Journal of Structural Geology 31 (2009) 752–755

Contents lists available at ScienceDirect

Journal of Structural Geology

journal homepage: www.elsevier.com/locate/jsg

Folding with thermal-mechanical feedback: A reply

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ARTICLE INFO

Article history:
Received 26 March 2009
Accepted 28 March 2009
Available online 7 April 2009

Keywords:
Folding
Boudinage
Thermodynamics
Reaction-diffusion equation

ABSTRACT

A unified theory of deformation at all scales is outlined. Processes operating during deformation and metamorphism can be coupled in the form of reaction-diffusion equations. Solutions to these equations depend on the specific processes that dominate the dissipation of energy. Hobbs et al. (2008) is concerned with a scale where deformation and conduction of heat dominate and this corresponds to the regional scale. Other papers present results for other length and time scales. Boudinage develops through these processes in materials where the strict Biot theory predicts no boudinage. The strict Biot theory is applicable only at the instant of instability and provides no information on the subsequent growth of the folds. Analytical results for growth to large amplitudes show that only one wavelength develops and not a spectrum of wavelengths as proposed by Treagus and Hudleston (in press) and others. The wavelength to thickness ratio that finally develops is strongly dependent on boundary conditions and so such ratios tell us nothing about the conditions of folding unless these boundary conditions are known. The processes involved in folding with thermal-mechanical feedback are identical for single- and multi-layer systems so that it requires little space to expand the discussion to multi-layers.

We thank Sue Treagus and Peter Hudleston for the opportunity to expand on our paper on the formation of folds through thermal-mechanical feedback (Hobbs et al., 2008) and to clarify some apparent omissions. Their comments address three main issues. (i) Our paper addressed folds at regional scales and did not demonstrate folds at finer scales such as one might observe at outcrop, hand specimen or thin section scales; as part of this issue we also promised a unified framework which does not appear obvious to Treagus and Hudleston from our paper. We also promised an application to boudinage. (ii) The wavelength to thickness ratios we quoted for natural folds are not comprehensive and representative of natural folds and in particular of that predicted by the Biot theory. (iii) Our paper concentrated on single layer folds and the real interest is in multi-layer folds to which we relegated a small amount of space. We address these three issues below.

1. A unified framework, the scale issue and boudinage

The deformation of rocks takes place together with other processes of interest to structural geologists including metamorphic mineral reactions, metamorphic differentiation, microstructural adjustments such as grain-size reduction, preferred orientation development, fracturing and melting. None of these processes are addressed within a Biot framework; our motivation is to develop a self-consistent framework where all the processes that operate during orogenesis are integrated within that framework. The processes mentioned are thermally activated and either consume or produce heat. Many silicate reactions not involving hydration are endothermic whereas reactions that involve hydration are commonly exothermic (Haack and Zimmermann, 1996). Inelastic deformation such as crystal plasticity, fracturing and frictional sliding (Wu et al., 2006) produce heat whereas grain-size reduction and melting consume heat. The important issue concerns the total heat budget of the deforming, reacting rock mass; this is where the coupling between all of the interesting processes arises and is why a thermodynamic approach supplies an integrating framework.

It is well known in many fields of science that systems involving $\aleph$ processes each of which produce or consume heat, evolve according to an equation of the form:

$$\frac{DT}{Dt} = \kappa_{ij}\frac{\partial^2 T}{\partial x_i \partial x_j} + \sum_{\aleph} \lambda^{\aleph} \exp\left(-\frac{E^{\aleph}}{RT}\right) \quad (1)$$

where DT/Dt is the time material derivative of the absolute temperature, T, κ_{ij} is the thermal diffusivity tensor and x_i is a spatial coordinate. $\lambda^{\aleph}$ is a parameter that is a measure of the dissipation for the $\aleph^{\text{th}}$ process; for thermal-mechanical and thermal-chemical processes it is the Gruntfest Number and the Damkoehler Number

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0191-8141/$ – see front matter © 2008 Published by Elsevier Ltd.
doi:10.1016/j.jsg.2009.03.014

respectively (Veveakis et al., in press). $E^{\aleph}$ is the activation energy for the $\aleph^{\text{th}}$ process. Eq. (1) is a special form of the reaction-diffusion equation and its form derives from an Arrhenius dependence of the relevant geological processes upon temperature. Eq. (1) is the Energy Equation derived in Hobbs et al. (2008). Coupled processes that obey (1) have been widely studied and the solutions of many of the equations involved are well known (Law, 2006). In (1), if T is replaced by c, the concentration of a mineral species, and the exponential dependence is replaced or augmented by non-linear terms involving c, then the result is the behaviour discussed by Ortoleva (1994) for a diverse range of processes including metamorphic differentiation. All of these relations can be derived using modern continuum thermodynamics as presented in Hobbs et al. (2008).

Eq. (1) is the basis of a unified self-consistent framework describing the evolution of structures seen in deformed rocks. Our approach and that of others, has been to study special cases of this complete coupling. Examples of these special cases are:

(i) The isothermal case where the strain-rate is small compared to the thermal diffusivity. This corresponds to the outcrop scale where chemical reactions are coupled to inelastic deformation. These conditions result in strain-rate softening and shear zones, folds and boudinage develop because of this rate dependent softening (Hobbs et al., in press).

(ii) The isothermal case where the strain-rate is small compared to the thermal diffusivity and both chemical reactions and chemical diffusion operate. This corresponds to the micrometer scale in metamorphic rocks (Regenauer-Lieb et al., 2009).

(iii) The case where the strain-rate is small compared to the thermal diffusivity, and λ is a non-zero Gruntfest Number. This corresponds to the regional scale where thermal-mechanical feedback is the dominant process. Shear zones, folds and boudinage again develop. These conditions are the topic of Hobbs et al. (2008).

(iv) The adiabatic case where the strain-rate is large compared to the thermal diffusivity and $\lambda^{\aleph}$ represents both the Gruntfest and the Damkoehler Numbers. This corresponds to seismic frictional slip within a thin localised zone where mineral reactions including melting operate (Veveakis et al., in press); this coupling is particularly important for understanding the development of thin zones of ultramylonite and pseudotachylite within wider mylonite zones.

Thus the deformation response of a rock depends on time and length scales as well as the details of the processes operating. In Hobbs et al. (2008) we chose the simplest of these situations where the strain-rate is small and only thermal-mechanical feedback operates. This necessitates a response at the regional scale but the other papers mentioned above begin to address some of the other scales. The common response is that the coupling of rate sensitive deformation processes to chemical reactions, mass diffusion and thermal transport results in strain hardening/softening as well as strain-rate softening/hardening. Strain-rate softening is fundamental in developing shear zones, folds and boudins since any small perturbation in strain-rate is self-enhancing and leads to rapid amplification of the instability as expected from (1). The initiation of instabilities in these materials depends on initial heterogeneities (Needleman, 1988) and hence the wavelength of folds is sensitive to these heterogeneities. As this instability grows, exothermic processes such as fracturing and silicate reactions involving hydration destabilise the folding process whereas endothermic processes such as non-hydrating silicate reaction or grain-size reduction stabilise the process for seismic deformations but destabilise deformation at slower strain-rates at the outcrop scale. The important point is that structures that form are similar at all scales. At fine scales the processes discussed by Ortoleva (1994) operate but are still governed by a diffusion-reaction equation.

Not only do shear zones and folds develop by these processes but so do boudins. One of the problems with the Biot type approach is that boudinage is not predicted to develop (Smith, 1977; Schmalholz et al., 2008) in power law viscous materials unless the stress exponent is relatively large (say >5). Strain-rate softening readily produces boudins even in Newtonian materials with viscosity ratios as low as 10 (Fig. 1); other examples are given in Hobbs et al. (in press).

Clearly one of the main issues facing proponents of the Biot type of theory is that although it predicts the development of folds in materials with a stress exponent less than 5 (so long as the boundary conditions are suitable), for identical materials and identical types of boundary conditions it predicts that boudinage will not form. This is quite unsatisfactory and seems to be glossed over by proponents of the Biot approach. We show in the papers mentioned above that if any form of rate dependent coupling is included in the mechanical response then shear zones, folds and boudins form readily even in materials where the Biot theory predicts no structures would form.

2. Wavelength to thickness ratios

We thank Sue Treagus and Peter Hudleston for the catalogue of wavelength to thickness ratios that have been measured by various workers. However, in unstable systems it is not possible without additional information to take the dispersion (growth rate versus wave-number) relations derived by a linear instability analysis and apply those results to the continued growth of the structure. The theory developed by Biot is, for the most part, a linear theory of low amplitude folding and strictly is only applicable within the approximations involved in the linear stability analysis. In contrast, two papers that address large amplitude, thick layer folding analytically are by Mühlhaus et al. (1994, 1998). In Mühlhaus et al. (1998) the results are for large amplitude folds with constant force boundary conditions and so are directly applicable to the arguments raised by Treagus and Hudleston (in press). The results presented in Figs. 5–9 in Mühlhaus et al. (1998) are not computer simulations; they are analytical solutions to the large amplitude problem. Although a spectrum of wavelengths may exist at small amplitudes (the region where the arguments of Treagus and Hudleston (in press) and the Biot theory are relevant) only a single wavelength is developed by the time large amplitude folds are

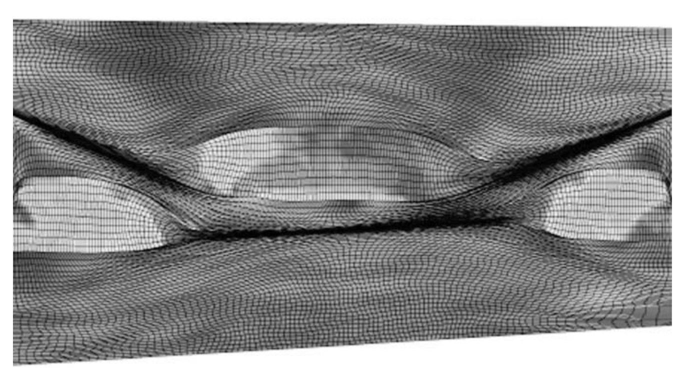

Fig. 1. Boudins developed in a two-layer sequence for pure shearing. Feldspathic layers embedded in quartzite. Parameters are identical to models in Table 4, Hobbs et al. (2008). Bulk extension 340%. Temperature 530 K.

formed. Thus we have to disagree with Treagus and Hudleston (in press) that the Biot theory predicts a range of wavelengths at finite amplitudes. The same conclusions follow for constant velocity boundary conditions (Mühlhaus et al., 1994) where single wavelengths are produced at much lower amplitudes than for constant force boundary conditions.

As we indicated in Hobbs et al. (2008) the wavelength to thickness ratio, Λ, which develops for a particular viscosity ratio for finite amplitude folds, using the Biot approach, depends on the boundary conditions for loading. Most treatments of the folding problem using a Biot type of approach assume that the deformation results from a constant force as would be imposed by a dead load. Under these conditions the folding amplification is driven by this load and the growth rate is exponential to large amplitudes. For small deflections (the range of validity of the Biot theory) it makes no difference if the boundary conditions consist of constant force or constant velocity or any combination of these; one gets identical behaviour. However Mühlhaus et al. (1994) shows that if the deformation continues past the point where the instability begins to grow (that is, folds start to grow) then the boundary conditions make a very large difference to the value of Λ that develops. It follows from Mühlhaus et al. (1998) that if the boundary conditions consist of a constant force then for large amplitude folding, Λ has one value and is that predicted by Sherwin and Chapple (1968) despite the comments of Treagus and Hudleston (in press). However for constant velocity boundary conditions, the force within the deforming layer rapidly drops to small values and fold growth due to this force stops (Mühlhaus et al., 1994). This is because the constant velocity boundary conditions preclude acceleration of the boundary and hence the force in the layer must drop to zero. This type of behaviour has been well documented for different boundary conditions for many systems (see Shawki, 1986, for a thorough treatment) and is true for multi-layers as well as single layers. Fold growth after the force in the layer has decreased is the result solely of homogeneous shortening but only one Λ survives to large amplitudes. The values of Λ that result for identical material properties and strains are quite different for the two types of boundary conditions so that quoting a value for Λ is not very informative unless one knows the boundary conditions. The data presented by Treagus and Hudleston (in press) are extremely interesting in light of the above discussion but certainly are not definitive when it comes to distinguishing various mechanisms for folding. These same comments apply to multi-layer models as well as to single layer folds.

We admit we were remiss in quoting Λ values of 2–4 for the folds described in Hobbs et al. (2008). The number 2 arises from the ideal case where shear zones inclined at 45° to the layer are repeatedly developed in the layer. This never develops to perfection and so as the folds grow any observer would note that values near 4 are common and values as high as 7 develop locally.

3. Single and multi-layer folds

We were not aware that the importance of a scientific result is proportional to the amount of space it occupies in a publication. We concentrated on single layer folds in Hobbs et al. (2008) in order to illustrate the principles involved, namely, that the viscosity decreases in the inner hinges of incipient folds due to thermal-mechanical feedback. This process is self-amplifying because of the feedback relations inherent in (1) and folds quickly amplify. This is true no matter how many layers exist and our exploration of the situation suggests that there is little interaction between layers; this is why we were careful to document the distances between the layers in Hobbs et al. (2008). Thus unlike the Biot approach, where it is important if layers are closer than an interaction distance, thermal-mechanical feedback processes are spatially localised to the immediate vicinity of the strain-rate perturbation. Thus once the principles are established for thermal-mechanical behaviour in a single layer it requires relatively little space to expand the discussion to multi-layers. The situation is different for the Biot approach where many papers continue to be published to explore the interaction between layers.

4. Concluding remarks

We reiterate that a framework based on modern continuum thermodynamics holds the promise for an integrated, self-consistent approach to understanding the development of structures and fabrics in structural geology. This is because such a framework is based on the heat budget for the deforming-reacting rock mass and describes the ways in which the energy dissipation is apportioned between the various processes operating. The relationship describing all of these processes can be derived from continuum thermodynamics and is a reaction-diffusion equation. The details of the apportionment of the dissipation are dependent on the spatial scale and the strain-rate relevant to the problem involved. We concentrated in Hobbs et al. (2008) on the regional scale because that is the simplest problem to tackle first. Nevertheless shear zones, folds and boudins develop readily at this scale in rocks with material properties such that these structures would not develop given a strict Biot mechanism. We show elsewhere that identical structures develop at all scales if the dominant coupling processes operating at those scales are considered (mineral reactions at the outcrop scale and mineral reactions plus chemical diffusion at the micro-scale). Given the fact that a variety of non-Biot mechanisms potentially exists for producing folds and that for some of these mechanisms, as well as the Biot mechanism, the wavelength to thickness ratio that develops for finite amplitude folds is strongly dependent on the boundary conditions, values of Λ are not diagnostic of any particular mechanism or any particular viscosity ratio given our present state of knowledge. We want to emphasise that an analytical solution to the Biot theory predicts only one wavelength at large deflections. Folding in multi-layer sequences arising from thermal-mechanical feedback is exactly the same as for single layers and does not require inordinate amounts of space to describe in a scientific publication once the process for single layers has been established.

Finally, the review by Hunt et al. (1997) points out that the Biot theory is a special case of a general equation that describes the growth of deflections in a layer. The Biot theory (as it is commonly expressed) assumes small deflections and that the constitutive relations of the layer and the embedding material are linear. This means that the growth rates of individual wavelengths are independent and hence the preoccupation with defining the fastest growing wavelength. If the constitutive relations are non-linear then the response can consist of localised packets of folds forming or even fractal geometries; the concept of a dominant wavelength no longer exists. The paper by Hobbs et al. (2008) is an example of this more complicated behaviour. We believe there is much to be learnt from folded rocks yet and that an exciting new period of observation is upon us. This means exploring the non-linear dynamics of folding and not restricting ourselves to linear, low amplitude theories.

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