Shear localisation during deformation of reactive thermo-visco-elastic-plastic materials

Robert Timms [a*], Richard Purvis [a] and John P. Curtis [b,c]

[a]*School of Mathematics, University of East Anglia, Norwich NR4 7TJ;*
[b]*AWE, Aldermaston, Berkshire RG7 4PR;*
[c]*Department of Mathematics, University College London, Gower Street, London WC1E 6BT.*
[*]r.timms@uea.ac.uk

Abstract: A one-dimensional model for the initiation of shear bands in a reactive material is developed, with an Arrhenius source term to model the chemical reaction occurring in the band. An inhomogeneity in the heat flux is used as the stimulus for localised plastic deformation, and the problem is treated as a perturbation to the elastic solution. In the analysis, the thin zone of localisation is identified as a boundary layer. It is found that the behaviour of the perturbations to the temperature and stress in the band are governed by three dimensionless parameters which are known in terms of various material properties. The resulting equations are solved numerically and a criterion for the onset of shear banding is discussed.

1   Introduction

Unintended low energy thermal or mechanical stimuli can lead to the accidental ignition of explosive materials. During such events, described as 'insults' in the literature, ignition of the explosive is caused by localised regions of high temperature known as 'hot spots'. Understanding the response of explosive materials to insults, and in particular understanding the mechanisms which cause the formation of hot spots, is of key importance in developing and maintaining safe procedures for working with explosives. Investigation of explosive response to insults through the use of numerical continuum mechanics methods, such as finite element models, often falls victim to problems such as severe mesh deformation [1]. Typically a very high resolution is required to overcome such issues, but this comes at the cost of computational resources and time. Additionally, large scale numerical codes do not always offer as much physical insight as small scale, simplified, analytical models.

Many mechanisms for hot spot generation are discussed in the literature [see 2, and references therein], and include adiabatic compression of trapped gas spaces, friction between impacting surfaces, local adiabatic shear, and heating at crack tips. Here we develop a one-dimensional model which investigates the role of localised shear, or shear banding, as an ignition mechanism resulting from an insult.

A common description of shear localisation is as follows. Consider a material which exhibits strain hardening, strain-rate hardening and thermal softening behaviour being placed under a uniform shear stress. In the early stages the response will be that of uniform shear strain; the material will undergo homogeneous deformation. As the strain is increased so that the material enters into the plastic regime, material hardening behaviour is observed. This hardening behaviour will be exacerbated by any geometric discontinuity or material inhomogeneity – the strain rate will be higher near the discontinuity, leading to further hardening behaviour. If the straining occurs at a high enough average strain rate (typically greater than 10^2 s^{-1}) there is insufficient time for the generated heat to be conducted away [3]. The material softens due to the localised temperature increase and, if this softening process dominates over the strain hardening effects, the material strength decreases. The local net softening of the material serves to concentrate the deformation into thin planar regions, known as shear bands. It is hypothesised that the concentration of thermal energy within such shear bands could trigger a localised reaction which may cause thermal runaway.

Shear localisation has been widely studied in inert materials (see [4, 5], for example), but there have been relatively few analytical studies on localised shear in explosive materials. In contrast to the dearth of analytical work, many experimental studies can be found in the literature. Evidence for localised shear within the explosive sample can be observed in recovered unexploded samples. Photographic evidence for adiabatic shear is given by Field et al. [6], showing ignition and propagation occurring in a shear band in a sample of high explosive. Notable analytical work on shear localisation in explosive materials includes [7–10] and the substantial work [11]. Also worthy of mention are the experimental works [12, 13]. It is in general concluded that localised shear is a prevalent hot spot mechanism, which manifests in many differing loading scenarios.

Here we present a model for the onset of localisation in a reactive material in which the reaction and localisation of plastic work occur on a similar timescale. We investigate the standard one-dimensional model for the initiation of a shear band, with the addition of an Arrhenius source term to model the chemical reaction occurring in the band. Motivated by [5] we use an inhomogeneity in the heat flux as the stimulus for localised plastic deformation, and treat the problem as a perturbation to the elastic solution. In the analysis, the thin zone of localisation (or shear band) is identified as a boundary layer.

In Section 2 the governing equations for the one-dimensional slab are presented in dimensional form. The constitutive law for the strain-rate is chosen to be that in [5], which is convenient for the asymptotic analysis in the following section. The governing equations are then recast in non-dimensional form using a thermal length scale, effectively placing the shear band an infinite distance from the edge of the plates, consistent with the physical observation that a shear band width is typically much smaller than the size of the slab. In Section 3 we give details of the boundary layer analysis used to obtain equations which govern the growth of the magnitudes of the perturbations to the temperature and stress at the centre of the band. In Section 4 the equations from the boundary layer analysis are expressed in terms of new non-dimensional parameters, and it is shown that the

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growth of the perturbations are controlled by three parameters which are know in terms of material properties. The results are compared with the inert case and a criterion for the initiation of reactive shear bands in discussed. We conclude in Section 5, where we give an example to demonstrate the role of the governing parameters, and suggest how the solution may differ if the onset of plastic localisation and onset of reaction occur on disparate timescales.

2   Mathematical Model

We consider a slab of reactive material of height $2L$ undergoing elastic-thermo-visco-plastic deformation, see Figure 1. In dimensional form the governing equations read:

$$\rho\tilde{v}_{\tilde{t}} = \tilde{s}_{\tilde{y}}, \qquad\qquad\text{momentum balance;} \qquad (1)$$

$$\rho c\tilde{T}_{\tilde{t}} = \kappa\tilde{T}_{\tilde{y}\tilde{y}} + \beta\tilde{s}\dot{\Gamma} + \rho\Omega A\exp\left(-\frac{E}{R\tilde{T}}\right), \qquad\text{energy balance;} \qquad (2)$$

$$\tilde{s}_{\tilde{t}} = G(\tilde{v}_{\tilde{y}} - \dot{\Gamma}), \qquad\qquad\text{elastic relationship;} \qquad (3)$$

$$\dot{\Gamma} = \dot{\Gamma}(\tilde{s}, \tilde{T}, \Gamma), \qquad\qquad\text{plastic flow law;} \qquad (4)$$

$$\Gamma = \int_0^{\tilde{t}} \dot{\Gamma}(t')\,\mathrm{d}t', \qquad\qquad\text{plastic strain.} \qquad (5)$$

Here the dependent variables are velocity $\tilde{v}(\tilde{y}, \tilde{t})$, stress $\tilde{s}(\tilde{y}, \tilde{t})$, temperature $\tilde{T}(\tilde{y}, \tilde{t})$, and plastic strain rate $\dot{\Gamma}(\tilde{y}, \tilde{t})$. The plastic strain $\Gamma(\tilde{y}, \tilde{t})$ is determined by integration of strain rate. The material constants ρ, G, c, κ, β, Ω, A, E and R, are the density, elastic shear modulus, specific heat, thermal conductivity, Taylor-Quinney coefficient, heat of reaction, rate constant, activation energy and molar gas constant, respectively.

On the top and bottom of the slab we impose the boundary conditions

$$\tilde{v}(\pm L, \tilde{t}) = \pm\tilde{v}_0, \quad \tilde{T}(\pm L, \tilde{t}) = \tilde{T}_0, \qquad (6)$$

with appropriate compliance of the stress. The initial conditions are taken to correspond to the uniform shearing solution

$$\tilde{v}(\tilde{y}, 0) = \tilde{\omega}\tilde{y}, \quad \tilde{s}(\tilde{y}, 0) = \tilde{s}_0, \quad \dot{\Gamma}(\tilde{y}, 0) = \tilde{\omega}, \quad \Gamma(\tilde{y}, 0) = 0, \quad \tilde{T}(\tilde{y}, 0) = \tilde{T}_0, \qquad (7)$$

where $\tilde{\omega}$ is the nominal strain rate. Specification of an initial stress $\tilde{s}_0 > 0$ corresponds to starting the physical problem nearer to the onset of plastic deformation [5].

In order to initiate a shear band it is necessary to introduce some external localised stimulus. Motivated by the work on inert shear bands by DiLellio and Olmstead [5], we consider an inhomogeneity in the heat flux placed at $\tilde{y} = 0$ as the stimulus for the formation of a shear band. The heat
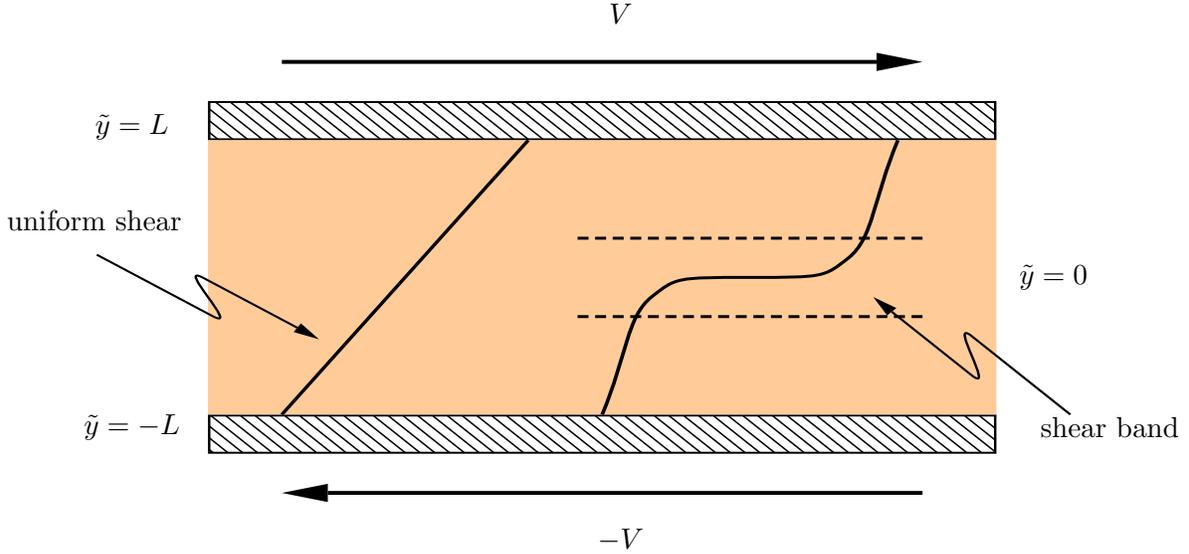
Figure 1: Schematic of uniform shearing vs. a shear band centered about $\tilde{y} = 0$.

flux disturbance is introduced as

$$\kappa \tilde{T}_{\tilde{y}}(0^-, \tilde{t}) = -\kappa \tilde{T}_{\tilde{y}}(0^+, \tilde{t}) = Q(\tilde{t}) \geq 0, \quad \tilde{t} > 0, \tag{8}$$

where $Q(\tilde{t})$ is assumed to be of small magnitude and short duration. Owing to symmetry considerations, we treat only the upper half plane, and solve the governing equations subject to the following conditions on the velocity and stress along the centreline

$$\tilde{v}(0, \tilde{t}) = 0, \quad \tilde{s}_{\tilde{y}}(0, \tilde{t}) = 0, \quad \tilde{t} > 0. \tag{9}$$

In the following we choose to adopt a strain-rate model which depends only on the stress and temperature. The analysis may be extended to account for hardening effects, but this introduces additional complexities. In the interest of obtaining a clear insight into how the reaction affects the onset of shear bands, and to allow for a more direct comparison with [5], the effects of strain hardening are not considered herein. We use the model proposed in [5] which accounts for thermal softening and strain rate dependence, and takes the following exponential form

$$\dot{\Gamma}(\tilde{s}, \tilde{T}) = \dot{\Gamma}^* \exp\{-[B_1^{-1}(\tilde{T}_{\mathrm{p}} - \tilde{T}) + B_2^{-1}(\tilde{s}_{\mathrm{p}} - \tilde{s})]\}, \tag{10}$$

where $\dot{\Gamma}^*$ is a dimensional reference strain-rate, and the constants $\tilde{T}_{\mathrm{p}}$ and $\tilde{s}_{\mathrm{p}}$ are the critical values of temperature and stress below which the plastic strain-rate is exponentially small. It is required that $\tilde{T}_{\mathrm{p}} > \tilde{T}_0$ and $\tilde{s}_{\mathrm{p}} > \tilde{s}_0$ so that the problem is started in the elastic stage in which plastic strain is initially negligible. The parameters B_1, B_2 are related to strain-rate sensitivity M and thermal

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sensitivity P via the definitions

$$M \equiv \frac{1}{\tilde{s}_{\mathrm{p}}} \frac{\partial \tilde{s}}{\partial \log \dot{\Gamma}} = \frac{B_2}{\tilde{s}_{\mathrm{p}}}, \quad P \equiv -\frac{\tilde{T}_{\mathrm{p}}}{\tilde{s}_{\mathrm{p}}} \frac{\partial \tilde{s}}{\partial \tilde{T}} = \left(\frac{B_2}{\tilde{s}_{\mathrm{p}}}\right) \Big/ \left(\frac{B_1}{\tilde{T}_{\mathrm{p}}}\right). \tag{11}$$

This strain-rate model is a good approximation of more typical power law models, but offers a form which is much more convenient for the boundary layer analysis to follow.

We introduce non-dimensional variables, which are related to the dimensional variables by

$$t = \tilde{t}/t^*, \quad y = \tilde{y}/l, \quad v = \tilde{v}/\tilde{v}_0, \quad s = \tilde{s}/\tilde{s}_0, \quad \dot{\gamma} = \dot{\Gamma}/\dot{\Gamma}_0, \quad T = \tilde{T}/\tilde{T}_0, \quad q = Q/q_0, \tag{12}$$

and the non-dimensional constants

$$t^* = \frac{\tilde{s}_0}{G\dot{\Gamma}_0}, \quad l = \left(\frac{\kappa \tilde{s}_0}{\rho c G \dot{\Gamma}_0}\right)^{1/2}, \quad \dot{\Gamma}_0 = \frac{\tilde{v}_0}{l}, \quad \Gamma_0 = t^* \dot{\Gamma}_0, \quad \omega = \frac{\tilde{\omega}}{\dot{\Gamma}_0},$$

$$\hat{\rho} = \frac{\kappa \dot{\Gamma}_0}{c \tilde{s}_0}, \quad \lambda = \frac{\beta \tilde{s}_0^2}{\rho c G \tilde{T}_0}, \quad \hat{E} = \frac{E}{R\tilde{T}_0}, \quad \hat{\Omega} = \frac{\Omega}{c\tilde{T}_0}, \quad \hat{A} = At^*, \quad q_0 = \frac{\kappa \tilde{T}_0}{l}. \tag{13}$$

The choice of the thermal length scale l allows us to make the simplifying assumption that the material sample occupies the space $-\infty < y < \infty$, which is consistent with the physical observation that shear bands are typically very thin compared with the sample size.

The non-dimensional governing equations for the shearing problem in the upper-half plane read

$$\hat{\rho} v_t = s_y, \tag{14}$$

$$T_t = T_{yy} + \lambda s \dot{\gamma} + \hat{\Omega}\hat{A} \exp\left(-\frac{\hat{E}}{T}\right), \tag{15}$$

$$s_t = v_y - \dot{\gamma}, \tag{16}$$

$$\dot{\gamma} = \frac{\dot{\Gamma}^*}{\dot{\Gamma}_0} \exp\left\{-\left[\frac{\tilde{T}_0}{B_1}(T_{\mathrm{p}} - T) + \frac{\tilde{s}_0}{B_2}(s_{\mathrm{p}} - s)\right]\right\}, \tag{17}$$

where $T_{\mathrm{p}} = \tilde{T}_{\mathrm{p}}/\tilde{T}_0 > 1$ and $s_{\mathrm{p}} = \tilde{s}_{\mathrm{p}}/\tilde{s}_0 > 1$ are the non-dimensional critical temperature and stress, respectively. Since we are neglecting hardening effects (i.e. strain dependence), the non-dimensional counterpart of (5) has been omitted.

3   Boundary Layer Analysis

We seek a solution of (14) – (17) in the form of a perturbation to the elastic ($\dot{\gamma} = 0$) solution. In the following analysis, a thin zone centred around $y = 0$ in which significant plastic work and reaction take place is identified. Outside of this region both the heating due to plastic work and heating due to reaction are exponentially small, and far from the centre of the localisation zone

the elastic solution remains valid. The solution in the thin zone around $y = 0$ is matched on to the elastic solution via an intermediate diffusive zone. The equations governing the behaviour of the perturbations to the elastic stress and temperature along the centreline will be obtained. The governing equations may be recast in the form

$$s_t = \hat{\rho}^{-1} \int_0^t s_{yy}(y, t') \, \mathrm{d}t' + \omega - \dot{\gamma}, \tag{18}$$

$$T_t = T_{yy} + \lambda s \dot{\gamma} + \hat{\Omega} \hat{A} \exp\left(-\frac{\hat{E}}{T}\right), \tag{19}$$

where (18) represents a combination of (14) – (16), and the velocity has been eliminated using the initial condition $v(y, 0) = \omega y$. The plastic strain-rate is still given by (17). These equations are to be solved subject to the initial and boundary conditions

$$s(y, 0) = 1, \qquad T(y, 0) = 1, \tag{20}$$

$$s_y(0, t) = 0, \qquad T_y(0, t) = -q(t), \qquad T(\infty, t) = 1. \tag{21}$$

In order to proceed with the boundary layer analysis we must identify a small parameter ε. This is introduced through the ratios B_1/T_0 and B_2/s_0 by the relations

$$\frac{B_1}{\tilde{T}_0} = \beta_1^{-1} \varepsilon, \quad \frac{B_2}{\tilde{s}_0} = \beta_2^{-1} \varepsilon, \quad 0 < \varepsilon \ll 1, \tag{22}$$

where β_1 and β_2 are $O(1)$ with respect to ε. Such a scaling is typical of material which exhibit shear banding [5]. It is assumed that the plastic strain rate function can be multiplicatively scaled [5], so that

$$\frac{\dot{\Gamma}^*}{\dot{\Gamma}_0} = \dot{\gamma}_0 \varepsilon^{-1/2}, \tag{23}$$

and the plastic strain-rate takes the non-dimensional form

$$\dot{\gamma}(s, T) = \dot{\gamma}_0 \varepsilon^{-1/2} \exp\{-\varepsilon^{-1}[\beta_1(T_{\mathrm{p}} - T) + \beta_2(s_{\mathrm{p}} - s)]\}, \tag{24}$$

where $\dot{\gamma}_0$ is $O(1)$ with respect to ε.

The non-dimensional parameter $\hat{\rho}$ is typically small in materials which exhibit shear banding effects so, in order to take advantage of this, we introduce the scaling

$$\hat{\rho} = \varepsilon \hat{\rho}_0, \tag{25}$$

where $\hat{\rho}_0$ is $O(1)$ with respect to ε.

We also exploit the largeness of the pre-exponential factor $\hat{A}$ by setting

$$\hat{A} = \hat{A}_0 \frac{\hat{E}^{1/2}}{T_\mathrm{R}} \exp\left(\frac{\hat{E}}{T_\mathrm{R}}\right), \tag{26}$$

where T_R is the non-dimensional critical reaction temperature, i.e. the temperature at which significant reaction first occurs, and $\hat{A}_0$ is $O(1)$ with respect to ε. The reaction temperature will later be used to identify a reaction time scale t_R. As in high activation energy asymptotic analyses (e.g. [14]), the small parameter ε, non-dimensional activation energy and the critical reaction temperature are related by

$$\varepsilon = \frac{T_\mathrm{R}^2}{\hat{E}}. \tag{27}$$

Both relations (22) and (27) are consistent when we consider materials in which onset of significant plastic work and onset of significant reaction occur over similar timescales, these we refer to as "reactive shear bands". For materials in which localisation of plastic work occurs well before significant reaction (or vice-versa) these relations should be adjusted so that the appropriate plastic or reaction properties are related through different powers of ε.

3.1 Elastic stage

In the initial stages of deformation the plastic strain-rate is initially exponentially small until the stress and temperature have risen sufficiently to make the argument of the exponent in (24) positive. Additionally, the Arrhenius source term is exponentially small until the critical reaction temperature T_R is reached. Thus, for early times the inert elastic solution of (18) – (19) is given by

$$T_\mathrm{e}(y,t) = 1 + \delta \int_0^t \frac{e^{-\frac{y^2}{4(t-t')}}}{[\pi(t-t')]^{1/2}} h(t')\,\mathrm{d}t', \tag{28}$$

$$s_\mathrm{e}(y,t) = 1 + \omega t, \tag{29}$$

see, for example, [15, p.75]. Here the heat flux inhomogeneity is represented as

$$q(t) = \delta h(t), \quad 0 \leq h(t) \leq 1. \tag{30}$$

The scaling of the heat flux is such that $0 < \varepsilon \ll \delta \ll 1$, so that δ is sufficiently large to introduce localisation but still small enough to be negligible in comparison with physical factors that control the evolution of the shear band. This early time solution will be used as the basis of our asymptotic analysis.

3.2 Onset of reactive shear band

Beyond the critical plastic threshold $\dot{\gamma}$ becomes large due to the multiplicative scaling. This motivates the definition of a critical time scale t_{p} at which the onset of significant plastic work occurs, i.e. the time at which the exponential in (24) becomes $O(1)$. Therefore t_{p} is defined by the smallest solution of

$$\beta_1[T_{\mathrm{p}} - T_{\mathrm{e}}(0, t_{\mathrm{p}})] + \beta_2[s_{\mathrm{p}} - s_{\mathrm{e}}(0, t_{\mathrm{p}})] = 0. \tag{31}$$

Given that the stimulus for the shear band is placed along the centreline, the plastic work first becomes significant near $y = 0$, and occurs at time $t = t_{\mathrm{p}}$. At this stage the solution will be a perturbation of the elastic solution (28) – (29). The temperature in the shear band will increase due to plastic work, until the critical reaction temperature is reached. As previously discussed, we consider the case where the subsequent reaction occurs on a similar timescale to the growth of the plastic work time. It is possible to consider a model in which the plastic and reactive behaviour occur on disparate timescales, but we restrict ourselves to the most critical case.

We introduce new independent variables ξ and τ such that

$$y = \varepsilon\xi, \quad t = t_{\mathrm{p}} + \varepsilon\tau, \quad \xi > 0, \quad \tau > -\frac{t_{\mathrm{p}}}{\varepsilon} \to -\infty, \tag{32}$$

which are appropriate to describe the inner solution in the boundary layer near $y = 0$, where the localised plastic straining first begins to occur. In order to identify the onset of the reaction we define a critical reaction timescale τ_{R} (related to the "original time" by $t_{\mathrm{R}} = t_{\mathrm{p}} + \varepsilon\tau_{\mathrm{R}}$) as the solution of

$$T_{\mathrm{R}} = T_{\mathrm{e}}(0, t_{\mathrm{p}} + \varepsilon\tau_{\mathrm{R}}) + \varepsilon T_1(0, \tau_{\mathrm{R}}) + o(\varepsilon), \tag{33}$$

where the function T_1 is still to be determined as part of the solution.

In the inner layer we expand the temperature and stress in powers of ε as

$$T = T_{\mathrm{e}}(\varepsilon\xi, t_{\mathrm{p}} + \varepsilon\tau) + \varepsilon T_1(\xi, \tau) + \varepsilon^{3/2} T_2(\xi, \tau) + \cdots, \tag{34}$$

$$s = s_{\mathrm{e}}(\varepsilon\xi, t_{\mathrm{p}} + \varepsilon\tau) + \varepsilon s_1(\xi, \tau) + \varepsilon^{3/2} s_2(\xi, \tau) + \cdots. \tag{35}$$

Physically we expect the solution in the shear band to be driven by plastic work and the chemical reaction. The chosen scalings in the expansion allow for the appropriate balance between the corrections to the temperature and stress and the plastic work and reaction terms in the governing equations (18) – (19). We expand the elastic parts of the solution as

$$T_{\mathrm{e}}(\varepsilon\xi, t_{\mathrm{p}} + \varepsilon\tau) = T_{\mathrm{e}}(0, t_{\mathrm{p}}) + \varepsilon(a\tau - b\xi) + o(\varepsilon), \tag{36}$$

$$s_{\mathrm{e}}(\varepsilon\xi, t_{\mathrm{p}} + \varepsilon\tau) = s_{\mathrm{e}}(0, t_{\mathrm{p}}) + \varepsilon\omega\tau + o(\varepsilon), \tag{37}$$

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where

$$a = T_{e_t}(0, t_p) = \delta \int_0^{t_p} [\pi(t_p - t')]^{-1/2} h'(t') \, dt', \quad b = -T_{e_y}(0, t_p) = \delta h(t_p). \tag{38}$$

Substitution of the expansions for the temperature and stress into (18) – (19) gives

$$\left[s_1 + \varepsilon^{1/2} s_2 + \cdots \right]_\tau = \hat{\rho}_0^{-1} \int_{-\infty}^\tau \left[\varepsilon^{-1} s_1 + \varepsilon^{-1/2} s_2 + \cdots \right]_{\xi\xi} d\tau' - \dot{\gamma}, \tag{39}$$

$$\left[T_1 + \varepsilon^{1/2} T_2 + \cdots \right]_\tau = \left[\varepsilon^{-1} T_1 + \varepsilon^{-1/2} T_2 + \cdots \right]_{\xi\xi} + \lambda \left[s_e + \varepsilon s_1 + \cdots \right] \dot{\gamma} + \hat{\Omega}\hat{A} \exp\left(-\frac{\hat{E}}{T} \right), \tag{40}$$

where the expansions of the plastic strain-rate and Arrhenius source term are given by

$$\dot{\gamma} = \dot{\gamma}_0 \varepsilon^{-1/2} \left\{ \exp[\beta_3 \tau - \beta_1 b\xi + \beta_1 T_1 + \beta_2 s_1] + o(1) \right\}, \tag{41}$$

and

$$\hat{\Omega}\hat{A} \exp\left(-\frac{\hat{E}}{T} \right) = \hat{\Omega}\hat{A}_0 \varepsilon^{-1/2} \exp\left\{ \frac{T_R^2}{\varepsilon} \left(\frac{1}{T_R} - \frac{1}{T_e(0, t_p) + \varepsilon(a\tau - b\xi + T_1) + o(\varepsilon)} \right) \right\}, \tag{42}$$

respectively. Here $\beta_3 = \beta_1 a + \beta_2 \omega < 0$. Using (33) we may rewrite the temperature expansion as a correction to the reaction temperature T_R, that is

$$\begin{aligned} T &= T_e(0, t_p) + \varepsilon(a\tau - b\xi + T_1) + o(\varepsilon) \\ &= T_e(0, t_p) + \varepsilon(a\tau_R + T_1(0, \tau_R)) + \varepsilon(a(\tau - \tau_R) - b\xi + T_1 - T_1(0, \tau_R)) + o(\varepsilon) \\ &= T_R + \varepsilon(a(\tau - \tau_R) - b\xi + T_1 - T_1(0, \tau_R)) + o(\varepsilon), \end{aligned} \tag{43}$$

so that (42) reads

$$\hat{\Omega}\hat{A} \exp\left(-\frac{\hat{E}}{T} \right) = \hat{\Omega}\hat{A}_0 \varepsilon^{-1/2} \exp\left\{ a(\tau - \tau_R) - b\xi + T_1 - T_1(0, \tau_R) + o(1) \right\}, \tag{44}$$

and we observe that the onset of reaction is delayed by the shift in time τ_R.

We now solve the sequence of boundary value problems which arise from considering powers of ε. At $O(\varepsilon^{-1})$ we have the problem

$$\int_{-\infty}^\tau s_{1_{\xi\xi}} \, d\tau = 0, \quad s_{1_\xi}(0, \tau) = 0, \quad s_1(\xi, -\infty) = 0, \tag{45}$$

$$T_{1_{\xi\xi}} = 0, \quad T_{1_\xi}(0, \tau) = 0, \quad T_1(\xi, -\infty) = 0. \tag{46}$$

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This has solution

$$T_1(\xi, \tau) = f_1(\tau), \quad f_1(-\infty) = 0, \quad s_1(\xi, \tau) = g_1(\tau), \quad g_1(-\infty) = 0, \tag{47}$$

where f_1 and g_1 are to be determined. We next solve the problem at $O(\varepsilon^{-1/2})$:

$$\int_{-\infty}^{\tau} s_{2\xi\xi} \, \mathrm{d}\tau = \hat{\rho}_0 \dot{\gamma}_0 \exp[\beta_3 \tau - \beta_1 b\xi + \beta_1 T_1 + \beta_2 s_1], \tag{48}$$

$$s_{2\xi}(0, \tau) = 0, \quad s_2(\xi, -\infty) = 0, \tag{49}$$

$$T_{2\xi\xi} = -\lambda\dot{\gamma}_0(1 + \omega t_\mathrm{p}) \exp[\beta_3 \tau - \beta_1 b\xi + \beta_1 T_1 + \beta_2 s_1]$$
$$- \hat{\Omega}\hat{A}_0, \exp[a(\tau - \tau_\mathrm{R}) - b\xi + f_1(\tau) - f_1(\tau_\mathrm{R})], \tag{50}$$

$$T_{2\xi}(0, \tau) = 0, \quad T_2(\xi, -\infty) = 0, \tag{51}$$

which has solution

$$T_2(\xi, \tau) = -\frac{\lambda\dot{\gamma}_0(1 + \omega t_\mathrm{p})}{\beta_1 b} \left(\xi + \frac{\exp(-\beta_1 b\xi)}{\beta_1 b}\right) \exp[\beta_3 \tau + \beta_1 f_1(\tau) + \beta_2 g_1(\tau)]$$
$$- \frac{\hat{\Omega}\hat{A}_0}{b} \left(\xi + \frac{\exp(-\beta_1 b\xi)}{\beta_1 b}\right) \exp[a(\tau - \tau_\mathrm{R}) - b\xi + f_1(\tau) - f_1(\tau_\mathrm{R})] + f_2(\tau), \tag{52}$$

$$s_2(\xi, \tau) = \frac{\hat{\rho}_0 \dot{\gamma}_0}{\beta_1 b} \left(\xi + \frac{\exp(-\beta_1 b\xi)}{\beta_1 b}\right) \frac{\mathrm{d}}{\mathrm{d}\tau}\{\exp[\beta_3 \tau + \beta_1 f_1(\tau) + \beta_2 g_1(\tau)]\} + g_2(\tau), \tag{53}$$

$$f_2(-\infty) = 0, \quad g_2(-\infty) = 0, \tag{54}$$

where f_2 and g_2 are to be determined.

In order to satisfy the boundary conditions away from the shear band we consider an outer layer, in which the appropriate independent variables are

$$y = \varepsilon^{1/2}Y, \quad t = t_\mathrm{p} + \varepsilon\tau, \quad Y > 0, \quad \tau > -\frac{t_\mathrm{p}}{\varepsilon} \to -\infty. \tag{55}$$

In this region both the plastic straining and reaction are negligible. Motivated by achieving a balance between the time derivative and diffusive terms in the governing equations [5], we introduce the expansions

$$T = T_\mathrm{e}(\varepsilon^{1/2}Y, t_\mathrm{p} + \varepsilon\tau) + \varepsilon T_1^O(Y, \tau) + \varepsilon^{3/2}T_2^O(Y, \tau) + \cdots, \tag{56}$$

$$s = s_\mathrm{e}(\varepsilon^{1/2}Y, t_\mathrm{p} + \varepsilon\tau) + \varepsilon s_1^O(Y, \tau) + \varepsilon^{3/2}s_2^O(Y, \tau) + \cdots. \tag{57}$$

For the analysis here we only require the leading order governing equations in the outer layer, which

read

$$s^O_{1_\tau} = \hat{\rho}^{-1} \int_{-\infty}^{\tau} s^O_{1_{YY}} \, \mathrm{d}\tau', \quad s^O_1(\infty, \tau) = 0, \quad s^O_1(Y, -\infty) = 0, \tag{58}$$

$$T^O_{1_\tau} = T^O_{1_{YY}}, \quad T^O_1(\infty, \tau) = 0, \quad T^O_1(Y, -\infty) = 0. \tag{59}$$

No boundary conditions are imposed at $Y = 0$. Instead we must perform an asymptotic matching between the inner and outer solutions. The inner expansion is expressed in terms of the outer variables and equated to the outer expansion in order to derive matching relations at $Y = 0$. The result is

$$\varepsilon T^O_1(Y, \tau) + \varepsilon^{3/2} T^O_2(Y, \tau) + \cdots = \varepsilon T_1(\varepsilon^{-1/2} Y, \tau) + \varepsilon^{3/2} T_2(\varepsilon^{-1/2} Y, \tau) + \cdots$$
$$= \varepsilon \left[f_1(\tau) - \frac{\lambda \dot{\gamma}_0 (1 + \omega t_\mathrm{p}) Y}{\beta_1 b} \exp(\beta_3 \tau + \beta_1 f_1(\tau) + \beta_2 g_1(\tau)) \right.$$
$$\left. - \frac{\hat{\Omega} \hat{A}_0 Y}{b} \exp(a(\tau - \tau_\mathrm{R}) - b\xi + f_1(\tau) - f_1(\tau_\mathrm{R})) \right] + O(\varepsilon^{3/2}), \tag{60}$$

$$\varepsilon s^O_1(Y, \tau) + \varepsilon^{3/2} s^O_2(Y, \tau) + \cdots = \varepsilon s_1(\varepsilon^{-1/2} Y, \tau) + \varepsilon^{3/2} s_2(\varepsilon^{-1/2} Y, \tau) + \cdots$$
$$= \varepsilon \left[g_1(\tau) + \frac{\hat{\rho}_0 \dot{\gamma}_0 Y}{\beta_1 b} \frac{\mathrm{d}}{\mathrm{d}\tau} \exp(\beta_3 \tau + \beta_1 f_1(\tau) + \beta_2 g_1(\tau)) \right] + O(\varepsilon^{3/2}), \tag{61}$$

which provides the boundary conditions

$$T^O_1(0, \tau) = f_1(\tau), \quad s^O_1(0, \tau) = g_1(\tau), \tag{62}$$

$$T^O_{1_Y}(0, \tau) = -\frac{\lambda \dot{\gamma}_0 (1 + \omega t_\mathrm{p})}{\beta_1 b} \exp(\beta_3 \tau + \beta_1 f_1(\tau) + \beta_2 g_1(\tau))$$
$$- \frac{\hat{\Omega} \hat{A}_0}{b} \exp(a(\tau - \tau_\mathrm{R}) + f_1(\tau) - f_1(\tau_\mathrm{R})), \tag{63}$$

$$s^O_{1_Y}(0, \tau) = \frac{\hat{\rho}_0 \dot{\gamma}_0}{\beta_1 b} \frac{\mathrm{d}}{\mathrm{d}\tau} \exp(\beta_3 \tau + \beta_1 f_1(\tau) + \beta_2 g_1(\tau)). \tag{64}$$

Solution of the leading order equations (58) – (59) subject to the boundary and flux conditions gives

$$T^O_1(Y, \tau) = \int_{-\infty}^{\tau} \left\{ \frac{\lambda \dot{\gamma}_0 (1 + \omega t_\mathrm{p})}{\beta_1 b} \exp \left[\beta_3 \tau' + \beta_1 f_1(\tau') + \beta_2 g_1(\tau') \right] \right.$$
$$\left. + \frac{\hat{\Omega} \hat{A}_0}{b} \exp[a(\tau - \tau_\mathrm{R}) + f_1(\tau) - f_1(\tau_\mathrm{R})] \right\} \times \exp \left[-\frac{Y^2}{4(\tau - \tau')} \right] \frac{\mathrm{d}\tau'}{[\pi(\tau - \tau')]^{1/2}}, \tag{65}$$

$$s^O_1(Y, \tau) = -\frac{\hat{\rho}_0^{1/2} \dot{\gamma}_0}{\beta_1 b} \exp \left[\beta_3(\tau - \hat{\rho}_0^{1/2} Y) + \beta_1 f_1(\tau - \hat{\rho}_0^{1/2} Y) + \beta_2 g_1(\tau - \hat{\rho}_0^{1/2} Y) \right]. \tag{66}$$

Imposing matching conditions between the inner and outer solution at $Y = 0$ gives a pair of coupled

nonlinear equations for the leading order temperature and stress perturbations in the shear band, namely

$$f_1(\tau) = \int_{-\infty}^{\tau} \left\{ \frac{\lambda \dot{\gamma}_0 (1 + \omega t_{\mathrm{p}})}{\beta_1 b} \exp\left[\beta_3 \tau' + \beta_1 f_1(\tau') + \beta_2 g_1(\tau')\right] \right.$$
$$\left. + \frac{\hat{\Omega}\hat{A}_0}{b} \exp[a(\tau - \tau_{\mathrm{R}}) + f_1(\tau) - f_1(\tau_{\mathrm{R}})] \right\} \frac{\mathrm{d}\tau'}{[\pi(\tau - \tau')]^{1/2}}, \tag{67}$$

$$g_1(\tau) = -\frac{\hat{\rho}_0^{1/2} \dot{\gamma}_0}{\beta_1 b} \exp\left[\beta_3 \tau + \beta_1 f_1(\tau) + \beta_2 g_1(\tau)\right]. \tag{68}$$

We note that $f_1(\tau) \geq 0$ and $g_1(\tau) \leq 0$ which is consistent with the physical observation that plastic deformation leads to an increase in the temperature and a decrease in the stress [5]. In particular, rapid growth (decay) of the temperature (stress) is associated with the formation of a shear band.

4 Results

In order to analyse the coupled equations (67) and (68) we introduce the new variables

$$f(\eta) = \beta_1 f_1(\tau), \quad g(\eta) = -\beta_2 g_1(\tau), \quad \eta = \beta_3 \tau + \log\left[\frac{\lambda \dot{\gamma}_0 (1 + \omega t_{\mathrm{p}})}{b \beta_3^{1/2}}\right], \tag{69}$$

and the parameters

$$\Lambda_{\mathrm{p}} = \frac{\beta_2 (\hat{\rho}_0 \beta_3)^{1/2}}{\beta_1 \lambda (1 + \omega t_{\mathrm{p}})}, \quad \Lambda_{\mathrm{R}} = \frac{\hat{\Omega}\hat{A}_0}{b \beta_3^{1/2}}, \quad \Lambda_{\mathrm{t}} = \frac{a}{\beta_3}. \tag{70}$$

Now (67) and (68) take the simplified form

$$f(\eta) = \int_{-\infty}^{\eta} [\pi(\eta - \eta')]^{-1/2} \left\{ \exp\left[\eta' + f(\eta') - g(\eta')\right] \right.$$
$$\left. + \Lambda_{\mathrm{R}} \exp\left[\Lambda_{\mathrm{t}}(\eta' - \eta'_R) + \beta_1^{-1}(f(\eta') - f(\eta'_R))\right] \right\} \mathrm{d}\eta', \tag{71}$$

$$g(\eta) = \Lambda_{\mathrm{p}} \exp\left[\eta + f(\eta) - g(\eta)\right], \tag{72}$$

and correspond to the magnitudes of the temperature and stress perturbations, respectively. The parameters Λ_{p} and Λ_{t} relate to the material properties, applied shearing motion and heat flux inhomogeneity, whereas the parameter Λ_{R} relates to the properties of the chemical reaction.

We first consider the case of vanishing reaction, Λ_{R}, as treated in [5]. Typically, equations (71) and (72) must be solved numerically to determine the behaviour of $f(\eta)$ and $g(\eta)$. However, there are a few cases which allow for analytical solution. When $\Lambda_{\mathrm{p}} = 0$ it follows that $g(\eta) = 0$, and it

can be shown that

$$f_{(\eta)} = -\frac{1}{2}\log(\eta^* - \eta) - \left[\eta^* + \log\frac{2}{\pi^{1/2}}\right] + o(1), \quad \eta \to \eta^*, \tag{73}$$

at some $\eta^* < \infty$. This analysis corresponds to a problem in combustion theory in which a half-space is heated by some constant thermal flux [16]. For the special case $\Lambda_p = 1$ (and $\Lambda_R = 0$) we have the exact solution $f(\eta) = g(\eta) = e^\eta$ for any Λ_t and β_1.
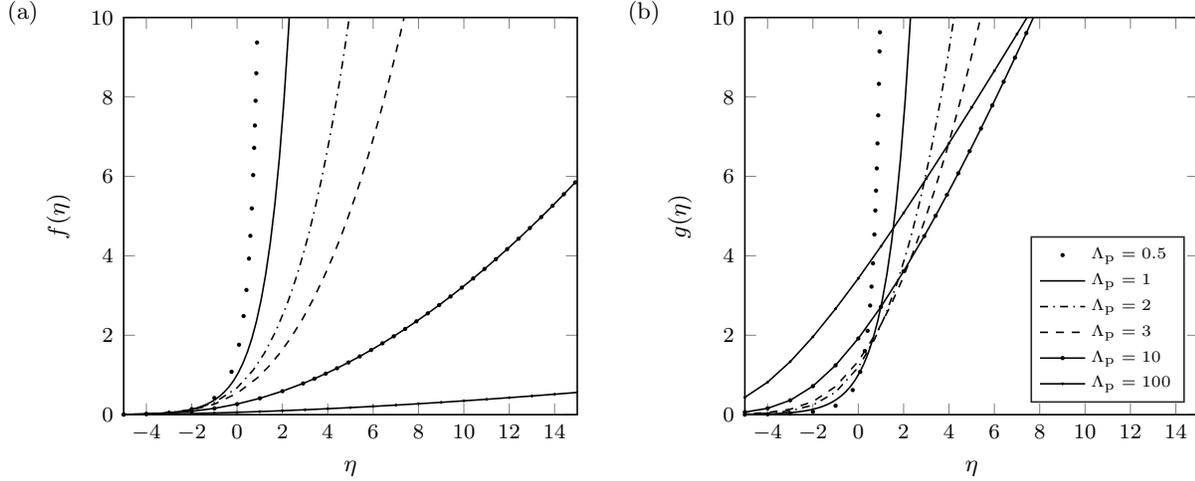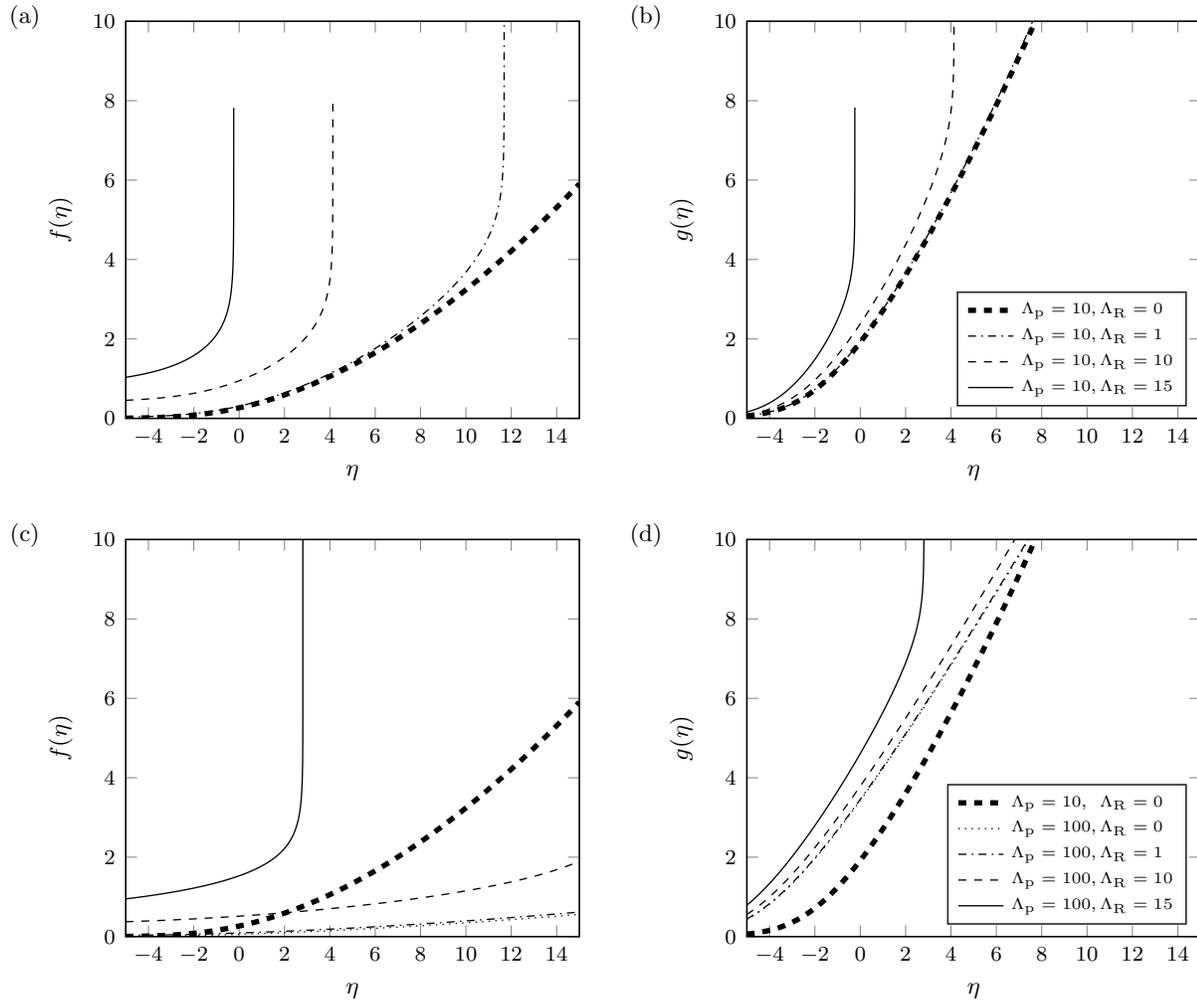

Figure 2: Magnitude of the perturbations to the temperature $f(\eta)$ and stress $g(\eta)$.

Figure 2 shows the numerical solutions of (71) and (72) for various values of the parameter Λ_p, along with the exact solution with $\Lambda_p = 1$. For $\Lambda_p = 1$ the magnitudes of the perturbations undergo exponential growth, with the growth becoming more rapid as Λ_p is decreased. In [5] it is argued that $\Lambda_p < 10$ provides a useful criterion for the onset of shear banding. This is motivated by adopting the position that the perturbations should remain $O(1)$ at the critical plastic time for plastic work $t = t_p$ ($\tau = 0$). Upon inclusion of a chemical reaction we will continue to use the solution given by $\Lambda_p = 10$ and $\Lambda_R = 0 = \Lambda_t$ as our criterion for formation of a shear band, and investigate how varying the properties of the reaction affects the solution.

In order to simplify the analysis to follow we note that $\beta_1 \sim O(1)$, and through an appropriate choice of scaling we can always set $\beta_1 = 1$. Further, we note that the parameter Λ_t, which is approximately the ratio of the growth rate of the centreline elastic solution to the non-dimensional shear rate, is typically $O(10^{-2})$. We choose to fix $\Lambda_t = 0.01$ and study a simplified two parameter system. Doing so allows us to focus on how the reaction properties affect the initiation of a shear band.

When $\Lambda_R \neq 0$ the equations governing the behaviour of $f(\eta)$ and $g(\eta)$ require numerical solution. Equations (71) and (72) are to be solved using an iterative numerical scheme, along with (33) to determine the critical reaction time $\eta_R = \beta_3 \tau_R + \log[\lambda\dot{\gamma}_0(1 + \omega t_p)b^{-1}\beta_3^{-1/2}]$. The numerical results

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Figure 3: Magnitude of the perturbations to the temperature $f(\eta)$ and stress $g(\eta)$. Panels (a) and (b) show results for fixed $\Lambda_{\mathrm{P}} = 10$ and various Λ_{R}, and panels (c) and (d) show results for fixed $\Lambda_{\mathrm{P}} = 100$ and various Λ_{R}. In all panels the thick dashed line shows solution associated with the shear band criterion $\Lambda_{\mathrm{P}} = 10$, $\Lambda_{\mathrm{R}} = 0 = \Lambda_{\mathrm{t}}$.

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are shown in Figure 3, with the shear band criterion shown as a thick dashed line. Panels (a) and (b) show the behaviour of $f(\eta)$ and $g(\eta)$ for fixed $\Lambda_{\mathrm{p}} = 10$ and varying Λ_{R}. Using the criterion in [5] we would expect to see a shear band in the case of an inert material. Here we observe that increasing Λ_{R} has the effect of initiating a shear band at an earlier time. Increasing Λ_{R} beyond a value of approximately 10 we can initiate a shear band for $\eta < 0$. Panels (c) and (d) show the numerical results for an increased value of $\Lambda_{\mathrm{p}} = 100$. For $\Lambda_{\mathrm{R}} < 10$ we observe that the growth of the temperature perturbation is slow when compared with the $\Lambda_{\mathrm{p}} = 10$ criterion, and that the magnitude of the stress perturbation is of a similar size at $\eta \sim 7$. However, as Λ_{R} is increased to 15 we see a significant increase in the growth rate of both the temperature and stress, clearly demonstrating that the inclusion of a chemical reaction can cause shear bands to initiate in a reactive material in conditions where no shear band would be seen in an inert material with similar material properties.

Figure 4 shows a sketch of the boundary in the $\Lambda_{\mathrm{p}} - \Lambda_{\mathrm{R}}$ plane which separates the region in parameter space where a shear band occurs and the region where a shear band does not occur, with fixed $\Lambda_{\mathrm{t}} = 0.01$. For $\Lambda_{\mathrm{p}} < 10$ a shear band is always initiated (using the criterion in [5]), irrespective of the reaction properties. However, the reaction may affect the growth rate of the temperature and stress perturbations once the band has formed. For $\Lambda_{\mathrm{p}} > 10$ a shear band is not observed when there is no reaction, but it is found that a shear band may be initiated by sufficiently increasing Λ_{R}. That is, for a sufficiently strong/fast reaction a shear band may be initiated in a material which would not otherwise undergo shear banding under the same load. The solid dashed line in Figure 4 may be viewed as a criterion for the onset of shear banding in reactive materials.
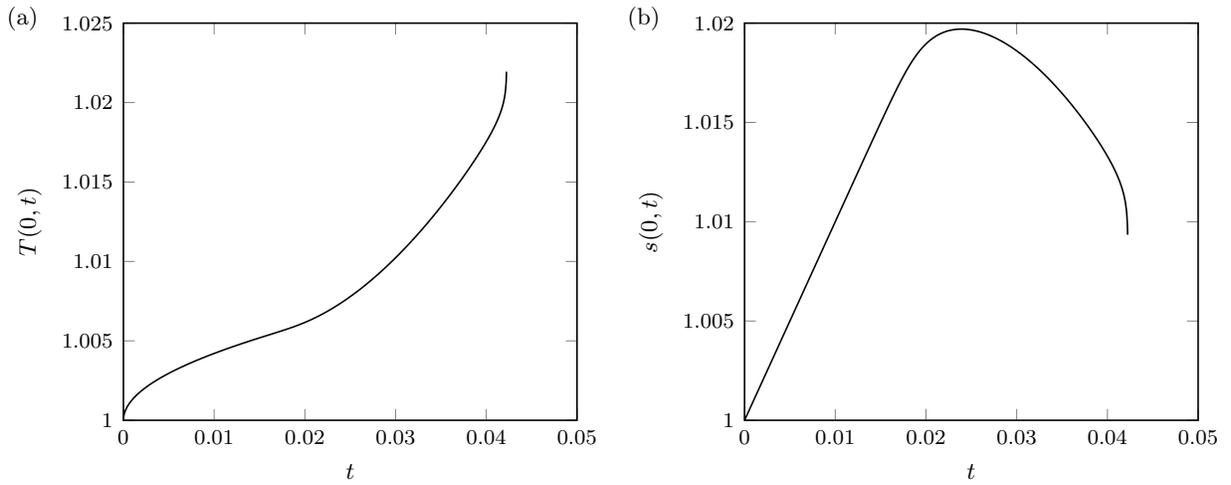
Figure 5 shows representative profiles of the centreline temperature $T(0, t)$ and stress $s(0, t)$ as a function of time t for a material in which the critical plastic and reaction temperatures are similar: $T_{\mathrm{p}} = 1.01$ and $T_{\mathrm{R}} = 1.02$, respectively. In this case the critical plastic and reaction times are calculated as $t_{\mathrm{p}} = 0.02$ and $t_{\mathrm{R}} = 0.0419$, respectively. The process can clearly be split into three distinct stages: the elastic stage, $t < t_{\mathrm{p}}$ where the is no significant plastic strain or reaction; the plastic stage, $t_{\mathrm{p}} \leq t < t_{\mathrm{R}}$; and the reaction stage, $t \geq t_{\mathrm{R}}$. The results agree well with a full numerical solution of (1) – (5) using a so-called "cohesive scheme", see [17] for details. In particular, the critical times for plastic work and reaction are well predicted by the asymptotic solution.

5   Conclusion

Here we have developed a model for shear bands occurring in reactive in materials motivated by the boundary layer analysis of [5]. The analysis allows for the full system of governing equations to be reduced to three coupled equation used to describe the behaviour of the perturbations to the centreline temperature and stress, as well as the critical reaction time. In contrast to the inert case, we find that the initiation of shear banding is controlled by three parameters instead of one. The simplified equations allow for the parameter space to be explored, and a criterion for the initiation
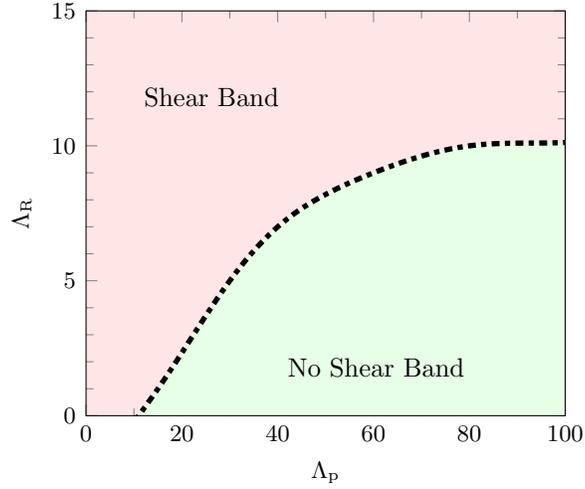
Figure 4: A sketch of the region in the $\Lambda_\mathrm{p} - \Lambda_\mathrm{R}$ plane in which a shear band is formed. The parameter Λ_t has been held fixed at a typical value of 0.01.

Figure 5: The centreline temperature $T(0,t) = T_\mathrm{e}(0,t) + \varepsilon T_1(t)$ and stress $s(0,t) = s_\mathrm{e}(0,t) + \varepsilon s_1(t)$ as a function of time $t = t_\mathrm{p} + \varepsilon\tau$. Here the critical plastic and reaction temperatures are $T_\mathrm{p} = 1.01$ and $T_\mathrm{R} = 1.02$, giving critical times $t_\mathrm{p} = 0.02$ and $t_\mathrm{R} = 0.0419$, respectively. The value of the small parameter was $\varepsilon = 10^{-2}$.

of shear bands based on known physical parameters has been suggested.

The usefulness of this analysis is primarily in assessing the tendency of a reactive material to form shear bands based on its material properties and the shear rate of the deformation. As an example we consider the reactive material LX-14. Using the parameter values given in [18], we have in SI units $\rho = 1.849 \times 10^3$, $G = 3.520 \times 10^9$, $c = 1.130 \times 10^3$, $\kappa = 4.390 \times 10^{-1}$, $M \approx 0.1$, $P \approx 1$, $\beta = 1$, $\tilde{\omega} = 10^3$, $\tilde{T}_0 = 3 \times 10^2$, $\tilde{s}_0 = 4 \times 10^7$, $\Omega = 5.950 \times 10^6$, $A = 5 \times 10^{19}$, $E = 2.206 \times 10^5$ and $R = 8.314$. By further assuming that $\tilde{T}_p \approx \tilde{T}_0$ and $\tilde{s}_p \approx \tilde{s}_0$, we find that $\Lambda_p \approx 1.4$ and $\Lambda_R \approx 10$, which is well within the range of values for which a shear band would be observed, even in the absence of any reaction. However, if the material were less sensitive to thermal softening, say $P = 0.1$, then we would find $\Lambda_p \approx 14$. In this case we would not expect a shear band if the material were inert, but we do expect a shear band when we take the reaction into consideration. From this we conclude that considering the behaviour of the reaction can be critical in determining whether or not localised plastic deformation will occur in an explosive material. The boundary layer analysis may also help to explain the charring and partial reaction observed in high explosives during experiments (e.g. [19]).

In this study it was assumed that the critical temperature for plastic work and reaction were similar in magnitude, so that the reaction occurs soon after the band has formed. In fact, the scalings are such that the onset of significant plastic work and onset of reaction effectively occur simultaneously. In reality this may not be the case and some adjustment to the analysis would be required. For the case where reaction occurs before significant plastic work (i.e. reactive materials which do not exhibit significant shear localisation) it can be shown that the problem reduces to that of [16]. In this instance the reaction is confined to a thin zone around the centreline, and the problem is effectively equivalent to the heating of a half-space of material with the boundary layer playing the role of a thermal flux applied at the boundary. On the other hand, if the reaction is significantly weak it may be observed that the shear band becomes fully developed before the reaction occurs. Solution of this problem would require imposing initial conditions consistent with those found inside a developed shear band and looking for a perturbation about the critical reaction temperature.

Acknowledgements

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