c} \rightarrow 0$, then $h_{cr} \rightarrow h'_{cr} = 0.014$, thus it tends
 388 to the case of pressurization alone as weakening mechanism (Sulem et al.
 389 (2011)). As $\frac{A_0}{T_c}$ increases, h_{cr} increases as well, reaching an upper threshold
 390 at $h_{cr}^m \approx 6$.

Figure 4: The critical hardening modulus h_{cr} as a function of A_0/T_c (logarithmic scale for A_0/T_c).

391 It is to be noted that as soon as h_{cr} reaches h_{cr}^m , then the maximum
 392 positive root changes from purely real to complex (Figure 4). This effect
 393 takes place at a critical $\frac{A_0}{T_c}$ (in this case $A_0^{cr} = 10^7 \text{ s}^{-1}$ for $T_c = 800^\circ\text{C}$) and
 394 signifies the onset of oscillatory instabilities due to the chemical reaction.
 395 The existence of oscillatory instabilities is questionable because when the
 396 temperature decreases below the given threshold the reaction stops. In other
 397 words, the linear stability analysis is not valid for non monotonous processes
 398 in case of non-linear behaviour. For this reason the exact type of these
 399 oscillatory instabilities, as well as their time evolution cannot be determined
 400 by the present linear stability analysis. To this end nonlinear analyses and
 401 time integration of the full system of equations is required, to determine
 402 whether imaginary eigenvalues may correspond to stick-slip type of instability
 403 (appearing as limit cycles on a phase diagram, as for example in Alevizos and
 404 Veveakis (2011))

405 5.2. Effect of thermal pressurization mechanism

406 As already mentioned and anticipated, when $\frac{A_0}{T_c} \rightarrow 0$, then $h_{cr} \rightarrow h'_{cr} =$
 407 0.014, thus the system is influenced by pressurization alone as weakening
 408 mechanism (Sulem et al. (2011)). However, when the reaction becomes strong
 409 and $\frac{A_0}{T_c}$ increases so that $h_{cr} \rightarrow h_{cr}^m$, the effect of thermal pressurization,
 410 compared to the chemical effect (i.e. the production of excess pore fluid due
 411 to CaCO_3 lattice breakdown and CO_2 production), is negligible. This fact
 412 becomes apparent in the Appendix A, where we compare the $s - \lambda$ curves
 413 of Figures 7b and 6b with the corresponding ones in the absence of thermal
 414 pressurization, appearing in Figure 8.

415 We notice that the same response is obtained, both for the magnitudes of

416 h , s and λ and for the type of instability (nodal instability for $A_0 = 10^6 \text{ s}^{-1}$
 417 and oscillatory for $A_0 = 10^7 \text{ s}^{-1}$, $T_c = 800^\circ\text{C}$). The pre-exponential factor
 418 for the considered depths cannot be realistically estimated, since it is pres-
 419 sure dependent (Lvov et al. (2002)) and there is a lack of experimental data
 420 at high pressures, however usually it is accepted to be more than 10^{10} s^{-1}
 421 (for example Dollimore et al. (1996) suggest a value of the order of 10^{15} s^{-1} ,
 422 used also by Sulem and Famin (2009)). Thus, we may conclude that at high
 423 temperatures where reaction is triggered (around T_c), and for the decompo-
 424 sition reaction considered, the main weakening mechanism of the two is the
 425 reaction, verifying the recent experimental findings of Han et al. (2007) and
 426 Ferri et al. (2010). However, as also discussed by Han et al. (2010) and De
 427 Paola et al. (2011) important weakening mechanisms like powder lubrication
 428 and flash heating (see also Rice (2006)) should not be excluded if one would
 429 like to model all the mechano-physical processes taking place in a fault, since
 430 they could have equal or even more dramatic role than chemical pressuriza-
 431 tion. In addition secondary chemo-mechanical effects like the breakdown of
 432 calcite grains expressed through the production of holes in the Calcite grains
 433 due to decarbonation reduce also the compressive strength, forcing the mi-
 434 crostructure to collapse. In this study we have excluded these mechanisms to
 435 emphasize on the two pressurization mechanisms, i.e. thermal and chemical
 436 pressurization.

437 However, we notice that the initial temperature for a 7-*km* fault is around
 438 200°C , far below the activation temperature $T_c \approx 800^\circ\text{C}$ of calcite decomposi-
 439 tion. Up to the temperature regime around T_c the reaction term is negligible
 440 and localization is driven by thermal pressurization, a fact that could not

441 be analyzed in this study due to the choice of the reference temperature T_c ,
 442 around which we linearized in Section 4.1, in order to emphasize on the re-
 443 action itself. As temperature increases the process is progressively localizing
 444 towards an ultimate shear-zone whose thickness is determined by the reac-
 445 tion itself. To address this claim, we proceed with a shear band thickness
 446 analysis.

447 5.3. Shear band thickness, Wavelength selection

448 Indeed, it is expected that at temperatures near T_c the width D of the
 449 PSZ of Fig.1 is influenced by the chemical reaction. To verify this claim we
 450 may plot the minimum selected wavelength against the ratio A_0/T_c (Figure
 451 5) to conclude that with increasing A_0/T_c , λ_m and thus D decrease. In the
 452 absence of chemical reaction, λ_m was calculated to be equal to about 187.
 453 The ultimate value for λ_m in the presence of a chemical reaction is around
 454 3, denoting that the PSZ may be an extremely localized structure, obtaining
 455 $\lambda_m = 300 \mu m$ when $d_{50} = 0.1 mm$ as is the case for fine sands, or even less if
 456 we consider possible average grain sizes from principal slipping zones, up to
 457 $10 \mu m$, in the lines of the field evidence provided by Smith et al (2011) and
 458 thoroughly discussed in the introduction.

459 Thus, indeed the onset of the reaction is taking place in an ultra local-
 460 ized zone, that could be significantly thinner than the initial one defined
 461 by thermal pressurization alone ($\lambda_m \sim 187$). This means that in a “non-
 462 reactive” fault thermal pressurization of pore fluids would result in a slipping
 463 zone of $18.7 mm$ thick (for a fault material with $d_{50} = 0.1 mm$), while un-
 464 der the same ambient conditions and slip rate, in a ”reactive” gouge (e.g.,
 465 calcite) chemical reaction would result in a slipping zone of $0.3 mm$.

Figure 5: The selected wavelength λ_m as a function of A_0/T_c

466 What have to be noted at this point, is that localizing mechanisms like
 467 flash heating and breakage have been neglected in this study, as discussed
 468 thoroughly in Sections 2 and 5.2. Including these mechanisms would provide
 469 a more realistic behaviour of the fault even at low temperatures where pres-
 470 surization or the chemical reaction are absent. In addition, the thickness of
 471 this ultimate structure (the PSZ) seems to push continuum theories to its
 472 limits, since the width of the structure is comparable to the size of the aver-
 473 age grain. However, we emphasize that in this study the average grain size
 474 used (d_{50}) is the one of the initial grain size distribution and that during the
 475 evolution of a chemical reaction, grains undergo chemical degradation and
 476 phase transitions that could significantly alter the average grain size, or even
 477 make the determination of grain size ambiguous if amorphization (Yund et al
 478 (1990); Brantut et al. (2008)) is the chemical reaction. As shown by Veveakis
 479 et al. (2010); Alevizos and Veveakis (2011) during shearing of faults we may
 480 identify a regime of lower temperatures, where mechanical effects determine
 481 the evolution of the system and a high temperature regime, where the reac-
 482 tion is triggered and dominates the response of the fault, irrespective of the
 483 mechanical behavior. Thus, the present Cosserat approach is valid up to the
 484 point that chemical reaction is fully set and determines all the mechanical
 485 effects of the fault, like grain size evolutions and rheological response. It is
 486 used in order to obtain an estimate of the thickness of the layer at which
 487 chemical reaction will be triggered. Pass this point, either discrete analyses
 488 or even higher order continuum theories (Stefanou et al. (2010)) must be ap-
 489 plied to account for the chemical reaction effects (for example by introducing
 490 varying d_{50}).

491 6. Discussion

492 Thermal instabilities were shown to be important at elevated temper-
493 atures, and to determine the stability of a fault even at regimes that are
494 considered to be stable under purely mechanical conditions. The formalism
495 presented here however revealed the importance of parameters that are not
496 well-constrained. In particular, the hardening modulus h of rock materials is
497 in principle varying with shear strain, while the parameters of the reaction A_0
498 and T_c strongly depend on the applied pressures at which the reaction takes
499 place (Lvov (2007), pp. 79) and several values can be found in the literature
500 (For example A_0 may vary from $10^2 s^{-1}$ to $10^{20} s^{-1}$ for calcite decomposition,
501 as discussed by Lvov et al. (2002)).

502 Therefore, in order to apply the presented theory in real faults, there
503 is a need of extensive laboratory testing of the strain-stress response of the
504 fault gouge materials and on the effect of pressure and temperature on this
505 response.

506 The results presented in this work could provide insight for the thermo-
507 mechano-chemical coupling occurring in soil materials. Given the stress-
508 strain response of the material, the ambient thermal conditions of the fault
509 determine whether the fault may weaken thermally or not. At lower tem-
510 peratures thermal pressurization may be triggered and cause softening at
511 positive, but near zero, hardening modulus. At higher temperatures, near
512 the activation of chemical reactions thermal softening induces a strong weak-
513 ening effect since it may take place at extremely high (positive) values of
514 the hardening modulus. Therefore at high temperatures even if the material
515 is mechanically stable (steep hardening regime) the triggering of a chemical

516 reaction would lead the system to instability and softening.

517 The model presented here contains parameters that need to be evaluated
518 from interdisciplinary experiments at conditions that match the ones met in
519 real faults at seismic depths. Parameters like those appearing in the reaction
520 rate of the chemical reaction (A_0 , T_c) or in friction laws of geomaterials that
521 would provide parameters like G_c should be evaluated before applying such
522 models in real cases.

523 7. Conclusions

524 In this work, we have used higher order continua considerations and al-
525 lowed to the fault material additional, rotational degree of freedoms, along
526 with the presence of a decomposition reaction. We have shown that the ill-
527 posed problem of simple shear of a saturated fault can be remedied when
528 accounting for the micro-inertia of the rotations and that, at temperatures
529 near its activation energy, the impact of the reaction is significant to the
530 stability of the mechanical problem and the localization of deformation.

531 We have shown that the width of the localizing shear zone at which dy-
532 namic weakening of faults take place depends strongly on the parameters of
533 the reaction, i.e. the pre-exponential factor A_0 and the activation temper-
534 ature T_c . Small values of the ratio $\frac{A_0}{T_c}$ correspond to broader zones, of the
535 order of few centimeters.

536 A. Linear Stability Analysis

537 By substituting the perturbation fields (22) into the linearized govern-
538 ing equations (18, 21), we obtain a homogeneous algebraic system for the

539 coefficients $U_1, U_2, \Omega, \Pi, \Theta$:

$$\begin{aligned}
 & \begin{bmatrix} \frac{s\delta\sigma(d+\epsilon+2c\mu)}{2h\lambda\sigma'} & \frac{s\delta\sigma(2f+(a+b)\mu)}{2h\lambda\sigma'} & 0 & -\frac{a\alpha_s s T_c \delta\mu\sigma + \alpha_s b s T_c \delta\mu\sigma + 2h\sigma'(sT_c + \chi)}{2hT_c\sigma'} & s + \frac{\eta}{\lambda^2} \\ -\frac{s\alpha\sigma(d+\epsilon+2c\mu)}{2h\lambda\sigma'} & \frac{s\alpha\sigma(2f+(a+b)\mu)}{2h\lambda\sigma'} & 0 & \frac{1}{\lambda^2} + \frac{s(a\alpha_s\alpha\mu)\sigma + \alpha_s b\alpha\mu\sigma + 2h\sigma'}{2h\sigma'} + \frac{\psi}{T_c} & 0 \\ -s^2I - \frac{d}{\lambda^2} & -\frac{f}{\lambda^2} & \frac{-d+\epsilon}{\lambda} & 0 & 0 \\ -\frac{c}{\lambda^2} & -s^2I - \frac{a}{\lambda^2} & 0 & \frac{\alpha_s(a+b)}{2\lambda} & \frac{1}{\lambda} \\ \frac{-d+\epsilon}{\lambda} & 0 & -2d + 2\epsilon - \frac{s^2I}{2} - \frac{g}{\lambda^2} & 0 & 0 \end{bmatrix} \begin{bmatrix} U_1 \\ U_2 \\ \Omega \\ \Pi \\ \Theta \end{bmatrix} = 0, \\
 & \hspace{15em} (23)
 \end{aligned}$$

540 where

$$\begin{aligned}
 a &= \frac{G + K - (\mu\beta K^2)/(G + H + K\beta\mu)}{\sigma}, \\
 b &= \frac{K - G - (\mu\beta K^2)/(G + H + K\beta\mu)}{\sigma}, \\
 c &= \frac{-(G\beta K)/(G + H + K\beta\mu)}{\sigma}, \\
 d &= \frac{G + G_c - (G^2)/(G + H + K\beta\mu)}{\sigma}, \\
 \epsilon &= \frac{G - G_c - (G^2)/(G + H + K\beta\mu)}{\sigma}, \\
 f &= \frac{-(\mu GK)/(G + H + K\beta\mu)}{\sigma}, \\
 g &= \frac{G}{\sigma}, \quad K = \frac{G}{1 - 2\nu}.
 \end{aligned} \tag{24}$$

541 A nonzero solution is possible only when the determinant of the linear
 542 system vanishes. This request results in a characteristic polynomial equation
 543 of degree 8 for the growth coefficient s . If a root has a positive real part,
 544 then the corresponding perturbation grows exponentially in time. Since a
 545 polynomial of degree 8 cannot admit an analytic solution, indicative values
 546 of the parameters have to be used in order to obtain numerical solutions

Figure 6: Real parts of the roots of the characteristic equation (growth coefficient s) as a function of the wavelength number λ , for $A_0 = 10^6$ and $T_c = 800$ (a) for $h \geq h_{cr} = 6$ where only negative roots appear, rendering the system stable, (b) for $h < h_{cr}$. The dashed curves represent the real part of complex roots whereas the solid curves depict the purely real roots (zero imaginary part). The wavelength at which the growth coefficient s obtains its maximum value is the one corresponding to the selected wavelength λ_m .

547 of the characteristic polynomial. To this end we consider the case of a 7-
548 km deep fault, of a gouge material having the parameters depicted in Table
549 4.2. With these values we obtain a critical value for the hardening modulus
550 $h_{cr} \approx 6$, such that for $h \geq h_{cr}$ all the roots of the polynomial equation have
551 negative real part, and thus the system is stable (Figure 6a). For $h < h_{cr}$
552 roots with positive real parts exist, bringing the system to instability (Figure
553 6b).

554 In order to asses the localizing effect of the chemical reaction, we may
555 plot the greatest root (i.e. the one corresponding to the instability mode
556 with the fastest growth in time) as a function of the wavelength λ . This
557 curve exhibits a maximum at $\lambda = \lambda_m$ so that a wavelength with the fastest
558 growth in time appears (Figure 6b)

559 In the absence of thermal pressurization (i.e. when $\Lambda = 0$ in the original

Figure 7: Real parts of the roots of the characteristic equation (growth coefficient s) as a function of the wavelength number λ , for $A_0 = 10^7$ and $T_c = 800$ (a) for $h \geq h_{cr} = 6$ where only negative roots appear, (b) for $h < h_{cr}$. The dashed curves represent the real part of complex roots, whereas the solid curves depict the purely real roots (zero imaginary part). The maximum root is complex in this case, denoting the onset of oscillatory instability.

560 set of equations), we rescale temperature with T_c , recalculate the roots of
 561 the characteristic polynomial and plot s against λ . By comparing the $s - \lambda$
 562 curves of Figures 7b and 6b with the corresponding ones in the absence of
 563 thermal pressurization, appearing in Figure 8, we may conclude that ther-
 564 mal pressurization is a secondary effect at elevated temperatures where the
 565 reaction sets in.

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Figure 8: Real parts of the roots of the characteristic equation (growth coefficient s) as a function of the wavelength number λ , in the absence of thermal pressurization for $T_c = 800^\circ\text{C}$ and (a) $A_0 = 10^6 \text{ s}^{-1}$, (b) $A_0 = 10^7 \text{ s}^{-1}$.

References

- Alevizos, S., Veveakis, E., 2011. Thermal and chemical mechanisms of frictional faults: Static and dynamic instabilities. *J. Mech. Phys. Solids* in print.
- Brantut, N., A. Schubnel, J.-N. Rouzaud, F. Brunet, and T. Shimamoto, 2008. High velocity frictional properties of a clay-bearing fault gouge and implications for earthquake mechanics, *J. Geophys. Res.*, 113, B10401, doi: 10.1029/2007JB005551.
- Brantut, N., Schubnel, A., Corvisier, J., Sarout, J., 2010. Thermochemical pressurization of faults during coseismic slip. *J. Geophys Res.* 115, B05314.
- Brantut, N., Sulem, J., Schubnel, A., 2011. Effect of dehydration reactions on earthquake nucleation: Stable sliding, slow transients and unstable slip. *J. Geoph. Res.* 116, B05304, doi:10.1029/2010JB007876.
- Brantut, N., R. Han, T. Shimamoto, N. Findling, and A. Schubnel, Fast

587 slip with inhibited temperature rise due to mineral dehydration: Evidence
588 from experiments on gypsum, *Geology*, 39 (1), 5962, 2011.

589 Chester, F., 1995. A geologic model for wet crust applied to strike-slip faults.
590 *J. Geophys. Res. - Solid Earth* 100, 13033–13044.

591 Chester, F., Chester, J., 1998. Ultracataclasite structure and friction pro-
592 cesses of the punchbowl fault, san andreas system, california. *Tectono-*
593 *physics*, 199–221.

594 Chester, F. M., Evans, J. P., Biegel, R. L., 1993. Internal structure and
595 weakening mechanisms of the san andreas fault. *J. Geophys. Res.* 98, 771–
596 786.

597 Chester, J. S., Goldsby, D. L., 2003. Microscale characterization of natural
598 and experimental slip surfaces relevant to earthquake mechanics, SCEC
599 Annu. Prog. Rep. 2003, South. Calif. Earthquake Cent., Los Angeles.

600 Chester, J.S., Chester, F.M., Kronenberg, A.K., 2005. Fracture surface en-
601 ergy of the Punchbowl Fault, San Andreas System. *Nature* 437, 133-136.

602 Cornet, F., Doan, M., Moretti, I., Borm, G., 2004. Drilling through the active
603 Aigion fault: the aig10 well observatory. *Comptes Rendus Geosciences*
604 336 (4-5), 395–406.

605 Di Toro, G., Han R., Hirose, T., De Paola, N., Nielsen, S., Mizoguchi, K.,
606 Ferri, F., Cocco, M., Shimamoto, T., 2011. Fault lubrication during earth-
607 quakes. *Nature*, vol. 471, 494-498.

608 De Paola, N., Hirose, T., Mitchell, T., Di Toro, G., Togo, T., Shimamoto, T.
609 2011. Fault lubrication and earthquake propagation in thermally unstable
610 rocks. *Geology*, vol. 39, pp. 35-38.

611 Dollimore, D., P. Tong, and K. S. Alexander (1996), The kinetic interpreta-
612 tion of the decomposition of calcium carbonate by use of relationships
613 other than the Arrhenius equation, *Thermochim. Acta*, 282/283, 13–27.

614 Famin et al., 2008, Earthquakes produce carbon dioxide in crustal faults,
615 *Earth and Planetary Science Letters*, 265, 487-497.

616 Ferri, F., Di Toro, G., Hirose, T., Shimamoto, T., 2010. Evidence of ther-
617 mal pressurization in high-velocity friction experiments on smectite-rich
618 gouges. *Terra Nova*, 22: 347-353, doi:10.1111/j.1365-3121.2010.00955.x.

619 Fisher, T.E. Tribochemistry. *Ann. Rev. Mater. Sci.* 18 303-323 (1988).

620 Garagash, D. I., Rudnicki, J. W., 2003a. Shear heating of a fluid-saturated
621 slip-weakening dilatant fault zone, 1, limiting regimes. *J. Geophys. Res.*
622 108.

623 Garagash, D. I., Rudnicki, J. W., 2003b. Shear heating of a fluid-saturated
624 slip-weakening dilatant fault zone, 2, quasi-drained regime. *J. Geophys.*
625 *Res.* 108.

626 Goren, L., Aharonov, E., 2007. Long runout landslides: The role of frictional
627 heating and hydraulic diffusivity. *Geophys. Res. Lett.* 34, L07301.

628 Goren, L., Aharonov, E., Anders, M. H., 2010. The long runout of the Heart

629 Mountain landslide: heating, pressurization, and carbonate decomposition.
630 J. Geophys. Res. 115, B10210.

631 Han, R., Shimamoto, T., Hirose, T., Ree, J., Ando, J., 2007. Ultralow friction
632 of carbonate faults caused by thermal decomposition. Science 316, 878–881.

633 Han, R., Hirose, T., and Shimamoto, T., 2010, Strong velocity weakening and
634 powder lubrication of simulated carbonate faults at seismic slip rate: Jour-
635 nal of Geophysical Research, v. 115, B03412, doi:10.1029/2008JB006136

636 Han, R. Takehiro Hirose, Toshihiko Shimamoto, Youngmin Lee and Jun-ichi
637 Ando, 2011, Granular nanoparticles lubricate faults during seismic slip,
638 Geology 2011;39;599-602

639 Hill, R., 1962. Acceleration waves in solids. J. Mech. Phys. Solids 10, 1–16.

640 Hirono, T. et al., 2007. A chemical kinetic approach to estimate dynamic
641 shear stress during the 1999 Taiwan Chi-Chi earthquake. Geophys. Res.
642 Lett. 34, L19308, doi:10.1029/2007GL030743.

643 Holcomb, D.J., Rudnicki, J.W., 2001. Inelastic constitutive properties and
644 shear localization in Tennessee marble, Int. J. Num. Anal. Meth. Geomech.
645 25, 109–129

646 Lachenbruch, A. H., Frictional heating, uid pressure, and the resistance to
647 fault motion, J. Geophys. Res., 85, 60976122, 1980.

648 Law, C., 2006. Combustion Physics. Cambridge University Press.

- 649 L'vov, B., 2007. Thermal Decomposition of Solids and Melts: New Ther-
650 mochemical Approach to the Mechanism, Kinetics and Methodology.
651 Springer.
- 652 L'vov, B. V., Polzik, L. K., Ugolkov, V. L., 2002. Decomposition kinetics
653 of calcite:a new approach to the old problem. *Thermochimica Acta* 390,
654 5–19.
- 655 Mandel, J., 1966. Conditions de stabilite et postulate de drucker. *Rheology*
656 and Soil Mechanics, 58–67.
- 657 Morgenstern, N. R., Tschalenko, J. S., 1967. Microscopic structures in kaolin
658 subjected to direct shear. *Geotechnique* 17, 309–328.
- 659 Muhlhaus, H. B., Vardoulakis, I., 1987. Thickness of shear bands in granular
660 materials. *Geotechnique* 37 (3), 271–283.
- 661 Nguyen, G. D., Einav, I., 2010. Nonlocal regularisation of a model based on
662 breakage mechanics for granular materials. *Int. J. Sol. Struct.* 47, 1350–
663 1360.
- 664 Noda, H., Shimamoto, T., 2005. Thermal pressurization and slip-weakening
665 distance of a fault: An example of the Hanaore fault, Southwest Japan.
666 *Bull. Seismol. Soc. Am.* 95 (4).
- 667 Pinyol, N., Alonso, E., 2010. Criteria for rapid sliding II.thermo-hydro-
668 mechanical and scale effects in Vaiont case. *Engineering Geology* 114,
669 211227.

670 Pittarello, L., Di Toro, G., Bizzarri, A., Pennacchioni, G., Hadizadeh,
 671 J., Cocco, M., 2008. Energy partitioning during seismic slip in
 672 pseudotachylyte-bearing faults (Gole Larghe Fault, Adamello, Italy).
 673 Earth and Planetary Science Letters, vol. 269, pp. 131-139.

674 Rice, J. R., 1975. On the stability of dilatant hardening for saturated rock
 675 masses. J. Geophys. Res. 80 (11), 1531 – 1536.

676 Rice, J. R., 2006. Heating and weakening of faults during earthquake slip. J.
 677 Geophys. Res. 111, B05311.

678 Rudnicki, J., Rice, J., 1975. Conditions for the localization of deformation in
 679 pressure sensitive dilatant materials. J. Mech. Phys. Solids 23, 371–394.

680 Sibson, R. H., Interaction between temperature and pore-fluid pressure during
 681 earthquake faulting a mechanism for partial or total stress relief, Nature,
 682 243, 6668, 1973.

683 Sibson, R.H., Thickness of the Seismic Slip Zone, Bull. Seism. Soc. Am., 93,
 684 1169-1178, 2003.

685 Smith, S. A. F., A. Billi, G. Di Toro, and R. Spiess, Principal slip zones in
 686 limestone: Microstructural characterization and implications for the seis-
 687 mic cycle (Tre Monti fault, Central Apennines, Italy), Pure Appl. Geo-
 688 phys., doi:10.1007/s00024-011-0267-5, 2011.

689 Sulem, J., 2007. Stress orientation evaluated from strain localisation analysis
 690 in Aigion fault. Tectonophysics 442, 3–13.

- 691 Sulem, J., Famin, V., 2009. Thermal decomposition of carbonates in fault
692 zones: slip-weakening and temperature-limiting effects. *J. Geophys. Res.*
693 114, B03309.
- 694 Sulem, J., Stefanou, I., Veveakis, E., 2011. Stability analysis of undrained
695 adiabatic shearing of a rock layer with Cosserat microstructure. *Granular*
696 *Matter* in press, doi:10.1007/s10035-010-0244-1.
- 697 Sulem, J., Vardoulakis, I., Ouffroukh, H., Perdikatsis, V., 2005. Thermo-
698 poro-mechanical properties of the aigion fault clayey gouge - application
699 to the analysis of shear heating and fluid pressurization. *Soils and Foun-*
700 *dations* 45, 97–108.
- 701 Stefanou I., Sulem J. and Vardoulakis I., 2010. Homogenization of inter-
702 locking masonry structures using a generalized differential expansion tech-
703 nique. *International Journal of Solids and Structures* 47, 1522–1536.
- 704 Tisato, N., Di Toro, G., De Rossi, N., Quaresimin, M., Candela T., 2011.
705 Experimental investigation of flash weakening in limestone. Submitted to
706 *Journal of Structural Geology*.
- 707 Yue, L., Shui, M. and Xu, Z. The decomposition kinetics of nanocrystalline
708 calcite. *Thermochimica Acta* 335 121-126 (1999).
- 709 Yund, R. A., M. L. Blanpied, T. E. Tullis, and J. D. Weeks, Amorphous ma-
710 terial in high strain experimental fault gouges, *J. Geophys. Res.*, 95 (B10),
711 15,589-15,602, 1990.

- 712 Vardoulakis, I., 1985. Stability and bifurcation of undrained, plane rectilin-
713 ear deformations on water-saturated granular soils. *Int. J. Numer. Anal.*
714 *Methods Geomech.* 9, 339–414.
- 715 Vardoulakis, I., 1986. Dynamic stability of undrained simple shear on water-
716 saturated granular soils. *Int. J. Numer. Anal. Methods Geomech.* 10, 177–
717 190.
- 718 Vardoulakis, I., 1996. Deformation of water-saturated sand: II. effect of pore
719 water flow and shear banding. *Geotechnique* 46 (3), 457–472.
- 720 Vardoulakis, I., 2002a. Dynamic thermo-poro-mechanical analysis of catas-
721 trophic landslides. *Geotechnique* 52, 157–171.
- 722 Vardoulakis, I., Sulem, J. (Eds.), 1995. *Bifurcation Analysis in Geomechan-*
723 *ics.* Blackie Acc. and Professional.
- 724 Veveakis, E., Alevizos, S., Vardoulakis, I., 2010. Chemical reaction capping
725 of thermal instabilities during shear of frictional faults. *J. Mech. Phys.*
726 *Solids* 58, 1175 – 1194.
- 727 Veveakis, E., Vardoulakis, I., Di Toro, G., 2007. Thermoporomechanics of
728 creeping landslides: The 1963 Vaiont slide, Northern Italy. *J. Geophys.*
729 *Res.* 112, F03026.
- 730 Wibberley, C., Shimamoto, T., 2005. Earthquake slip weakening and asperi-
731 ties explained by thermal pressurization. *Nature* 426 (4), 689–692.
- 732 Wibberley, C. A. J., Shimamoto, T., 2003. Internal structure and perme-

733 ability of major strike-slip fault zones: The median tectonic line in mid
734 prefecture, southwest japan. J. Struct. Geol. 25, 59–78.

735 Wibberley , C.A.J, Graham, Y., Di Toro, G., 2008. Recent advances in the
736 understanding of fault zone internal structure: a review. In "The Internal
737 Structure of Fault Zones - implications for mechanical and fluid flow prop-
738 erties", Eds. C.A.J. Wibberley, W. Kurz, J. Imber, R.E. Holdsworth and
739 C. Collettini, Special Volume of the Geological Society of London, Vol.
740 299, pp. 5-33.