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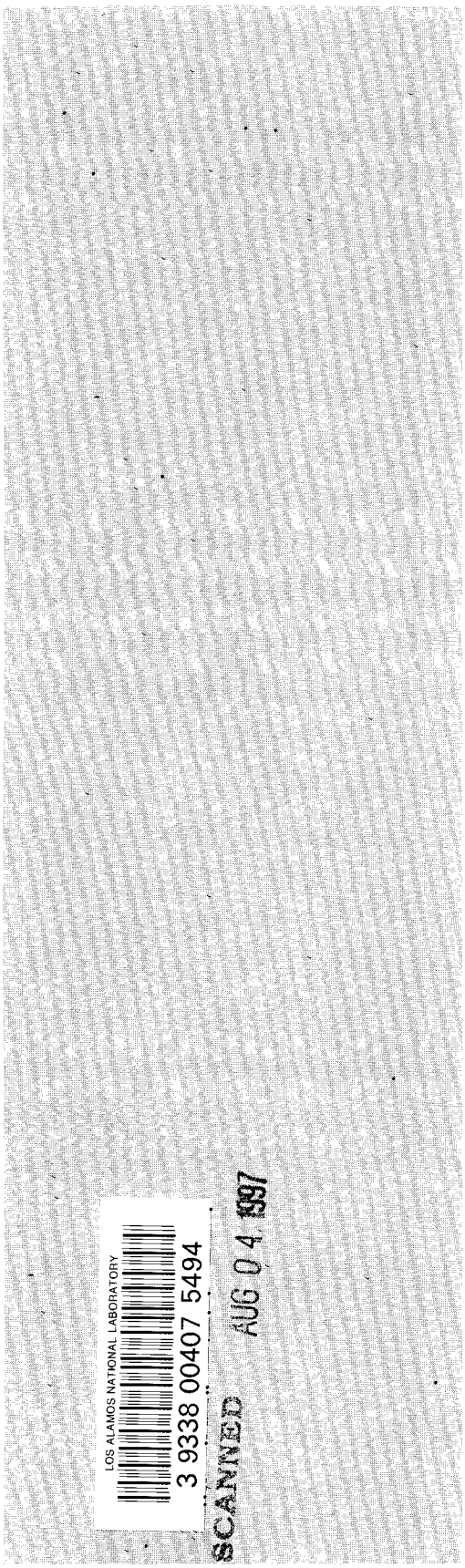

A Model for Shear-Band Formation and High-Explosive Initiation in a Hydrodynamics Code

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A MODEL FOR SHEAR-BAND FORMATION AND HIGH-EXPLOSIVE INITIATION IN A HYDRODYNAMICS CODE

by

Jerry F. Kerrisk

ABSTRACT

This report describes work in progress to develop a shear band model for MESA-2D. The object of this work is (1) to predict the formation of shear bands and their temperature in high explosive (HE) during a MESA-2D calculation, (2) to then assess whether the HE would initiate, and (3) to allow a detonation wave initiated from a shear band to propagate. This requires developing a model that uses average cell data to estimate the size and temperature of narrow region (generally much narrower than the cell size) that is undergoing shear within the cell. The shear band temperature (rather than the average cell temperature) can be used to calculate the flow stress of the material in the cell or to calculate heat generation from reactive materials. Modifications have been made to MESA-2D to calculate shear band size and temperature, and to initiate HE detonation when conditions warrant. Two models have been used for shear-band size and temperature calculation, one based on an independent estimate of the shear band width and a second based on the temperature distribution around the shear band. Both models have been tested for calculations in which shear band formation occurs in steel. A comparison of the measured and calculated local temperature rise in a shear band has been made. A model for estimating the time to initiation of the HE based on the type of HE and the temperature distribution in a shear band has also been added to MESA-2D. Calculations of conditions needed to initiate HE in projectile-impact tests have been done and compared with experimental data. Further work is needed to test the model.

INTRODUCTION

Shear Bands

Shear bands are narrow regions of high shear strain that can form in a material undergoing rapid (adiabatic) shearing (Olson and Mescall 1981, Merzer 1982, Hartley et al. 1987, Wright 1987, O'Donnell and Woodward 1988, Coleman and Newman 1989, Flockhart et al. 1991, Chou et al. 1991, Duffy and Chi 1992). The process concentrates a continuing shear strain that was occurring more or less

uniformly over a wide region into a narrow region with a width in the micron (10^{-6} m) range. Heat generation from plastic work (or viscous heating after the material melts) can raise the temperature of material of the shear band well above that of the surrounding material. The formation of shear bands has been proposed as one of the localization mechanisms that leads to the explosion of high explosives (HE) under impact conditions below those needed for shock initiation (Winter and Field 1975, Frey 1981, Dienes 1986).

The formation of a shear band in a region that was undergoing homogeneous shear occurs as the result of an instability (Bai 1982, Burns and Trucano 1982, Coleman and Newman 1989, Loret and Prevost 1990, Sluys 1992). Most investigators predict the instability to start when additional shear strain will decrease the flow stress, that is when $dY/d\varepsilon \leq 0$, where Y is the flow stress and ε is the strain. In most phenomenological models, Y is a function of strain (ε), strain rate (ε'), and temperature (T). For these models this criterion can be expressed as

$$dY/d\varepsilon = (\partial Y/\partial \varepsilon) + (\partial Y/\partial \varepsilon')\, \partial \varepsilon'/\partial \varepsilon + (\partial Y/\partial T)\, \partial T/\partial \varepsilon \leq 0. \qquad (1)$$

For essentially all normal materials Y increases with increasing strain and strain rate but decreases with increasing temperature; that is, $(\partial Y/\partial \varepsilon)$ and $(\partial Y/\partial \varepsilon')$ are positive and $(\partial Y/\partial T)$ is negative. Y will increase initially with increasing strain. If shearing occurs rapidly enough so that heat generated from plastic work cannot be redistributed (adiabatic shearing), a point can be reached beyond which subsequent strain will decrease Y. This is when shear bands are presumed to form (Bai 1982). If a material was perfectly homogeneous, shear bands would probably not form. However, normal variations in material properties and specimen geometry lead to small regions of slightly higher strain or temperature during deformation. These are the regions where shear band formation occurs once the criterion expressed by Eq. (1) is met.

Most experimental work on the formation of shear bands has been done with metals (Olson and Mescall 1981, Merzer 1982, Hartley et al. 1987, O'Donnell and Woodward 1988, Coleman and Newman 1989, Flockhart et al. 1991, Chou et al. 1991, Duffy and Chi 1992). Observed shear bands generally have a width much less than their length. Experiments with metals have indicated disturbed regions associated with shear bands of widths less than a micron for strong shock loading conditions (Grady and Kipp 1987) to several hundred microns at moderate strain rates (~500/s) (Merzer 1982). In addition to the strain rate, the conditions of the test and the properties of the specimen are important parameters in determining the shear band width.

Attempts to model shear band formation have varied from analytical and numerical solutions for the formation and growth of shear bands in model systems in simple shear (Burns and Trucano 1982, Iwakuma and Nemat-Nasser 1982, Coleman and Hodgdon 1985, Molinari and Clifton 1987, Coleman and Hodgdon 1988, Needleman 1988, Coleman and Newman 1989, Batra and Kim 1990, Wright 1990) to numerical models of more realistic experiments (Olson and Mescall 1981, Loret and Prevost 1990, Chou et al. 1991, Flockhart et al. 1991). Because shear band widths tend to be much less than realistic cell sizes in numerical calculations, calculated shear band widths will depend on cell size,

tending to decrease with decreasing cell size. However, even with appropriate cell sizes, proper shear band widths will not be calculated unless the constitutive equations includes rate terms (visco-plastic behavior) or higher-order spatial derivatives (Loret and Prevost 1990, Sluys 1992). Neither of these features is available in MESA-2D.

HE Initiation

HE will initiate when subject to a high enough shock pressure. This shock-to-detonation (SDT) process is understood at a phenomenological level and conditions leading to SDT are usually predictable. However, HE samples, particularly confined samples, can explode when impacted under conditions less severe than needed for SDT (Frey et al. 1979, Howe et al. 1981, Roberts and Field 1993) or when subject to rapid shear (Boyle et al. 1989). These explosions (they may or may not be detonations) are generally explained as localized heating in the HE leading to pressure buildup within the confinement and subsequent reaction of a large fraction of the HE in the sample (Frey et al. 1979). One feature of these explosions is the long delay between impact of a projectile and the explosion (it can be hundreds of microseconds) compared to tests where SDT occurs (usually less than ~10 μs delay).

Modeling impacts into realistic HE systems usually requires cell sizes greater than ~0.1 mm. These cell sizes would not resolve shear band widths even if the proper constitutive behavior were available. However, the generality of a numerical model that accounts for overall material flow in an impact situation is needed to address realistic accident situations. These constraints have led to the work on a shear band model for MESA-2D described here.

Shear Band Model

The objective of this work is to model impacts into confined HE and predict whether a detonation or explosion will occur as the result of localized heating in regions with large shear. The first step is to incorporate a model that calculates shear band behavior (formation, width, and temperature) within a cell in MESA-2D. This is essentially a mechanical model. For realistic systems, the cell sizes available will be much larger than the width of a shear band. Thus, a subcell model that estimates shear band parameters based on the average cell behavior is being pursued. The second step is to add a model to estimate the time to initiation of the HE in a cell based on the type of HE and the temperature distribution in a shear band. This is a thermo-chemical model. The third step is to allow a detonation wave started in one or a few cells with shear bands to propagate through the HE. This is a transition-to-detonation. The following represent an outline of the model:

1) a criterion for shear band formation in a cell,

2) energy dissipation in the shear band,

3) the shear band width and temperature calculation,

4) feedback to the constitutive model,

5) for HE, an energy release calculation, and

6) for HE, a transition to detonation.

The first four items are part of the mechanical model, the fifth item is the thermo-chemical model, and the sixth item is the transition-to-detonation model.

MECHANICAL MODEL FOR SHEAR BAND FORMATION

The mechanical model for shear band formation in MESA-2D is based on the concept that after a shear band forms, plastic work or viscous heating that would have been distributed over a region around the shear band is concentrated within the shear band. The model has been implemented on an individual cell basis, that is, calculations for each cell are done independently. This feature may be modified in the future if logic that connects shear bands across cell boundaries is needed. At present, the shear band model can be applied to only one material in a calculation and only the Johnson-Cook (JC) strength model can be used for that material. Although it is an empirical model, the JC strength model has sufficient flexibility to capture the strain and strain-rate hardening and the thermal softening effects needed to develop shear bands in a calculational situation.

Criterion for Shear Band Formation

The criterion for shear band formation in a cell is given by Eq. (1). The JC strength model calculates the tensile flow stress (Y) as a product of terms involving strain hardening, strain-rate hardening, and thermal softening,

$$Y = [Y_0 + B\varepsilon^n]\ [1 + C\ln(\varepsilon'^*)]\ [1 - T^{*m}]\ , \qquad (2)$$

where Y_0 is the yield stress at zero strain, quasi static conditions (low strain rate), and room temperature; ε is the equivalent plastic strain; $\varepsilon'^* = (\varepsilon'/\varepsilon'_0)$ is a dimensionless strain rate with $\varepsilon'_0 = 1/s$; $T^* = (T - T_0)/(T_m - T_0)$ is a dimensionless temperature with T = the sample temperature, T_0 = initial (room) temperature, and T_m = the melting temperature; and B, C, n, and m are constants. From Eq. (1) and the assumption the $\partial\varepsilon'^*/\partial\varepsilon = 0$,

$$dY/d\varepsilon = [nYB\varepsilon^{(n-1)}/(Y_0 + B\varepsilon^n)]\ -\ [(\partial T/\partial\varepsilon)mYT^{*(m-1)}/(1 - T^{*m})\ \Delta T_m]\ , \qquad (3)$$

where $\Delta T_m = T_m - T_0$. Assuming that the plastic work that leads to a temperature increase of the material occurs as strain at the flow stress, $\partial T/\partial\varepsilon = Y/\rho C_v$, where ρ is the density and C_v is the heat capacity of the material. Thus, $dY/d\varepsilon$ can be calculated as

$$dY/d\varepsilon = [nYB\varepsilon^{(n-1)}/(Y_0 + B\varepsilon^n)]\ -\ [mY^2T^{*(m-1)}/(1 - T^{*m})\ \rho\ C_v\ \Delta T_m]\ . \qquad (4)$$

The criterion for shear band formation is checked at the end of each advection time step in subroutine MUSER (see Appendix). If $dY/d\varepsilon > 0$, no further action is taken. If $dY/d\varepsilon \leq 0$, the model proceeds to calculate the width and temperature of the shear band.

Energy Dissipation in the Shear Band

For cells in which the shear band formation criterion is met and the shear band temperature (T_{sb}) is below the melting temperature, $Y > 0$ and plastic work can be done. (The calculation of T_{sb} and the feedback to the constitutive equations are discussed below.) In this case, the amount of plastic work accumulated over the last time step (ΔQ_{pw}) as calculated by the normal MESA-2D model for the cell is assumed to be deposited in the shear band.

As T_{sb} approaches T_m, the plastic work goes to zero. A model for viscous heating from shear flow was added to account for heating in the shear band above T_m. The viscous heating rate in a cell is calculated as

$$q_{vs} = \mu V[f(\partial u/\partial y + \partial v/\partial x)]^2 \ , \qquad (5)$$

where μ is the viscosity of the material, V is the cell volume, u and v are the x (or r) and y (or z) direction velocities as determined by the MESA-2D hydrodynamics, and f is the ratio of the velocity gradient in the shear band to the velocity gradient calculated from u and v. The quantity f is calculated as $W_{sb}/(\Delta x\, \Delta y)^{0.5}$, where W_{sb} is the width of the shear band, and Δx and Δy are the cell sizes in the x (or r) and y (or z) directions. This relation assumes that the entire variation of velocity occurs across the shear band, a reasonable assumption based on observations with metals (Coleman and Newman 1989, Duffy and Chi 1992). The viscous heating in the cell over a time step is calculated as $\Delta Q_{vs} = q_{vs}\, \Delta t$, where Δt is the time step.

To avoid a discontinuous change in the energy dissipation at $T_{sb} = T_m$, the viscous heating is phased in over the range $0.9T_m \le T_{sb} \le T_m$. Thus, the energy dissipated in the shear band (ΔQ) is

$$\Delta Q = \Delta Q_{pw} \qquad \text{if } T_{sb} < 0.9\, T_m \ , \qquad (6a)$$

$$\Delta Q = \Delta Q_{pw} + 10[(T_{sb}/T_m) - 0.9]\, \Delta Q_{vs} \qquad \text{if } 0.9\, T_m < T_{sb} < T_m \ , \qquad (6b)$$

$$\Delta Q = \Delta Q_{vs} \qquad \text{if } T_{sb} > T_m \ . \qquad (6c)$$

Width and Temperature of the Shear Band

The width and temperature of the shear band are interrelated quantities. The greater the width is for a given energy generation, the lower the temperature will be. Two models have been used to calculate the width and temperature of a shear band once the formation criterion is met. The work of Grady and Kipp (1987) is based on the mechanical and thermal dynamics of the shear band. The temperature-distribution model is based on the transient temperature distribution established from energy deposition at a plane of symmetry.

Grady and Kipp Model. The model developed by Grady and Kipp (1987) was adapted to meet the needs of the calculation within MESA-2D. The width of a shear band is calculated as

$$W_{sb} = [9\, \rho^3\, C_V^2\, \lambda^3 / (Y_s^3\, \alpha^2\, \varepsilon)]^{0.25} \ , \qquad (7)$$

where λ is the thermal diffusivity, Y_s is the flow stress in shear ($Y_s = Y/(3)^{0.5}$), and $\alpha = -(1/Y)(\partial Y/\partial T)$. The increase in temperature of the shear band as a result of the energy dissipation ΔQ over the time Δt is

$$\Delta T_{sb}^{n} = \Delta T_{sb}^{o} + \{[\Delta Q/(2C_v f)] - \eta \Delta T_{sb}^{o}\} / (1 + \eta) \quad (8)$$

where ΔT_{sb}^{o} and ΔT_{sb}^{n} are the old and new values of $(T_{sb} - T_{cell})$, f is defined above associated with Eq. (5), and $\eta = 4 \lambda \Delta t / (W_{sb})^2$. Only one-half the energy ($\Delta Q/2$) is used because the shear band is symmetric and heat flow in both directions. Before shear band formation starts in a cell, ΔT_{sb} is set to zero.

Temperature-Distribution Model. This model calculates the temperature distribution around a plane with a heat source on the plane and heat loss into an infinite medium. One-half the energy ($\Delta Q/2$) is assumed to flow in each direction. Figure 1 shows a sketch of the temperature distribution set up in a cell by this system with a number of variables defined. The assumption that heat flows into an infinite medium is based on the approximation that the widths of the shear band (W_{sb}) and thermal pulse (2δ) are small compared to the cell size.

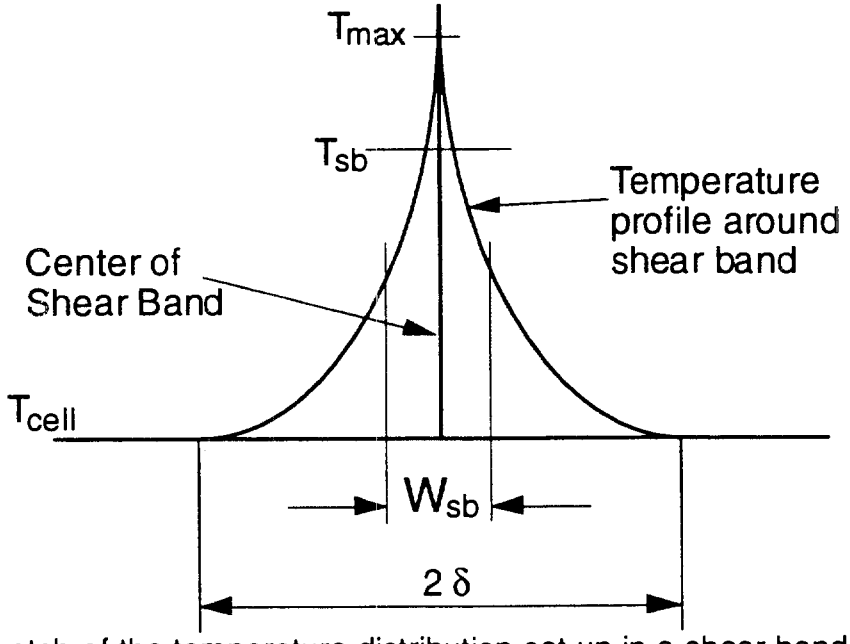

Fig. 1. Sketch of the temperature distribution set up in a shear band region with the Temperature-Distribution model.

The temperature distribution is approximated by a method call the Integral Method (Rohsenow and Hartnett 1975, Özisik 1980). The temperature profile is assumed to be a polynomial of the form $T = (T_{max} - T_{cell})[1 - (x/\delta)]^{\beta}$, where x is the distance measured from the plane of symmetry, δ is the distance that the thermal pulse has penetrated, T_{max} is the temperature on the plane of symmetry, and β is an integer (usually $2 \leq \beta \leq 6$). If q(t) is the energy flux on the plane x = 0 and $Q = \int q(t)\, dt$, then

$$\delta = [\beta (\beta + 1) \alpha Q / q(t)]^{0.5} , \quad (9)$$

and

$$T_{max} - T_{cell} = q(t) \delta / (\beta k) , \quad (10)$$

where k is the thermal conductivity. If q(t) is constant for a time t, then

$$\delta = [\beta (\beta + 1) \alpha t]^{0.5} . \quad (11)$$

For the MESA-2D calculation, $q(t) = \Delta Q \rho (\Delta x \Delta y)^{0.5} / \Delta t$ and $Q = \sum \Delta Q \rho (\Delta x \Delta y)^{0.5}$, where ΔQ is the energy deposited in a cell for a given time step (see Energy Dissipation in Shear Band section above) and the sum is over all time steps for which the shear band is active in the cell. The parameter β was taken as 3. For cells in which the shear band has been active in previous time steps but is inactive in a given time step, the above formulation fails. In that case, changes in δ and T_{max} are approximated as

$$\delta_{new} = [\delta_{old}^2 + \beta (\beta + 1) \alpha \Delta t]^{0.5} , \quad (12)$$

and

$$(T_{max} - T_{cell})_{new} = (T_{max} - T_{cell})_{old} (\delta_{old} / \delta_{new}) , \quad (13)$$

where the subscript 'old' refers to the previous values of the variables.

As shown in Fig. 1, the shear band width (W_{sb}) and temperature (T_{sb}) were taken as fractions of 2δ and ($T_{max} - T_{cell}$). The width of the shear band was taken as the width where ($T_{sb} - T_{cell}$) = 0.5 ($T_{max} - T_{cell}$). This gives

$$W_{sb} = 2 \delta [1 - (0.5)^{(1/\beta)}] . \quad (14)$$

The shear band temperature was taken as

$$T_{sb} = T_{cell} + 0.75 (T_{max} - T_{cell}) . \quad (15)$$

Although the Temperature-Distribution Model assumes a temperature distribution exists from the center of the shear band outward, most of the subsequent treatment uses a single temperature (T_{sb}) to characterize the shear band. This will be modified for the calculation of energy generation in a shear band in HE.

Melting of the Material in the Shear Band. As the temperature of the material in the shear band goes through the melting temperature (T_m), the heat of melting (ΔH_m) is accounted for. Melting is assumed to occur over a temperature range, $0.99T_m \leq T \leq 1.01T_m$. An effective heat capacity, $C_v^m = C_v + \Delta H_m/(0.02T_m)$, is assumed over this temperature range.

Feedback to the Constitutive Model

Once a shear band has formed in a cell, the effect of the shear band is communicated to the MESA-2D constitutive model by calculating the flow stress of the material in that cell using the shear band temperature (T_{sb}) rather than the average cell temperature. This feature has only been implemented for the JC strength model.

RESULTS OF CALCULATIONS FOR NONREACTIVE MATERIAL

The shear band model has been used to calculate shear band formation and behavior for three experiments in which shear bands have been observed in nonreactive material. In two of the experiments (Chou et al. 1991, and O'Donnell and Woodward 1988), the comparisons between observed and calculated behavior have been qualitative. These calculations were used to assess the dependence of the model predictions on cell size. In one experiment (Duffy and Chi 1992), temperatures in the shear band were measured as the shear band formed. A comparison of the measured and calculated local temperature rise in a shear band was made for this experiment.

Experiment of Chou et al. (1991)

In this experiment, a hard steel projectile was used to impact a target specimen under conditions such that a plug could form in the target. Shear band formation was observed near the edge of the plug (see Fig. 2). Two-dimensional, axisymmetric calculations of the experiment were done with MESA-2D. The calculations were done for only one of the target materials used in the experiments (martensitic steel tempered at 400 °C), one projectile impact velocity (0.005 cm/μs), and one backup hole diameter (0.127 cm). The indentor

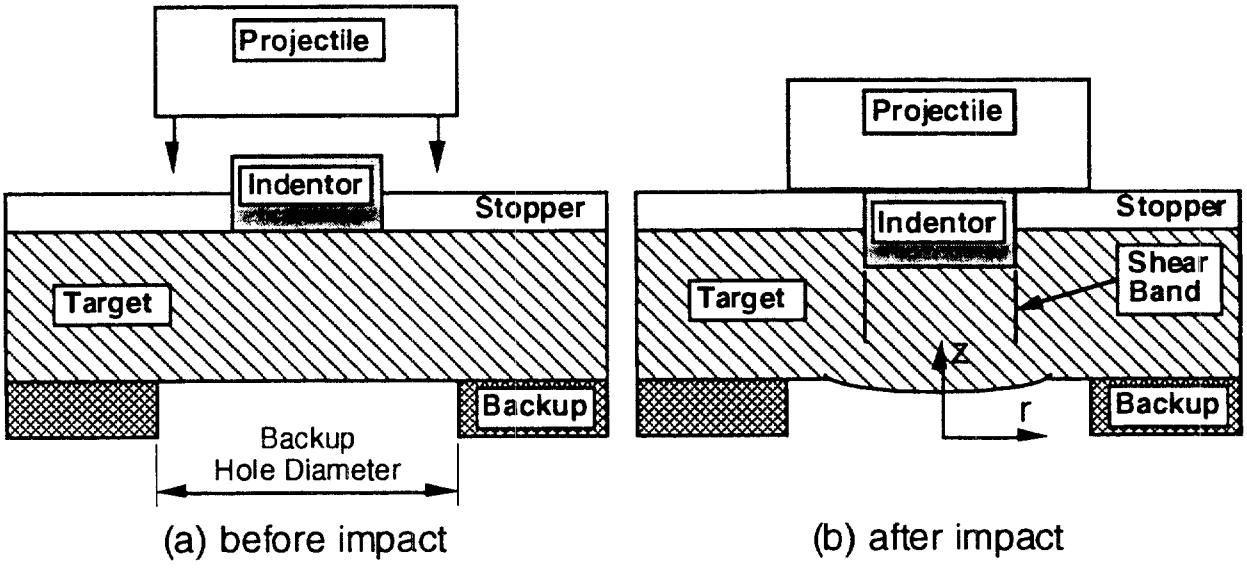

Fig. 2. Sketch of experiment of Chou et al. (1991).

diameter was 0.635 cm, the target diameter was 2.54 cm, and the target thickness was 0.635 cm. Indentor penetration of ~0.2 cm into the target was followed. This required a calculation to ~50 μs. Johnson-Cook strength parameters for the target were taken from Chou et al. (1991). They matched the parameters given by Johnson and Holmquist (1989) for S-7 tool steel. The indentor and backup ring (see Fig. 2) were modeled as high-density, high-strength materials so that they experienced essentially no deformation. The steel was modeled with a SESAME equation of state (SESAME 4270); this gives material temperatures directly.

Calculations were done using the Temperature-Distribution Model with four cell sizes, 0.08-, 0.04-, 0.02-, and 0.01-cm cells. Figure 3 shows a sequence of plastic strain contour plots for the calculation with 0.01-cm cells without the shear band model. The growth of the region of high strain is evident. Figure 4 shows a similar sequence for the same cell size with the shear band model. Note that the shear band length requiring 40-50 μs without the shear band model (Fig. 3) is accomplished in 10-15 μs with the shear band model (Fig. 4). In the experiment modeled here, a shear band length of ~0.6 cm was measured for a depth of penetration of ~0.05 cm (~12 μs into the calculation). This observation is consistent with the calculational result with the shear band model, but is more rapid than the result without the shear band model.

There is also a significant difference in the behavior of the temperature in the vicinity of the shear band with and without the shear band model. Without the model, cell temperatures in the vicinity of the shear band (r = ~0.3-0.35 cm) decrease and the width of the affected region increases with increasing cell size. Figure 5a shows cell temperatures as a function of radius along a line z = ~0.4 cm (~0.2 cm above the bottom of the target) at 50 μs into the calculation without the shear band model. With 0.08-cm cells, the peak temperature is only ~800 k compared to ~1500 k with 0.01-cm cells. Figure 5b shows temperatures (cell temperatures outside the shear band region and shear band temperatures near the shear band) for the same cell sizes with the shear band model. The peak temperatures are nearly the same. The location of the shear band shifts slightly in both cases as the cell size varies. This is caused by a change in resolution with cell size.

Although the late-time shear band temperature (Fig. 5b) shows good agreement for the various cell sizes used, the approach to a steady state does not. Figure 6 is a plot of the shear band temperature (T_{sb}) of a representative cell as a function of time for the four cell sizes. A late time (beyond ~25 μs), T_{sb} is at the melting temperature. Changes in temperature are moderated by the heat of melting. However, the rise from the initial temperature starting at ~8 μs is very erratic. This is caused by a highly variable amount of plastic work in the cells. Figure 7 is a plot of T_{sb} and the plastic work (ΔQ_{pw}) for the calculation with 0.01-cm cells. The plastic work varies over several orders of magnitude during the rise in T_{sb}. These variations do not have a large effect when spread out over the entire cell, but they have a significant effect in the much smaller shear band within the cell.

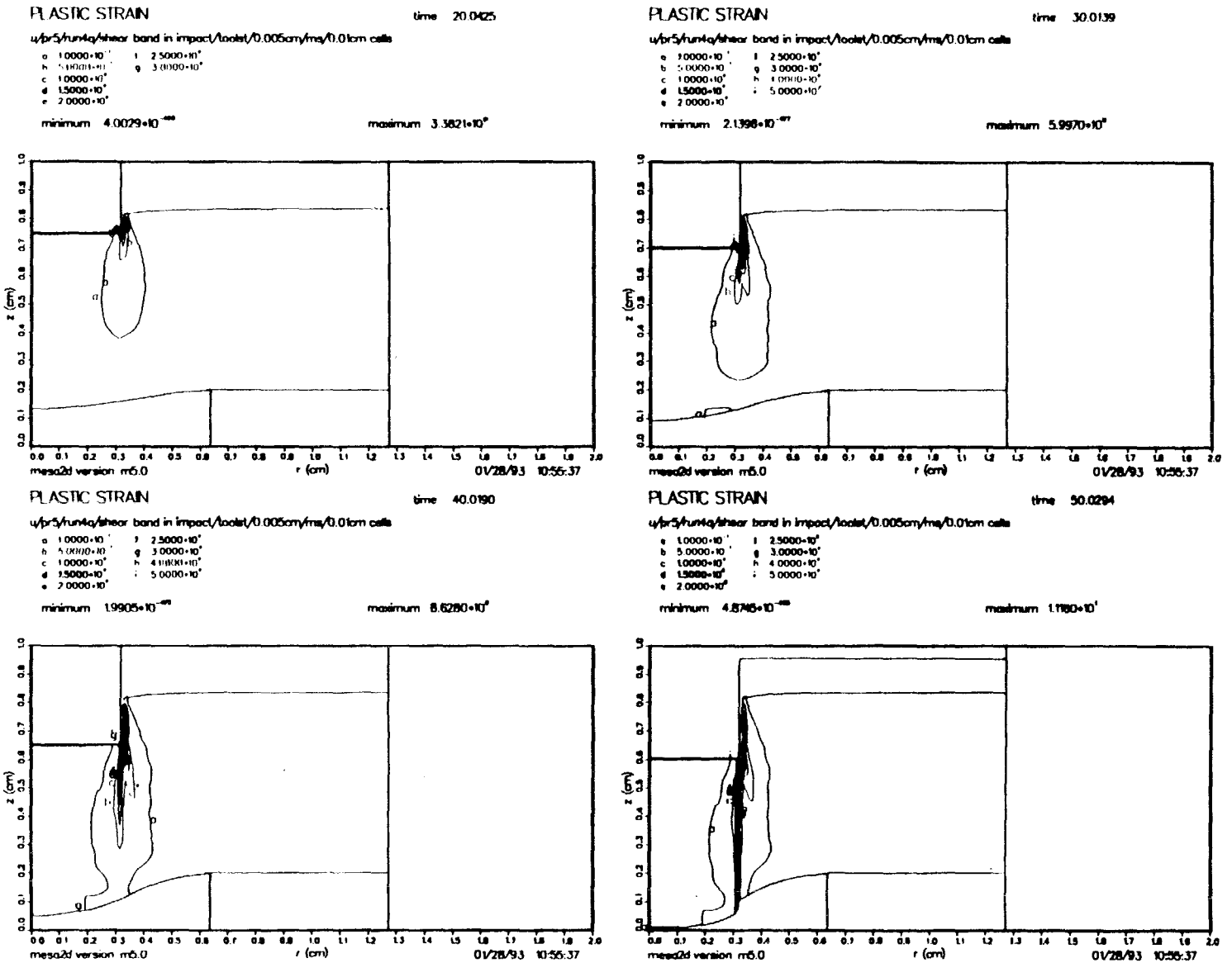

Fig. 3. Plastic strain contours at 20, 30, 40, and 50 μs for the calculation with 0.01-cm cells without the shear band model. Experiment of Chou et al. (1991).

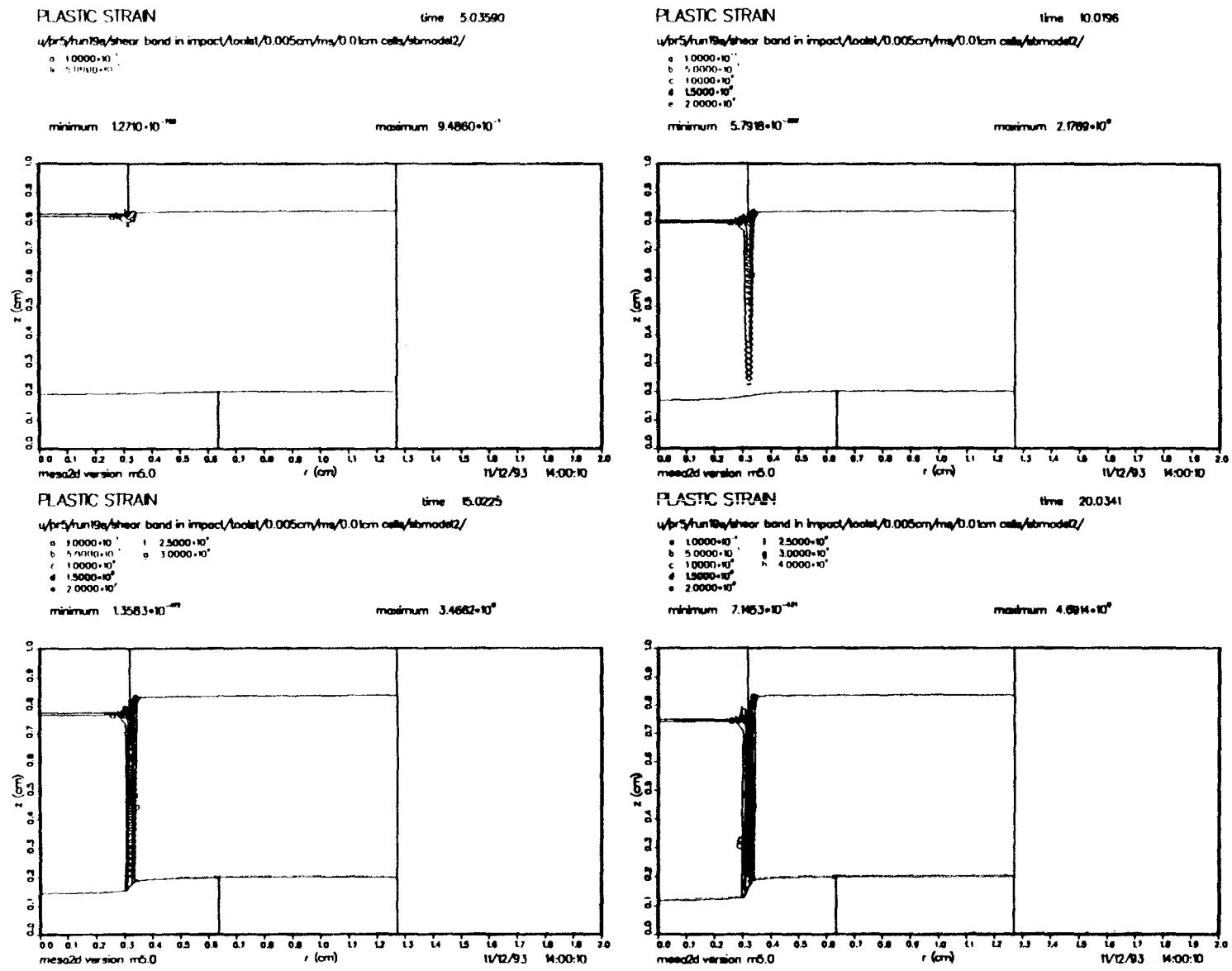

Fig. 4. Plastic strain contours at 5, 10, 50, and 20 μs for the calculation with 0.01-cm cells with the shear band model. Experiment of Chou et al. (1991).

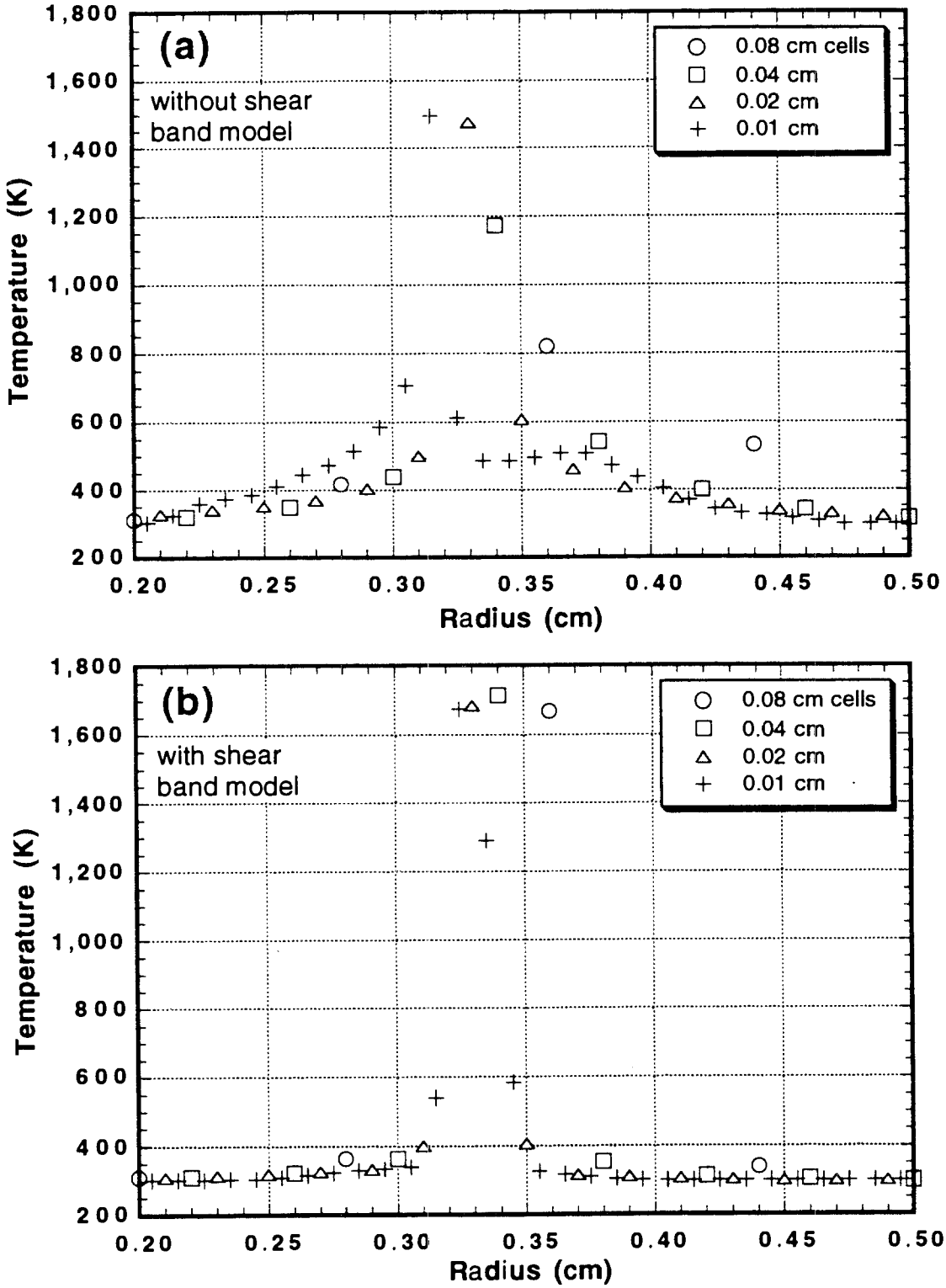

Fig. 5. Cell temperatures as a function of radius along a line z = ~0.4 cm at 50 μs for the experiment of Chou et al. (1991). Calculations (a) without and (b) with the shear band model.

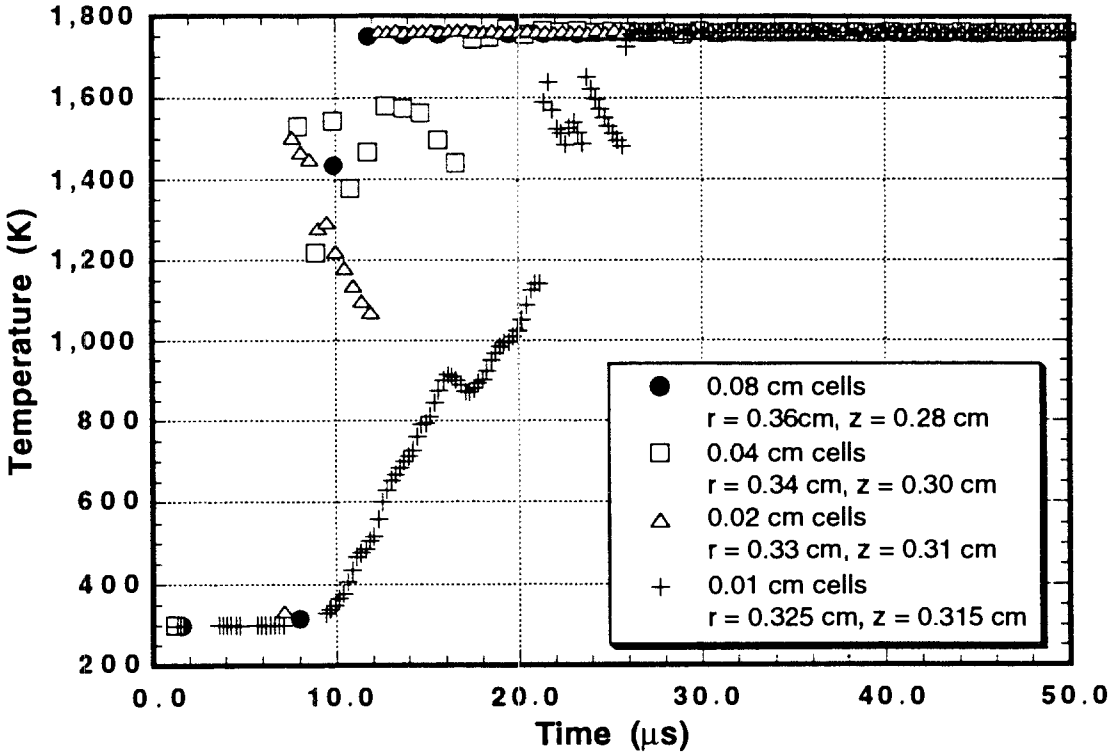

Fig. 6. Shear band temperature as a function of time for a representative cell from calculations of the experiment of Chou et al. (1991) with four cell sizes.

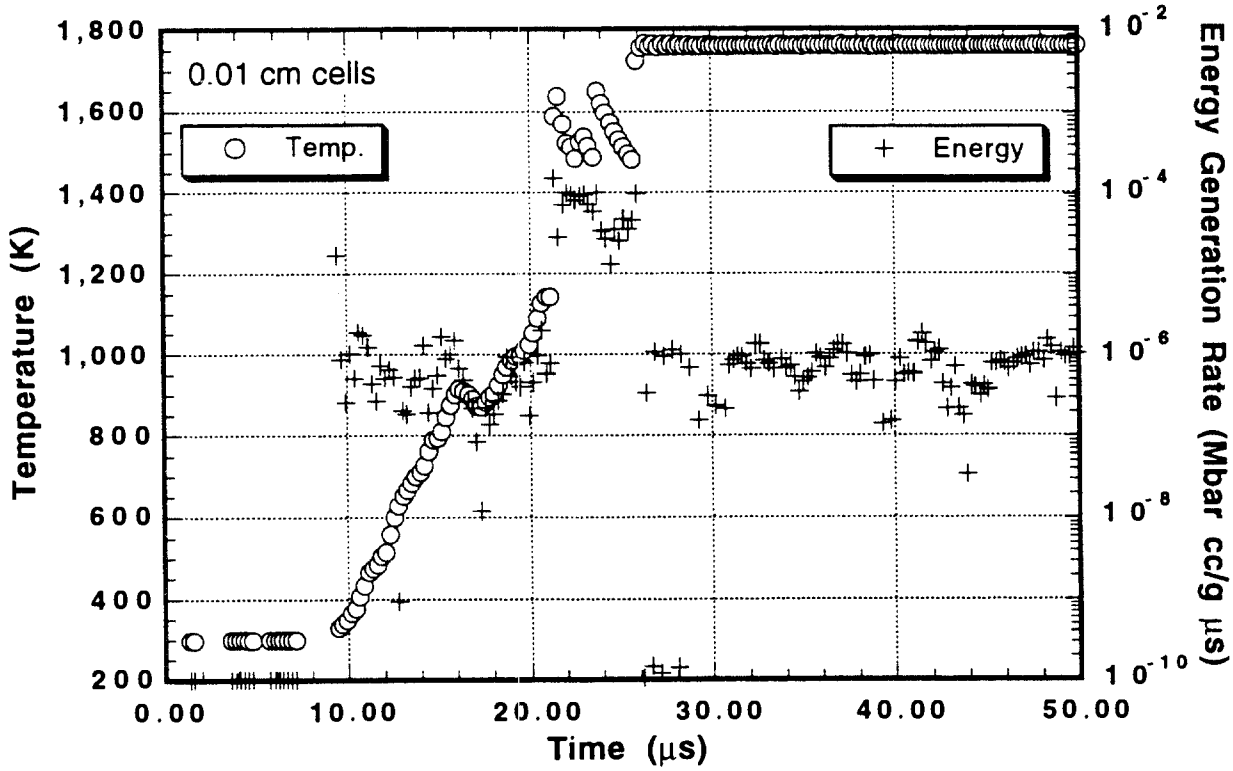

Fig. 7. Shear band temperature (T_{sb}) and energy generation rate as a function of time for a representative cell from calculations of the experiment of Chou et al. (1991).

Figure 8 is a plot of shear band width (W_{sb}) of a representative cell as a function of time for the four cell sizes. There is relatively good agreement for the three larger cell sizes. However, for the 0.01-cm cells there is a sharp drop in W_{sb} at 21 μs. This corresponds to the jump in T_{sb} and ΔQ_{sb} in this calculation (see Fig. 7). The behavior in this particular cell is not necessarily paralleled in other cells in the shear band.

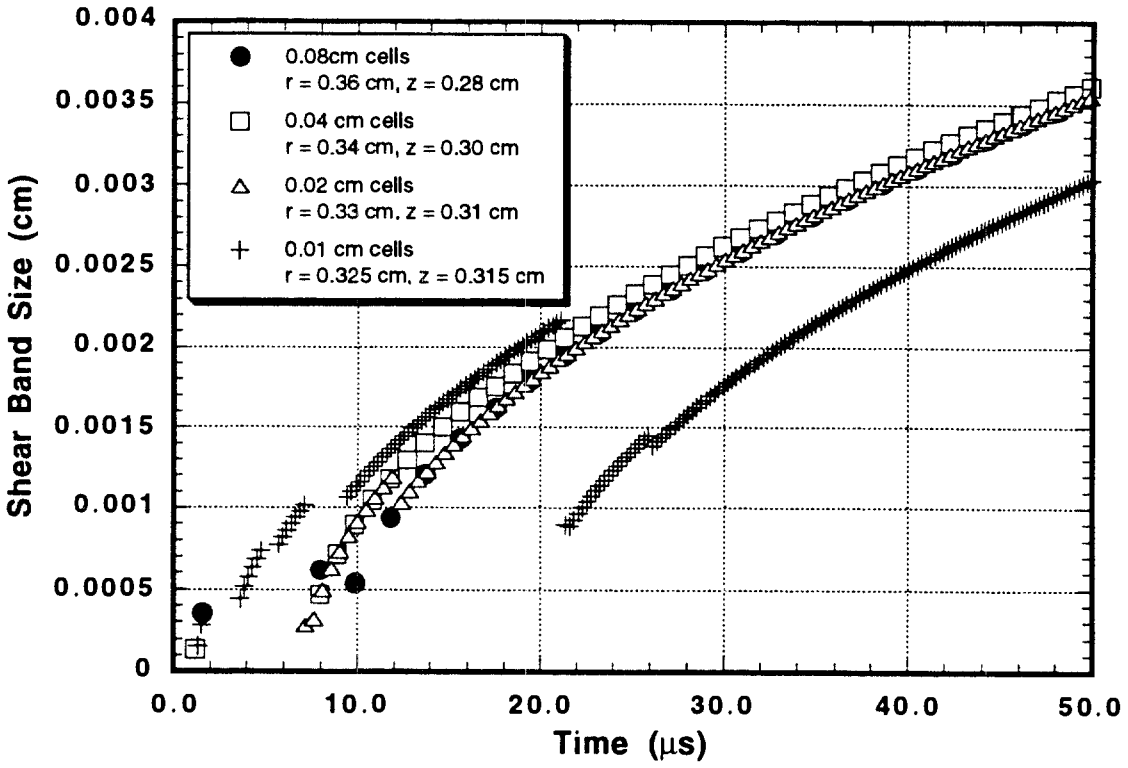

Fig. 8. Shear band width (W_{sb}) as a function of time for a representative cell from calculations of the experiment of Chou et al. (1991) with four cell sizes.

A similar set of calculations at the four cell sizes was done using the Grady and Kipp Model. The shear band size is about an order of magnitude smaller than with the Temperature-Distribution Model. This leads to lower shear band temperatures that continue to increase out to 50 μs. At that time they are below melting for all four cell sizes. In these calculations, values of T_{sb} show a cell-size effect, increasing with decreasing cell size. At 50 μs, T_{sb} ranges from ~900 k for 0.08-cm cells to ~1700 k for 0.01-cm cells.

One quantitative comparison was done with this experiment. Figure 9 shows a plot of shear band length as a function of penetration depth of the indentor for calculations with and without the shear band model compared with experimental results of Chou et al. (1991). The calculations with the shear band model used the Temperature-Distribution Model. With the shear band model, the agreement is quite good (probably better than warranted by the model). Without the shear band model, MESA-2D predicts much shorter shear band lengths for a given penetration depth.

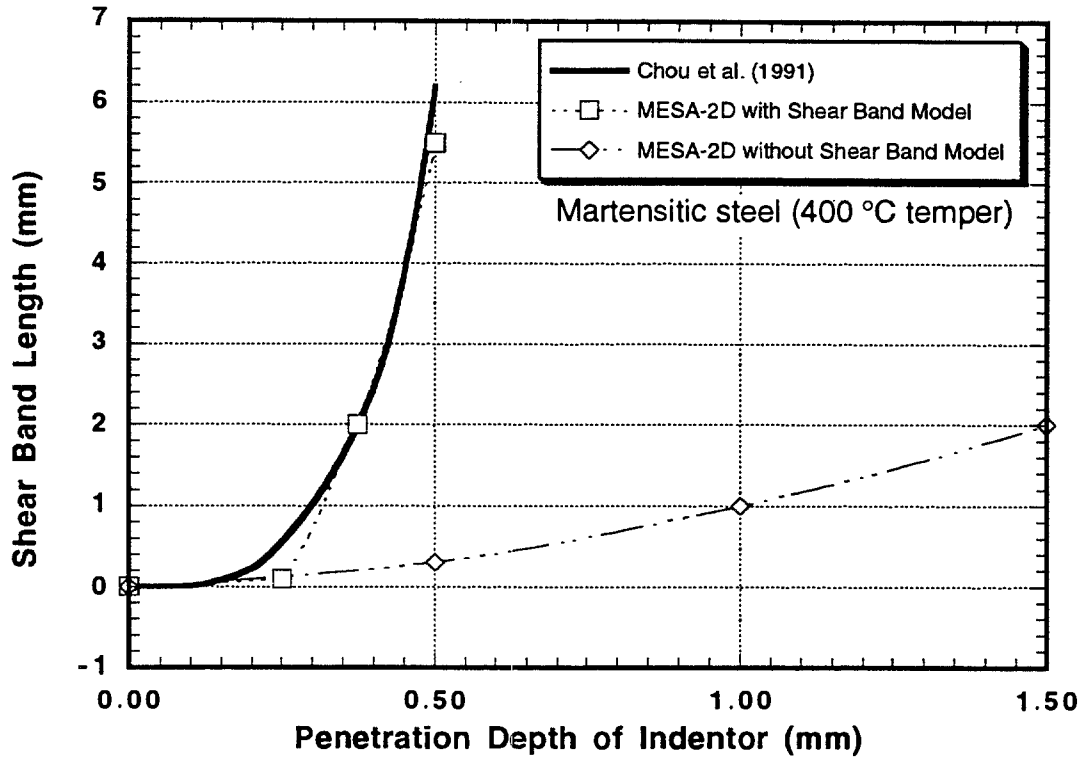

Fig. 9. Comparison of calculated and observed shear band width length as a function of penetration depth.

Experiment of O'Donnell and Woodward (1988)

In this experiment, cylinders of 2024 T351 aluminum were compressed in a drop-weight apparatus (see Fig. 10). Shear bands develop along slip planes in the cylinders. This experiment is interesting because the shear bands display a conical geometry and are thus at some angle to the mesh lines in a calculation. This phenomenon is also discussed by Flockhart et al. (1991). Two-dimensional, axisymmetric calculations of this experiment were done with MESA-2D. The calculations were done for one impact velocity (0.01 cm/μs) and to one compression (average strain of 0.5). Only the upper right quadrant of the experiment was modeled ($r > 0$ and $z > 0$).

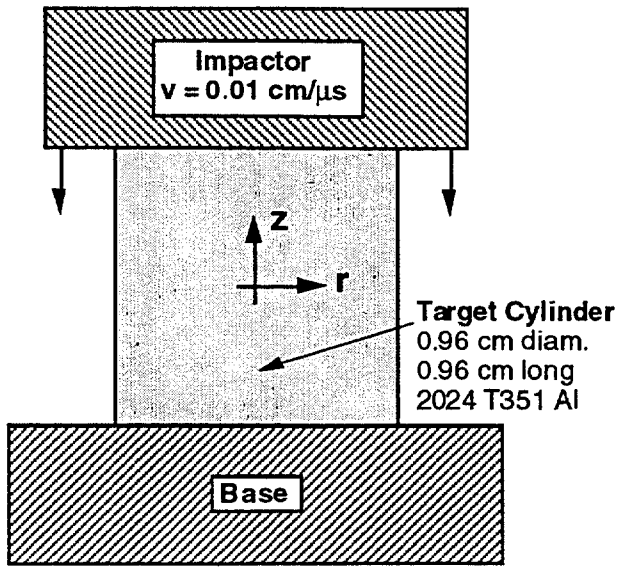

Fig. 10. Sketch of experiment of O'Donnell and Woodward (1988).

The impactor and base were modeled as a high-density, high-strength material so that they experienced little or no deformation. Johnson-Cook strength parameters for the Al target cylinder were taken from Johnson and Holmquist (1989). This material was modeled with a SESAME equation of state (SESAME 3717); this gives material temperatures directly. Calculations were run to 24 μs, at which time the Al cylinder was compressed to ~55% of its initial length.

Calculations were done with and without the shear band model (using the Temperature-Distribution Model for shear band calculations) with two cell sizes, 0.01- and 0.005-cm cells. Figure 11 shows a sequence of plastic strain contours plots for the calculation with 0.005-cm cells with the shear band model. The growth of the shear band starting at the upper right-hand corner of the Al cylinder is evident. The appearance of the plastic strain contours without the shear band model is similar to Fig. 11; however, the range of plastic strains within the shear band is about half what it is with the shear band model. The location of the shear band is similar to that shown in Fig. 3a of O'Donnell and Woodward (1988), which is for the material modeled here to essentially the same compression.

Figure 12 is a plot of temperature as a function of z (r = 0.4 cm) at 24 μs. Data shown as points are from calculations with the shear band model; data shown as curves are from calculations without the shear band model. Without the shear band model there is a variation in the width and maximum temperature of the high-strain region with cell size. With the shear band model, maximum temperatures are quite close, but there is still a variation in the width of the high-strain region with cell size. Figure 13 is a plot of shear band temperature (T_{sb}) of a representative cell as a function of time for the two calculations with the shear band model. The agreement is good - considerably better than seen in the previous experiment. In these calculations, values of the plastic work used to calculate T_{sb} showed much less variation than seen in the previous experiment (Fig. 7).

Experiment of Duffy and Chi (1992)

In this experiment, a cylindrical sample (thin-walled tube) was deformed dynamically in a torsional Kolsky bar. Shear bands developed at preexisting defects (thinner tube-wall regions). Shear band initiation and development were observed by high-speed photography and temperatures were measured with infrared temperature detectors. Within the shear band region, temperatures up to ~900 k were observed. Because this is a three-dimensional system, a number of approximations were made to model it with MESA-2D. The thin-walled tube was assumed to be cut and rolled out flat and modeled in x-y geometry (see Fig. 14). The section modeled was 0.5 cm in the x direction and 0.26 cm in the y direction. The defect could not be modeled as a thinned region because this dimension is normal to the x-y plane. Instead, the melting temperature of the defect region (0.06 cm wide) was reduced from a nominal value of 1800 k to 1725 k.

Calculations were done for HY-100 steel at an average strain rate of 0.0015/μs. Temperature measurements as a function of time and position were reported in

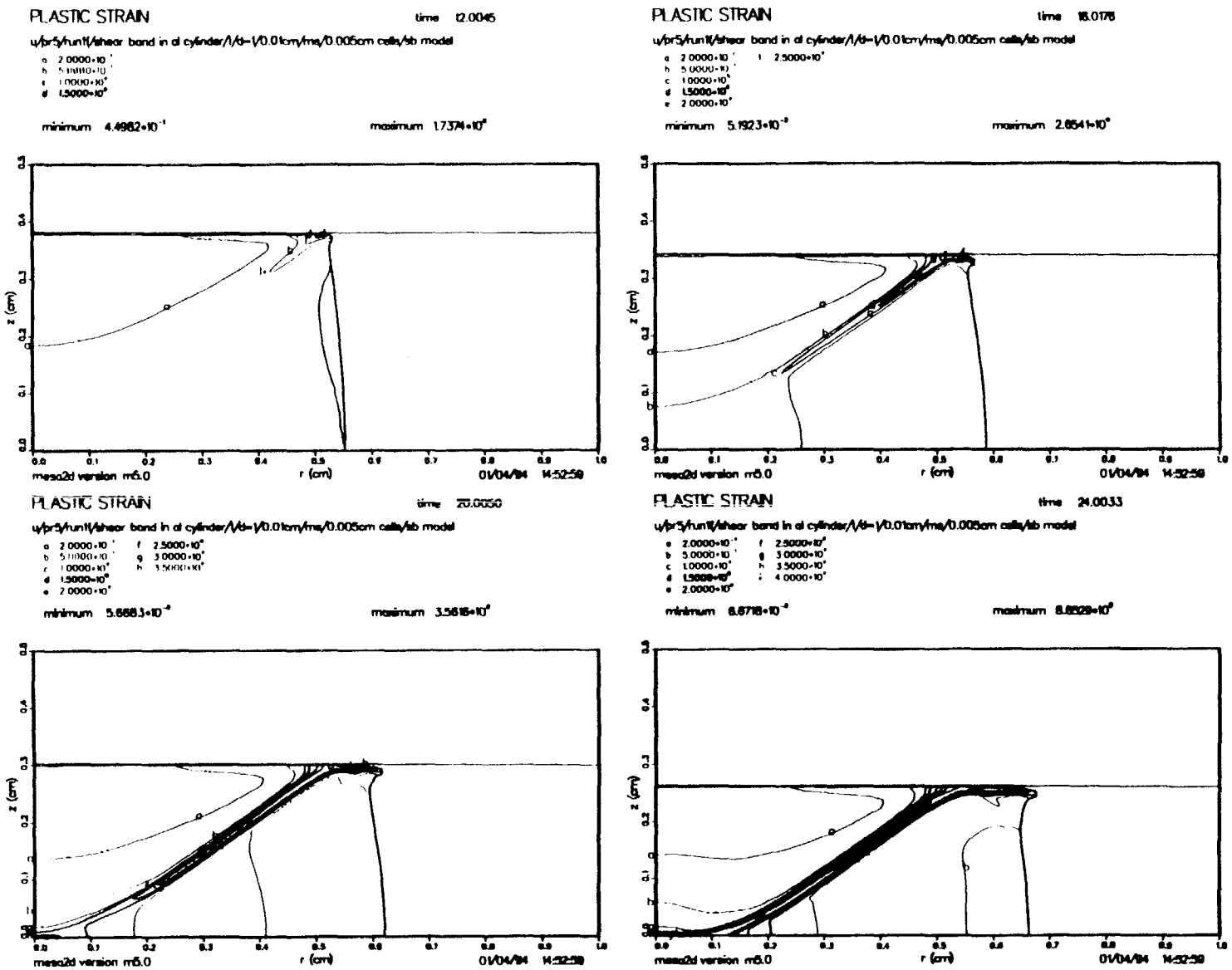

Fig. 11. Plastic strain contours at 12, 16, 20, and 24 μs for the calculation with 0.005-cm cells with the shear band model. Experiment of O'Donnell and Woodward (1988).

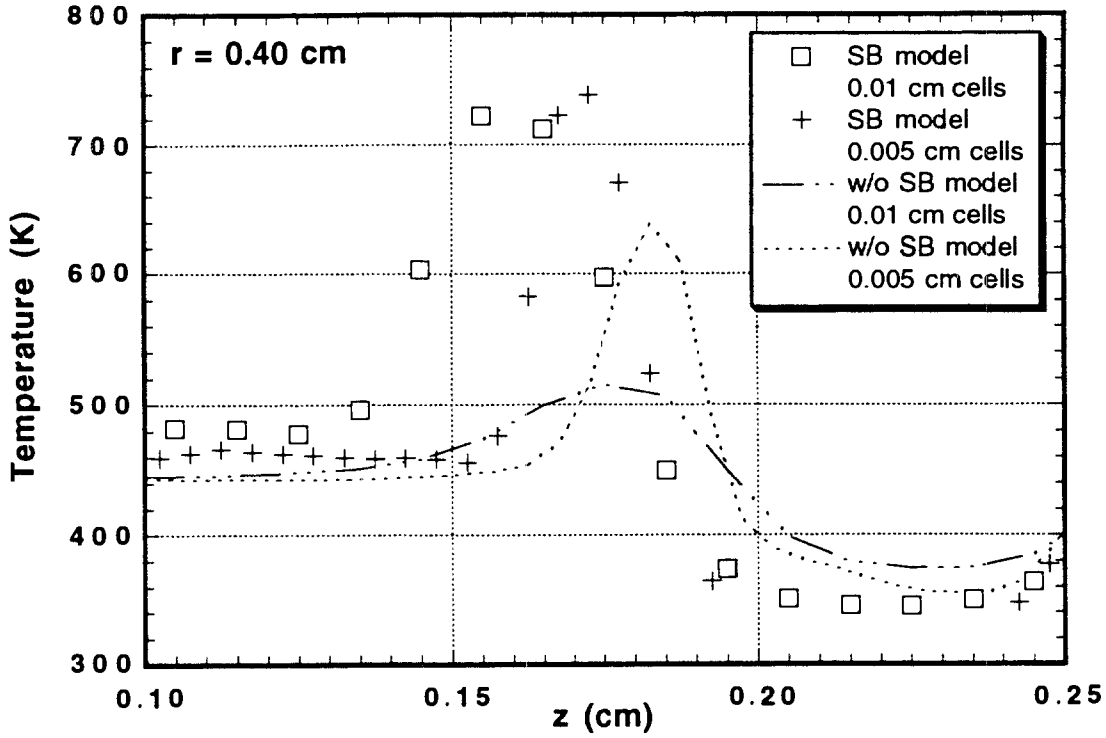

Fig. 12. Cell temperatures as a function of z along a line r = ~0.4 cm at 24 μs for the experiment of O'Donnell and Woodward (1988).

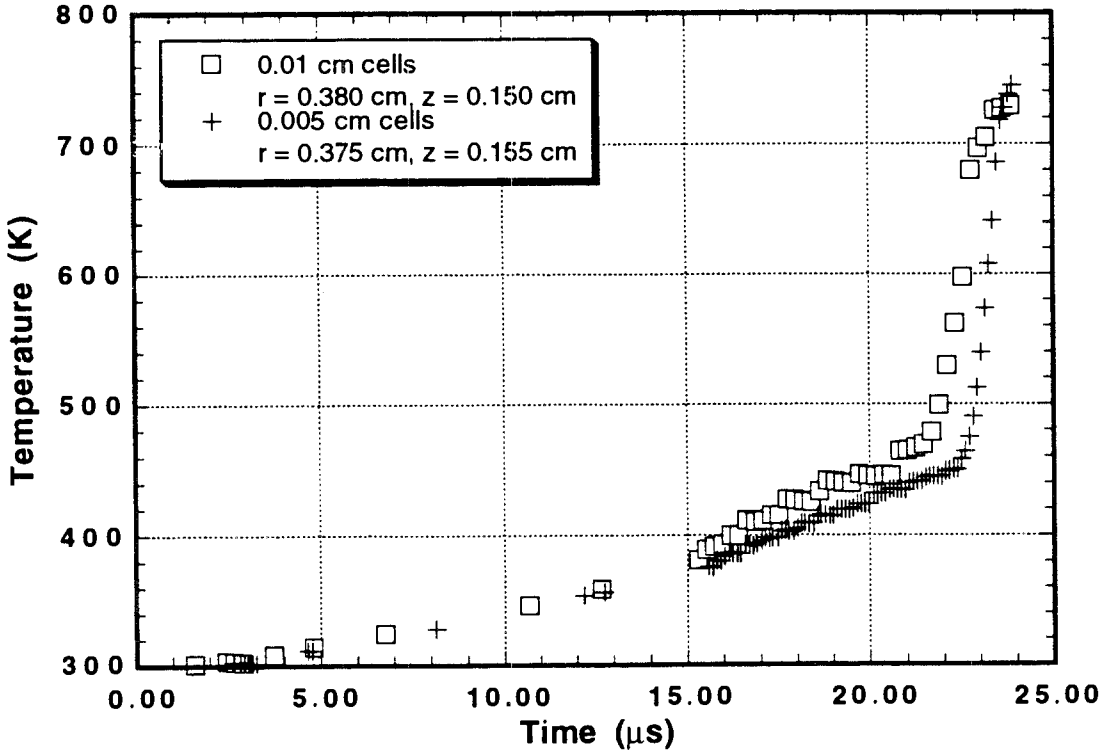

Fig. 13. Shear band temperature as a function of time for a representative cell from calculations of the experiment of O'Donnell and Woodward (1988) with two cell sizes.

Fig. 14 of Duffy and Chi (1992) for these conditions. Johnson-Cook strength parameters for HY-100 steel were taken from Johnson and Holmquist (1989). The average strain rate (γ') is related to the fixed boundary velocity (v) as $\gamma' = v/0.13$ cm. This gives $v = 0.0002$ cm/μs for $\gamma' = 0.0015/\mu s$. The steel was modeled with a SESAME equation of state (SESAME 4270); this gives material temperatures directly.

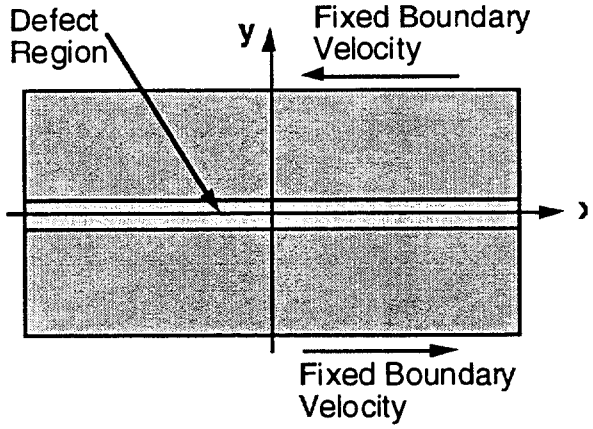

Fig. 14. Sketch of experiment of Duffy and Chi (1992).

Calculations were done with and without the shear band model (using the Temperature-Distribution Model and the Grady-Kipp Model for shear band calculations) with one cell size, 0.01- cm cells. The experiment modeled developed a shear band at an average strain of ~0.35 (at ~250 μs assuming a strain rate of 0.0015/μs). However, calculations consistently showed shear band formation at an average strain of ~0.65 (~430 μs) when the nominal HY-100 parameters were used. Figure 15 is a plot of shear stress as a function of average strain for two experimental cases using HY-100 steel ($\gamma' = 0.0015/\mu s$ and $0.0012/\mu s$) and for the calculation. There is a significant difference in the two experimental results that seem greater than can be ascribed to the relatively small difference in strain rate. Duffy and Chi (1992) do not discuss this difference. The calculated shear stress before formation of the shear band is in good agreement with the experimental results. However, shear band formation occurs much later. This may be related to the shear band model, the strength model for HY-100 steel, or the magnitude of the simulated defect used in these calculations. Duffy and Chi (1992) show (for another material) that the strain at which shear band formation starts is a function of the magnitude of the defect (see their Fig. 5a). Increasing the magnitude of the defect decreases the strain at which shear band formation starts. They did not report the magnitude of the defect in the HY--100 specimen for which temperature measurements were made.

A comparison of observed and calculated shear band temperatures was made by plotting temperature as a function of time from the start of shear band formation. The temperature rise in the material prior to the start of shear band formation is not large and has only a minor effect on temperatures in the shear band. Figure 16 is a plot of shear band temperature as a function of time for the experiment and for calculations with the two shear band models. The result from the Temperature-Distribution Model matches the experimental temperature better than the result from the Grady-Kipp Model. The difference between the two calculational temperatures is similar to that seen for calculations of the experiment of Chou et al. (1991); the Grady-Kipp Model for the shear band gives lower temperatures than the Temperature-Distribution Model.

Duffy and Chi (1992) indicate that their samples often fractured some time after shear band formation. The MESA-2D calculations done here do not include fracture. For that reason, plastic strain and temperature increase continue well beyond the strain at which fracture would occur. The result in Fig. 16 shows calculated temperatures continuing to increase beyond the point where fracture probably occurred in the experiment (~30 μs after the start of shear band formation).

For the experiment shown in Fig. 16, Duffy and Chi (1992) report a shear band width (W_{sb} in the notation here) of 20 μm a. The calculated value of W_{sb} (with the Temperature-Distribution Model) at 30 μs after the start of shear band formation is ~15 μm.

Discussion

Calculations were done for three experiments in which shear bands have been observed. Without the shear band model, MESA-2D predicts regions of high shear strain in the proper locations, but temperatures in these regions were a function of cell size, increasing with decreasing cell size. Using the Temperature-Distribution Model for shear band characterization reduced the variation of shear band temperature with cell size. However, calculations of the experiment of Chou et al. (1991) showed very erratic behavior of shear band temperatures

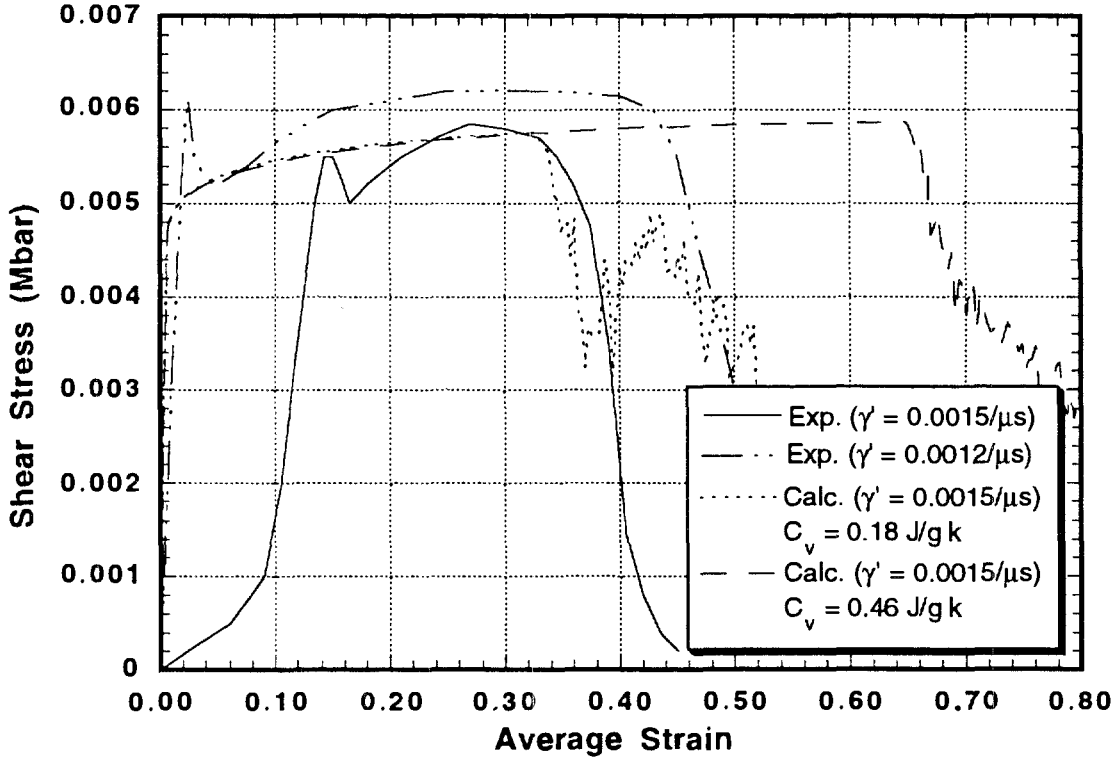

Fig. 15. HY-100 steel shear stress as a function of average strain for two experiments of Duffy and Chi (1992) and for one calculation.

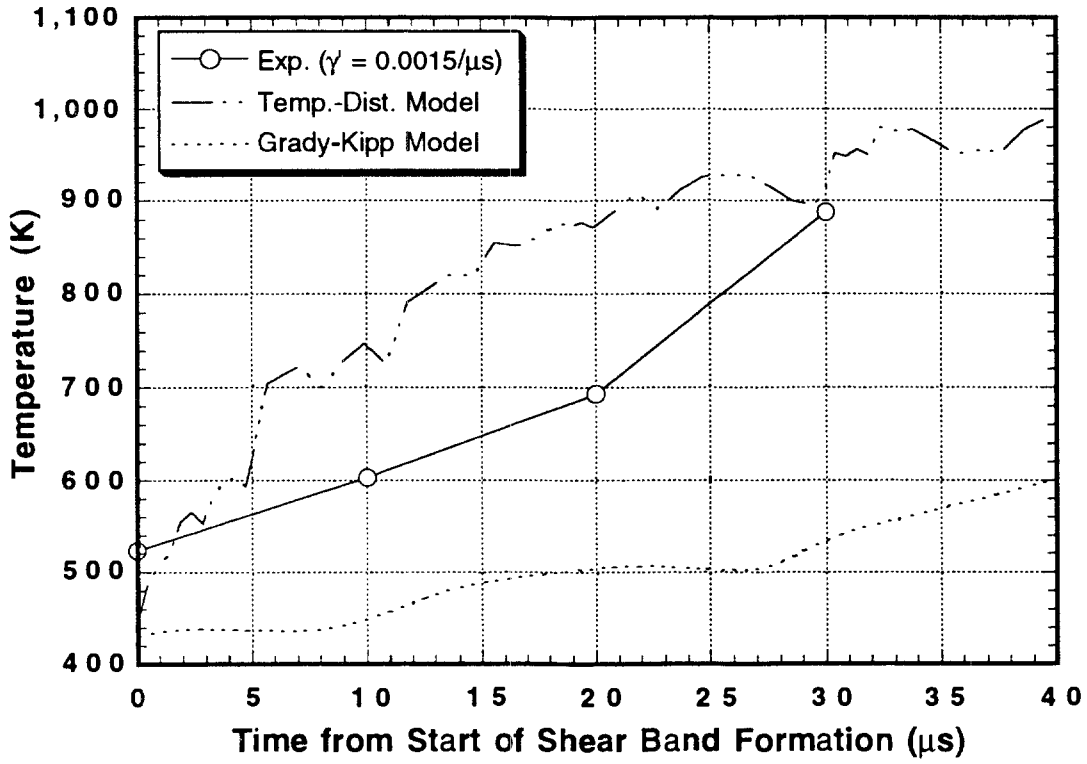

Fig. 16. Shear band temperature as a function of time HY-100 steel for one experiment of Duffy and Chi (1992) and for calculations using the Temperature-Distribution and Grady-Kipp shear band models.

as a function of cell sizes from the start of shear band formation to melting (see Fig. 6). In spite of this, calculated variation of shear band length with penetration depth was in good agreement with experimental results (see Fig. 9). Shear band temperatures calculated for the experiment of O'Donnell and Woodward (1988) are more consistent (see Fig. 13).

Calculated shear band temperatures were compared with observed temperatures from the experiment of Duffy and Chi (1992). The Temperature-Distribution Model for shear band behavior shows better agreement with the observations than the Grady and Kipp Model (see Fig. 16). The agreement with the experimental temperatures is fair.

At this point, calculations using the shear band model in MESA-2D give more consistent behavior than calculations without the model. However, calculated heat generation in the shear band, and thus shear band temperatures, fluctuate during a calculation (see Fig. 7). These variations may represent a stability problem, in which feedback between temperature (or energy generation) and flow stress lead to fluctuations in both quantities. Melting provides a damping mechanism, but there appears to be little damping below the melting point. This problem needs some consideration because the transition from heating in HE to detonation may be sensitive to small temperature variations.

THERMO-CHEMICAL MODEL FOR HE INITIATION

Localized high temperatures in a reactive material such as HE can lead to decomposition that further increases the temperature. At some point the heat release is fast enough to initiate an explosion or detonation. This process was demonstrated experimentally by Rogers (1975) for macroscopic samples of a number of common explosives. Rogers used his data to determine constants in an equation that relates the heat generation rate (Q') to the absolute temperature (T) for the explosives,

$$Q' = Q\, z\, e^{-E/RT}, \tag{16}$$

where Q (a heat of reaction), z (a pre-exponential factor), and E (an activation energy) are constants characteristic of each explosive and R is the gas constant (8.3144 J/mol K). Figure 17 shows a plot of Q' as a function of T for four common explosive materials (TNT, HMX, RDX, and TATB) calculated from Eq. (16).

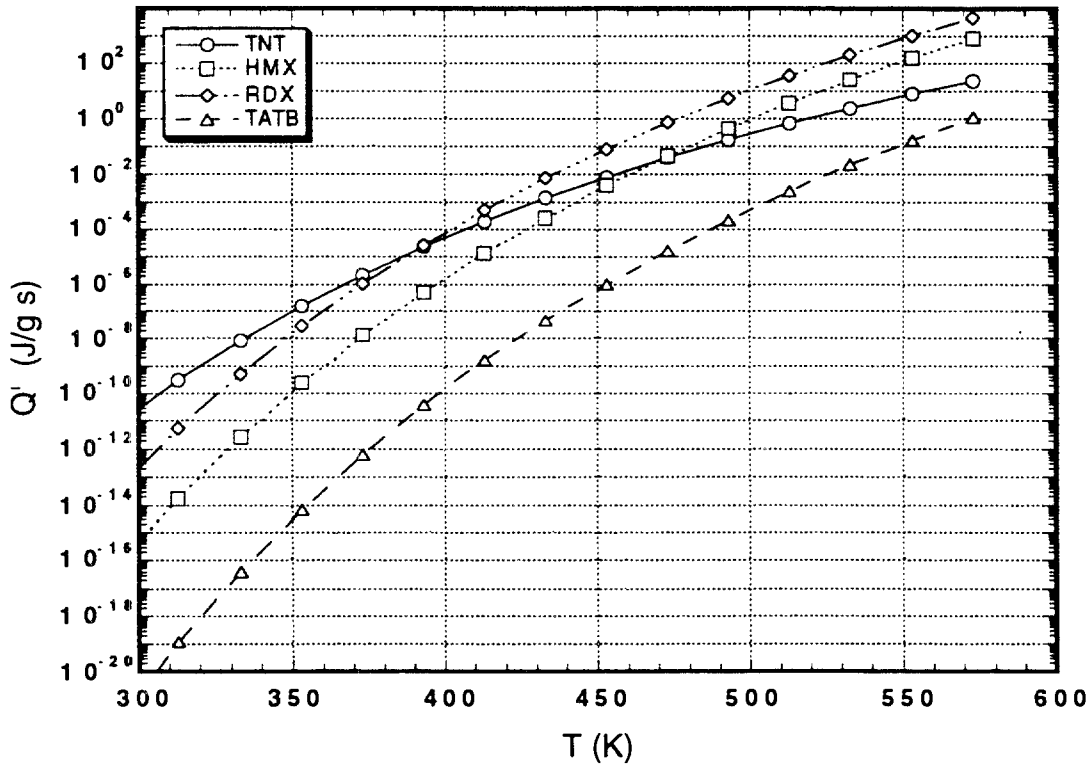

Fig. 17. Heat generation rate (Q') as a function of absolute temperature (T) for four common explosives from Rogers (1975).

The idea of a chemical heat release of the form of Eq. (16) was combined with a conductive heat-loss mechanism by Frank-Kamenetskii (1939, 1942) to show that when a high-enough temperature is reached in a particular geometry, there is no longer a mathematical solution to this problem. Dienes (1986) extended this formulation to include mechanical heating from plastic work in a shear band. This formulation is a steady-state model. Given a fixed geometric region (one-dimensional) of a reactive material (normally a slab, cylinder, or sphere), there is

a surface temperature above which a solution to the combined heat-generation (chemical and mechanical) and conductive heat-loss problem is no longer possible. Below this critical surface temperature, the one-dimensional temperature distribution in the region can be calculated; above the critical temperature, the temperature distribution cannot be calculated. The material properties (Q, z, E, and thermal conductivity), the mechanical heat generation rate (Q'_m), and the size of the region define the problem. Although this steady-state formulation already includes the effects of mechanical heating, incorporating it into the transient shear band model discussed above would be difficult.

Frank-Kamenetskii (1969) also describes a transient treatment for this problem. In the transient treatment, a one-dimensional region is assumed to have a uniform temperature. Based on the material properties (Q, z, E, thermal conductivity, and heat capacity) a characteristic heat transfer time (τ_q) and characteristic temperature rise time from the chemical heat generation (τ_{adHE}) can be defined as

$$\tau_q = \rho C_p r^2 / e \delta_{cr} k , \tag{17}$$

and

$$\tau_{adHE} = (C_p / Q z) (R T_0^2 / E) e^{-E/RT_0} , \tag{18}$$

where ρ is density, C_p is heat capacity, r is the characteristic size of the region (the distance from the center to the surface), k is thermal conductivity, δ_{cr} is 0.88 for planer systems, T_0 is the temperature of the surroundings, and e = 2.71828... The reduced temperature difference between the region and surroundings, θ, is defined as

$$\theta = E (T - T_0) / R T_0^2 . \tag{19}$$

Frank-Kamenetskii (1969) developed an equation for θ in terms of τ_q and τ_{adHE},

$$d\theta/dt = (e^{\theta} / \tau_{adHE}) - (\theta / \tau_q) , \tag{20}$$

and defined an induction time, τ_i, as

$$\tau_i = \int d\theta / [(e^{\theta} / \tau_{adHE}) - (\theta / \tau_q)] , \tag{21}$$

where the limits on the integral are from zero to infinity. In reduced form, this equation is

$$\tau_i / \tau_{adHE} = \int d\theta / [(e^{\theta}) - (\gamma \theta)] , \tag{22}$$

where $\gamma = \tau_{adHE} / \tau_q$. Figure 18 shows plots of τ_{adHE} as a function of T_0 for RDX and TNT (top) and τ_q as a function of r for typical HE properties. For these plots, Q, z, and E were taken from Rogers (1975), ρ = 1.715 g/cm^3, C_p = 1.2 J/g K, and k = 0.00219 w/cm K. Figure 19 show a plot of a numerical

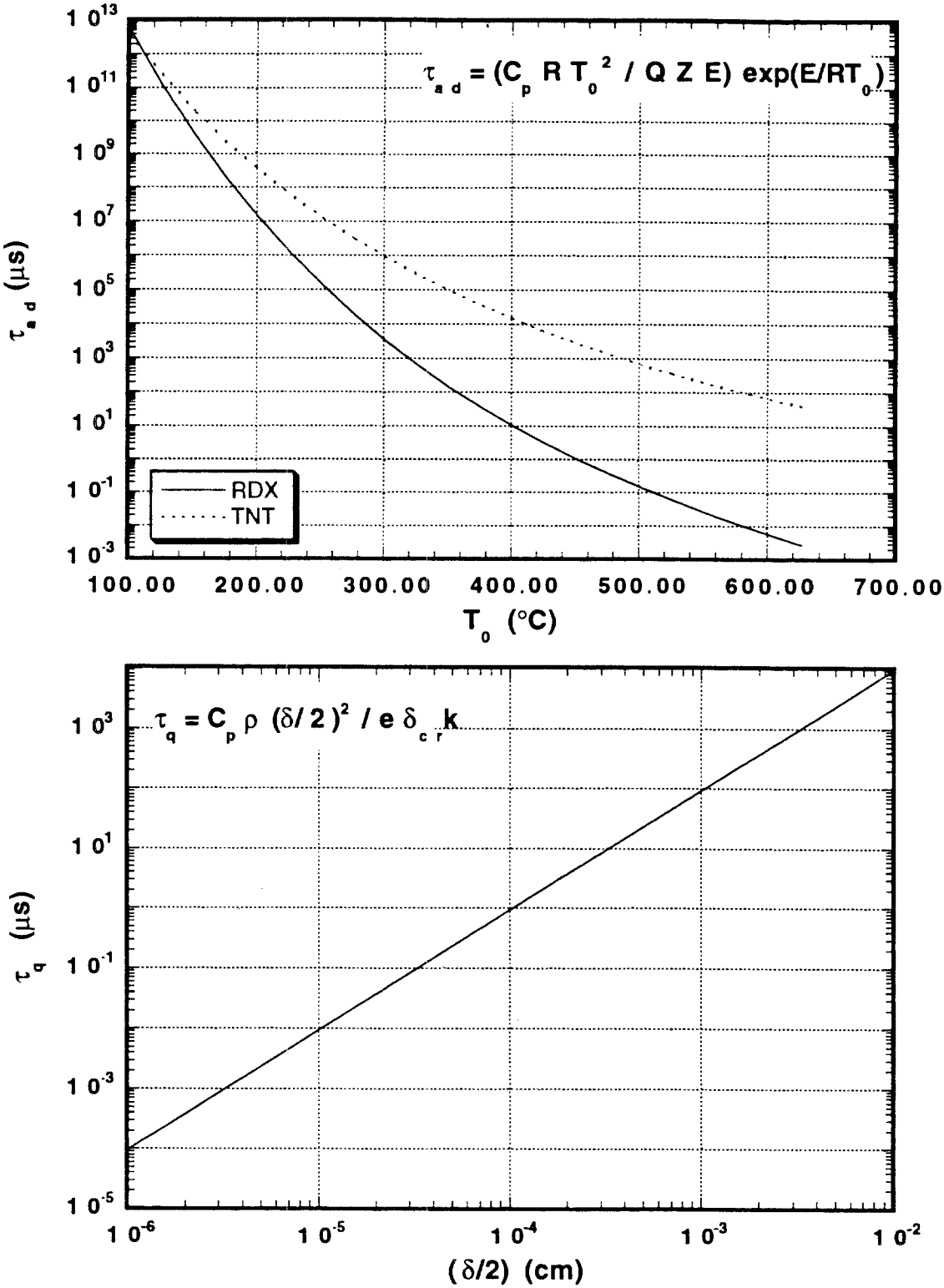

Fig. 18. τ_{adHE} as a function of T_0 for RDX and TNT (top) and τ_q as a function of r (bottom).

evaluation of (τ_i/τ_{adHE}) as a function of θ_{max}, where zero is the lower limit and θ_{max} is the upper limit of the integral in Eq. (22), for selected values of γ. Numerical evaluation of this integral is relatively easy; for practical values of the parameters, an upper limit of θ = ~5 can be used. Figure 20 shows (τ_i/τ_{adHE}) as a function of γ as calculated from a numerical evaluation of Eq. (22). As γ approaches e = 2.718... from below, (τ_i/τ_{adHE}) approaches infinity. Thus, for $\gamma > e$, no explosion occurs because the induction time is infinite. For $\gamma < e$, an explosion is possible.

The effect of mechanical heating can be included in this model in a manner analogous to the chemical heat generation. Define a characteristic temperature rise time from mechanical heating as

$$\tau_{adM} = (C_p / Q_M) (R T_0^2 / E) , \qquad (23)$$

where Q_M is the mechanical heating rate (in units of J/g s for example). The mechanical heating rate is assumed constant. Equation (20) is then modified to include this term as

$$d\theta/dt = (e^{\theta} / \tau_{adHE}) - (\theta / \tau_q) + (1 / \tau_{adM}) . \qquad (24)$$

Finally, the equation for the induction time in reduced units (Eq. 22) is given as

$$\tau_i / \tau_{adHE} = \int d\theta / [(e^{\theta}) - (\gamma \theta) + \beta] , \qquad (25)$$

where $\beta = \tau_{adHE} / \tau_{adM}$.

A graphical representation of the existence of an explosion limit that is inherent in Eq. (24) is shown in Fig. 21. The heavy line labeled exp(θ) in Fig. 21 represents the first term on the right-hand side in Eq. (24), the chemical heat generation term. If $\beta = 0$, the remainder of the terms on the right-hand side are represented by the solid lines in Fig. 21, labeled 1, 2, and 3. They are straight lines through the origin with slope γ. The line labeled 1 is, for some values of θ, above the heat generation curve. This implies that $d\theta/dt \leq 0$ for some θ and no explosion. The line labeled 3 is everywhere below the heat generation curve. This implies an explosion for this value of γ. The explosion limit is indicated by the line labeled 2, which is tangent to the chemical heat generation curve. This condition is defined by $e^{\theta} = \gamma \theta$ and $d(e^{\theta}) / d\theta = d(\gamma \theta) / d\theta$. The solution to these equations is $\theta = 1$ and $\gamma = e = 2.718...$

If β, which is never negative, is positive, the remainder of the terms on the right-hand side of Eq. (24) are represented by the dashed lines in Fig. 21, labeled 4 and 5. The magnitude of β represents an offset in the lines, which still have slope γ. The dashed line labeled 4 has the same slope as the line labeled 2. For β positive, this line is everywhere below the heat generation curve. Thus, adding mechanical heating ($\beta > 0$) would move the system from being just at the explosion limit to an explosion. The line labeled 5 is tangent to the chemical heat generation curve and is an explosion limit for this value of β. By the same

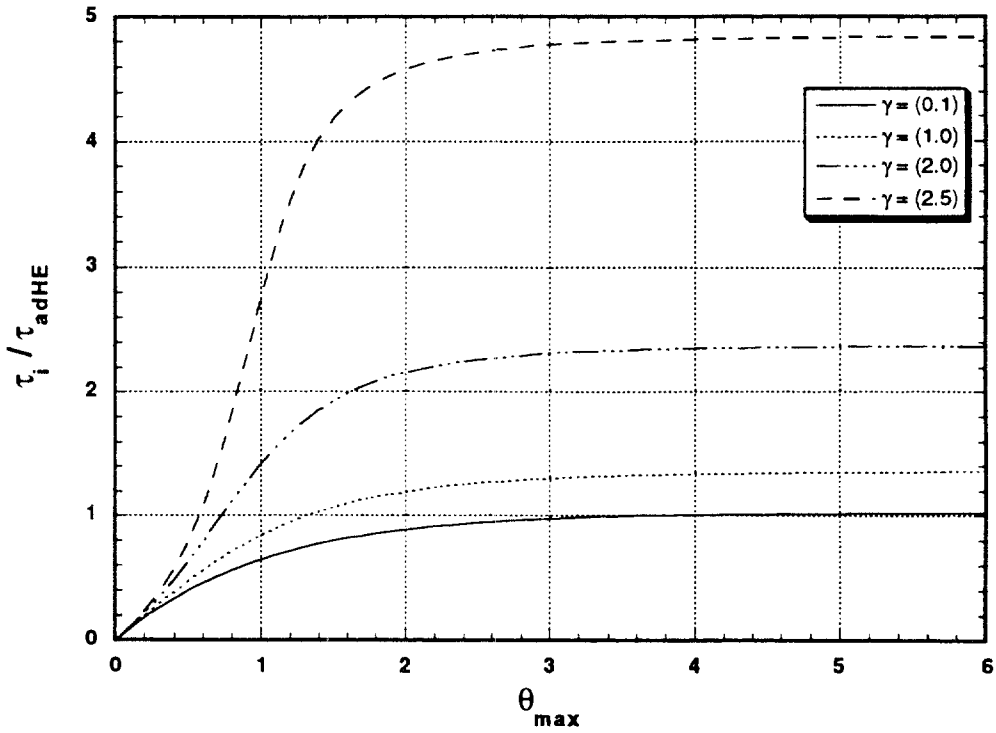

Fig. 19. (τ_i/t_{adHE}) as a function of θ_{max}, where zero is the lower limit and θ_{max} is the upper limit of the integral in Eq. (22).

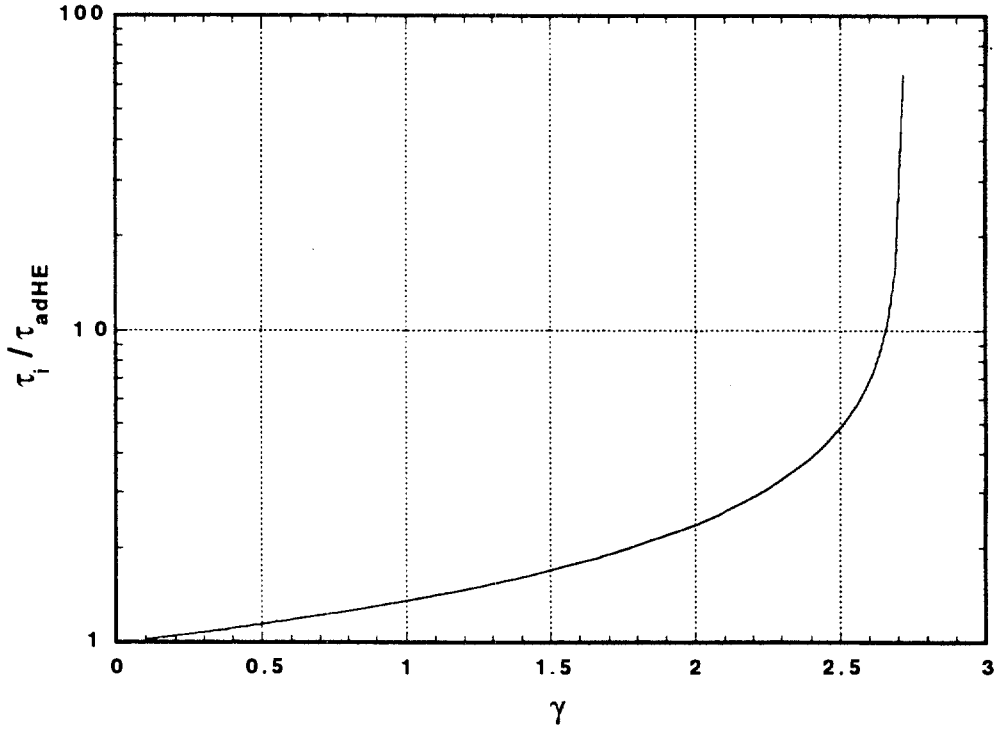

Fig. 20. τ_i/t_{adHE} as a function of γ as calculated from Eq. (22).

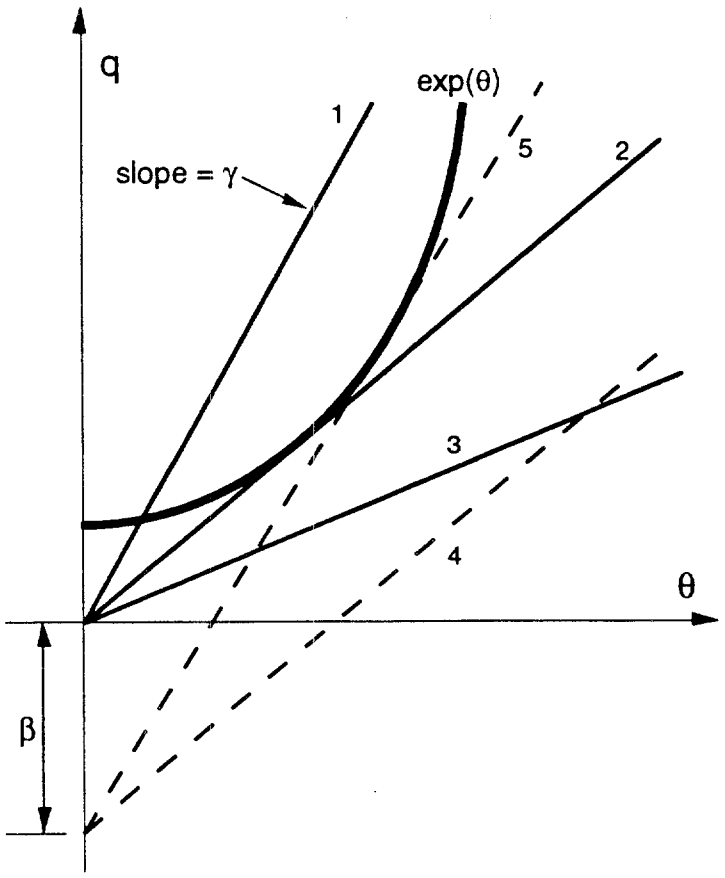

Fig. 21. Graphical representation of explosion limits from Eqs. (24) and (25).

reasoning as above, this condition is defined by $e^{\theta} = (\gamma\theta - \beta)$ and $d(e^{\theta}) / d\theta = d(\gamma\theta - \beta) / d\theta$. The solution of these equations is

$$\theta = \ln(\gamma) = 1 + (\beta/\gamma) \tag{26}$$

and

$$\beta = \gamma[\ln(\gamma) - 1]. \tag{27}$$

Thus, we have an explosion limit that is a function of the mechanical heat generation rate (represented by β). Figure 22 show the relation between β and γ that defines the explosion limit when mechanical heating is present. An explosion is possible if $\theta > \ln(\gamma)$ and $\beta > \gamma[\ln(\gamma) - 1]$. For β small (Q_M small), the explosion limit approaches $\gamma = e$.

Determining that an explosion is possible does not guarantee that the explosion will occur in a reasonable length of time. This is where an estimation of the induction period (Eq. 25) is required. Figure 23 is a plot of the induction period calculated from Eq. (25) for RDX for a region of characteristic size (r) 1×10^{-4} cm.

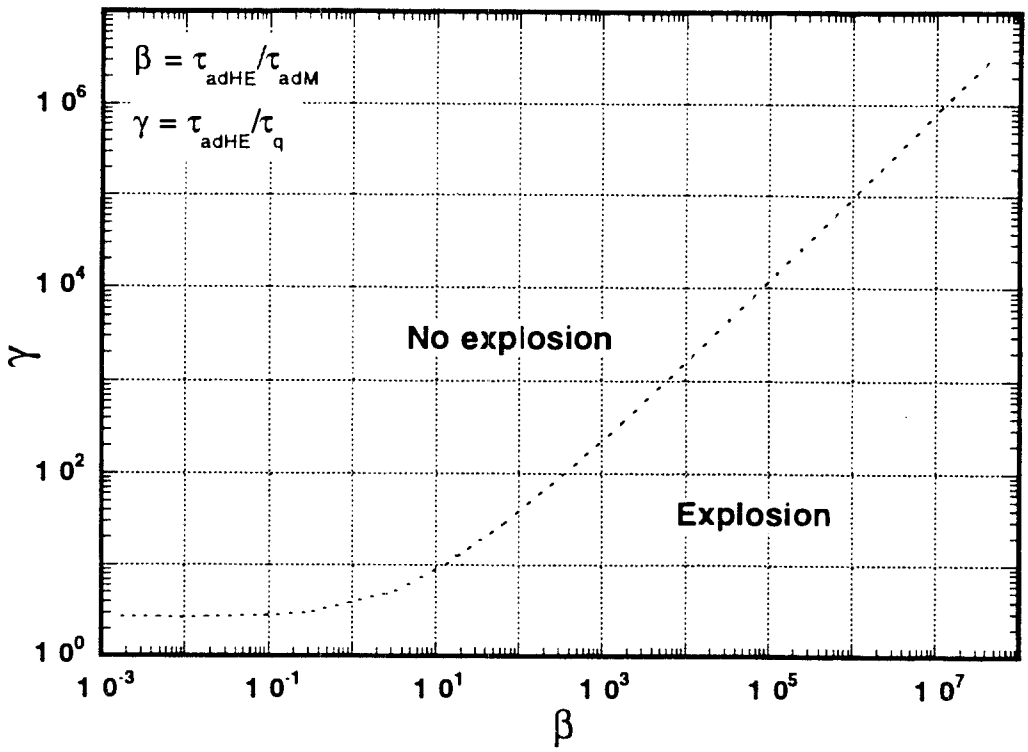

Fig. 22. Relation between β and γ that defined by Eq. (27).

For Q_M less than about 10 J/g μs, the induction period becomes infinite for T_0 equal to ~420 °C; thus, no explosion would occur below that temperature. For Q_M equal to 100 J/g μs, an explosion would not occur below ~320 °C. The shift is an indication that mechanical heat generation of this magnitude is beginning to affect the system. For Q_M equal to 300 J/g μs, an explosion would occur for T_0 less than 100 °C with an induction period of ~1 μs. At this level, mechanical heat generation dominates the system.

The method defined by Eqs. (23) through (26) was implemented in MESA-2D (see subroutine MUSER in Appendix). At each time step, the value of θ (defined in Eq. (19)) was calculated as

$$\theta = E\,(T_{max} - T_{cell}) / R\,T_{cell}^2 \quad , \tag{28}$$

where T_{max} and T_{cell} are defined in Fig. 1. In addition, Q_M is defined as ΔQ (see Eqs. (6)) and r is defined as δ (see Fig. 1). Values of γ and β are calculated from calculated values of τ_q, τ_{adHE}, and τ_{adM} (see Eqs. (17), (18), and (23)). If, based on the criteria of Eqs. (26) and (27), an explosion is possible, a value of τ_i is calculated from Eq.(25). Otherwise, τ_i is set to a large value. The fraction of HE reacted in each cell (f_{HE}) starts at zero at the beginning of a calculation and is incremented at each time step by

$$f_{HE}(new) = f_{HE}(old) + (dt / \tau_i) \quad , \tag{29}$$

where dt is the time step. If the value of f_{HE} becomes greater than 0.9, it is

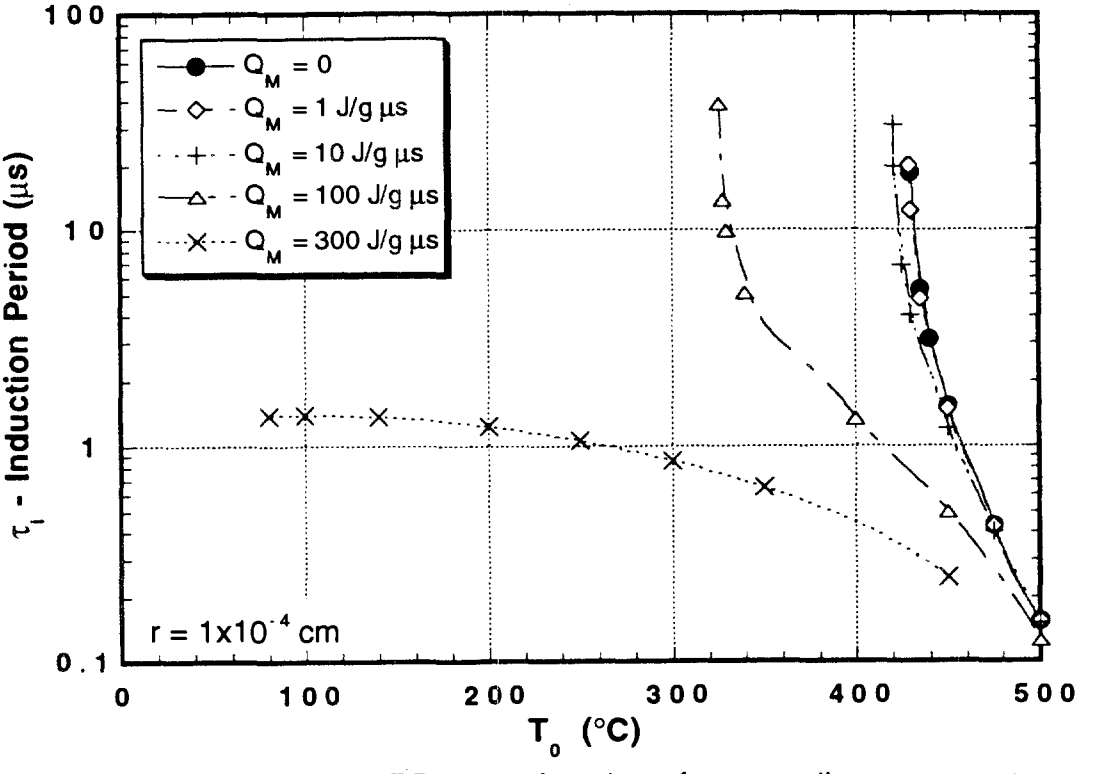

Fig. 23. Induction period for RDX as a function of surroundings temperature (T_0) for various values of Q_M.

assumed that all the HE in the cell reacts. This involves adding the reaction energy of the HE to the cell energy and replacing the EOS of the material in the cell with a JWL EOS for the HE.

TRANSITION TO DETONATION

The question of whether a group of cells, whose HE has reacted, will transition to a detonation is answered by use of the dynamic burn model already available in MESA-2D. In this model, unreacted HE in a cell reacts if the cell energy is greater than some predetermined amount (characteristic of the HE) and $d(q_{av}) / dt < 0$, where q_{av} is the artificial viscosity in the cell. Reaction consists of adding the reaction energy to the cell material and changing the EOS to a JWL for the HE. Thus, local material flow and shocks can influence cells adjacent to those that have reacted as a result of the shear band model. If the effects are large enough and over a large enough volume of material, reactions initiated by shear band formation can transition to a detonation.

RESULTS OF CALCULATIONS FOR REACTIVE MATERIAL

It has been more difficult to find experiments that can be used to test this model on reactive material. Most experiments are not two dimensional. One set of calculations was done to determine the threshold velocity needed to initiate a confined HE sample. The experiments are reported by Frey et al. (1979). They fired cylindrical steel projectiles of various mass into 105-mm artillery rounds containing Comp. B. They observed that the impact velocity needed to just

initiate the explosion was the ballistic limit of the projectile. This is a three-dimensional experiment. A two-dimensional version was used to test the shear band model discussed here. Figure 24 shows a sketch of the experiment as modeled. The model is axisymmetric so that the target is a sphere. For the calculations, the case was assumed to be 1006 steel and the projectile was assumed to be HY-130 steel. The Johnson-Cook (JC) strength model was used for both (Johnson and Holmquist 1989). The Comp. B was modeled as solid before reaction and with a JWL EOS after reaction. The JC strength model was also used for Comp. B. The JC parameters (see Eq. 2) were:

Y_0 = 0.00054 Mbar,
B = 0,
C = 0.1,
n = 1,
m = 1, and
melt energy = 9.4×10^{-4} Mbar-cc/g.

The strength parameters were estimated from the data of Pinto and Wiegand (1993) and Wiegand et al. (1991). Other parameters were:

$C_p = 1.2 \times 10^{-5}$ Mbar-cc/g K,
$k = 2.2 \times 10^{-14}$ Mbar-cc/cm s K, and
heat of melting = 5.9×10^{-4} Mbar-cc/g.

The viscosity of the Comp. B was estimated from the model proposed by Frey (1981) with his parameters. The chemical heat generation parameters for RDX were used (Rogers 1975).

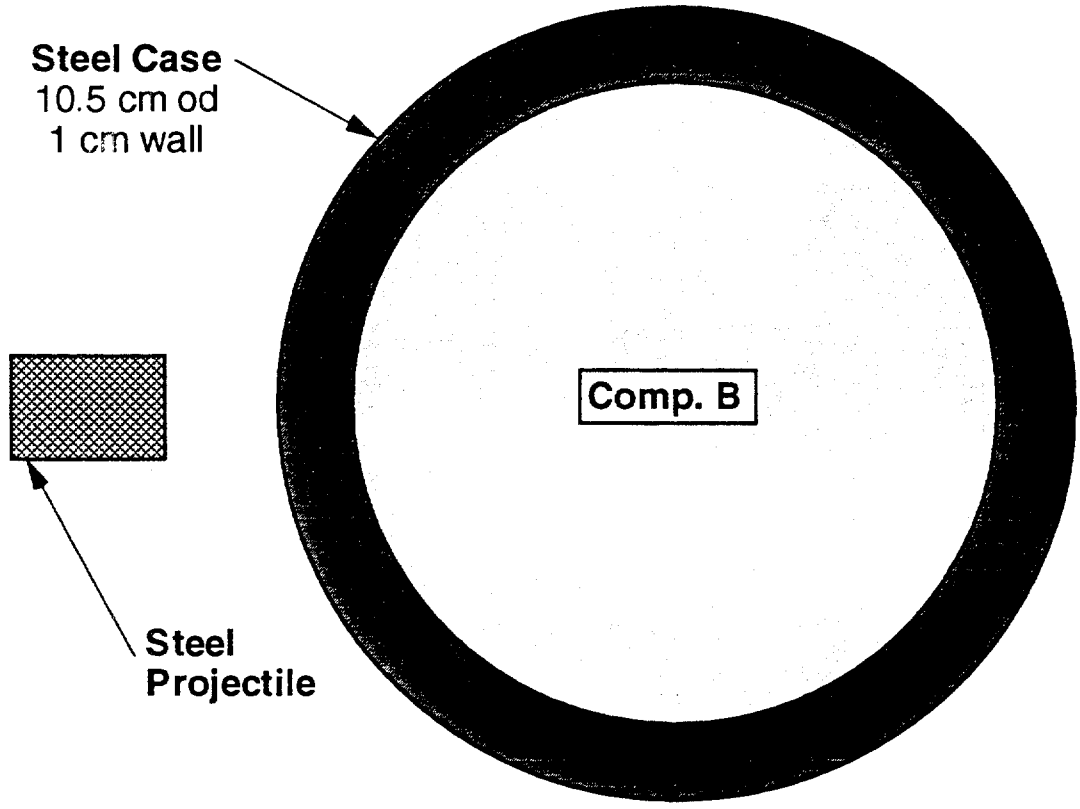

Fig. 24 Sketch of experiment used to model HE initiation.

Calculations were done for projectiles of mass 50 and 100 g with length/diameter ratio of 1. Figure 25 shows a plot of the maximum shear band temperature rise as a function of time for the impact of a 100-g projectile into the cased HE target shown in Fig. 24. Results for five impact velocities are shown. At 0.065 and 0.070 cm/μs there is no reaction of the HE. At 0.075 and 0.085 cm/μs, HE reaction starts and transitions to a detonation; this is indicated by the sharp rise in temperature at ~135 μs. These calculations were stopped at 150 μs. At 0.080 cm/μs the maximum temperature rise stays at ~100 °C (just above where the yield strength becomes zero); some HE reaction occurs, but it does not transition to a detonation. It is not clear why the behavior of the model is not more consistent at 0.075 and 0.080 cm/μs impact velocities.

Figure 26 shows a plot of projectile mass as a function of impact velocity in which results for the 50- and 100-g projectiles are shown compared with a line that defines the experimental no-explosion(lower velocity)/explosion transition (Frey et al. 1979). The calculated velocities at which reaction transitions to an explosion are higher than observed by Frey et al. (1979). However, the calculated transition velocities are about the ballistic limit for the conditions of the calculation. This difference may be related to an uncertainty in the properties of the steel case and projectile; they were not reported by Frey et al. (1979) so that the strength models noted above were only estimates. Calculations of the ballistic limit of 100-g projectiles into this target (with non-reactive HE) using a number of different strength models for the case and projectile showed that the ballistic limit was a strong function of the ratio of Y_0 of the projectile to Y_0 of the case (see Fig. 27).

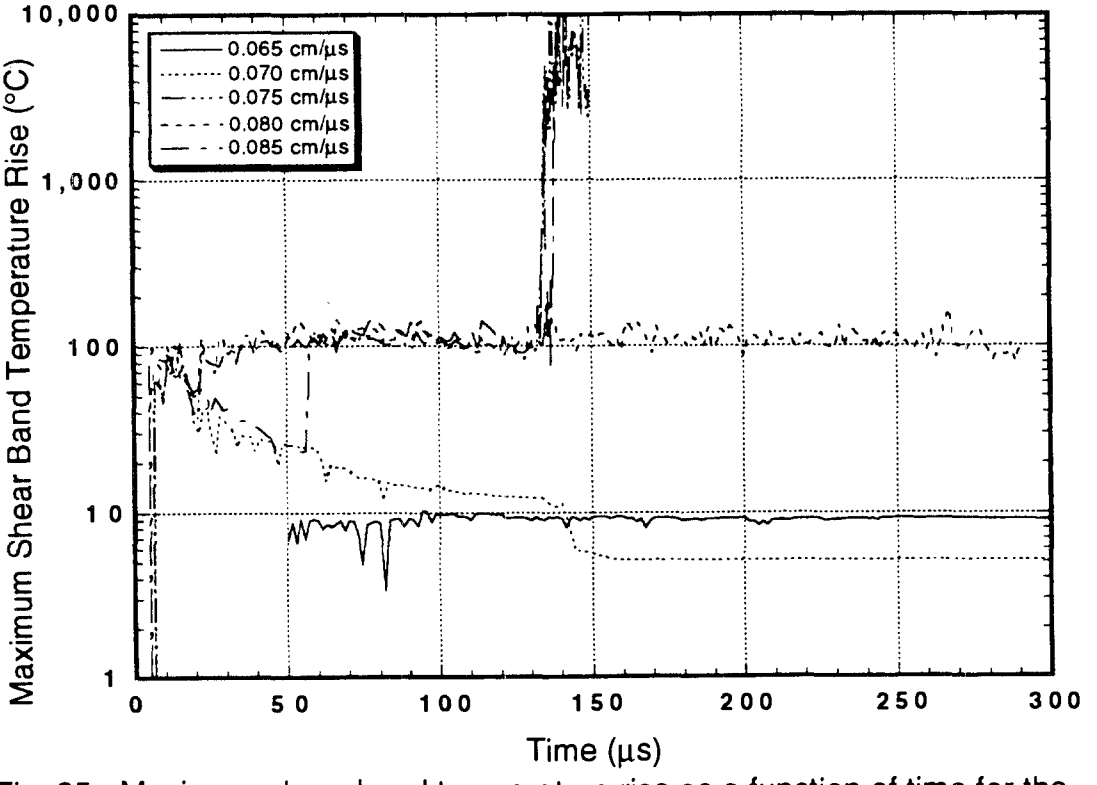

Fig. 25. Maximum shear band temperature rise as a function of time for the impact of a 100-g projectile into the cased HE target shown in Fig. 24.

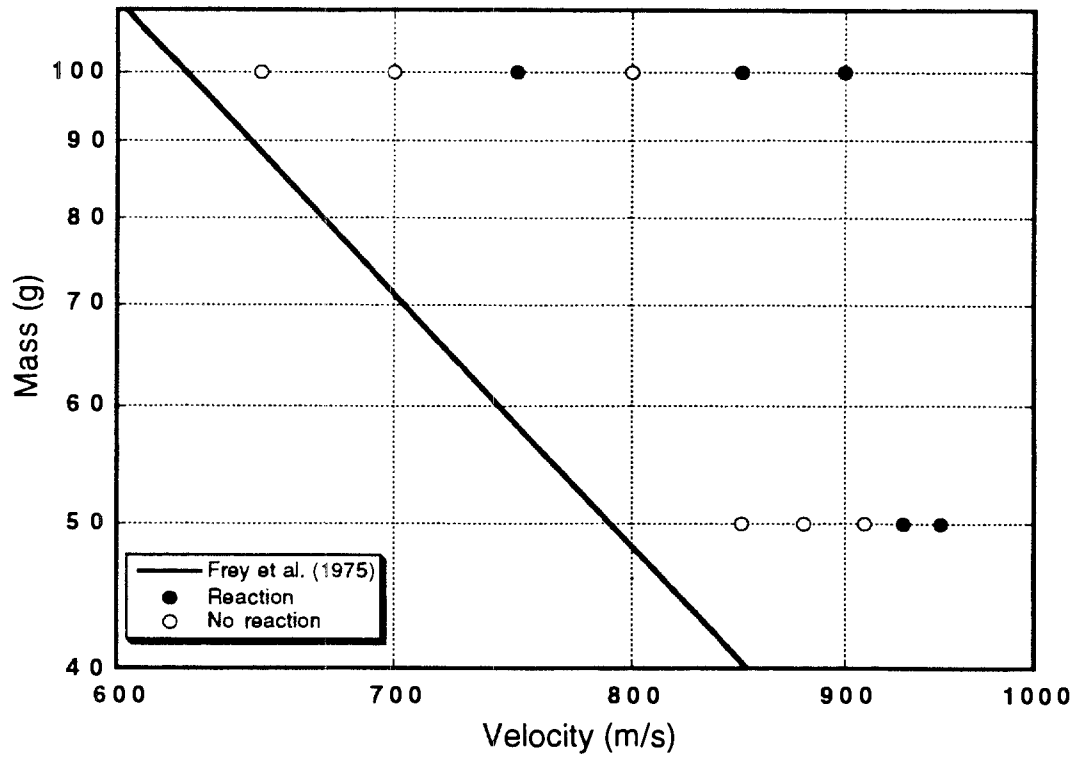

Fig. 26. Correlation of projectile mass and velocity that produces an explosion for the system shown in Fig. 24.

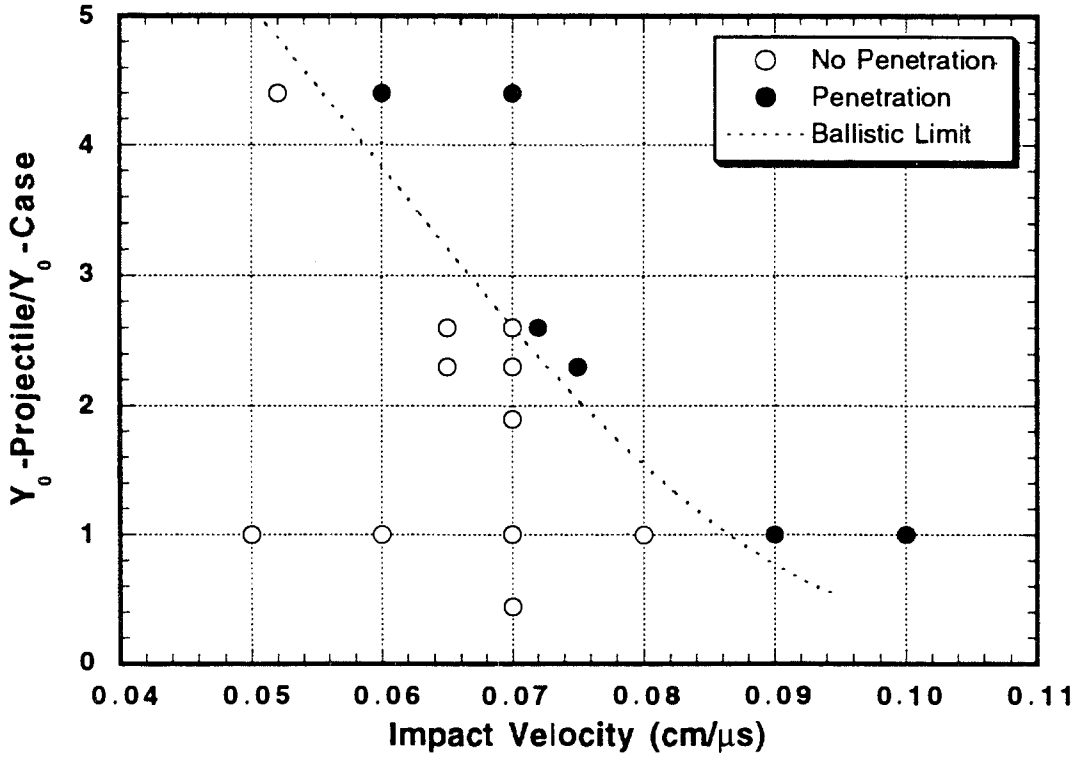

Fig. 27. Ballistic limit for a 100-g projectile impacting the target shown in Fig. 24. Y_0 is the JC strength parameter.

DISCUSSION

This report describes work in progress to develop a shear band model for MESA-2D. The object of this work is (1) to predict the formation of shear bands and their temperature in high explosive (HE) during a MESA-2D calculation, (2) to then assess whether the HE would initiate, and (3) to allow a detonation wave initiated from a shear band to propagate. This is a very complex process and has necessitated many approximations to complete a working model. The approach of coupling the model to a hydrocode was taken to allow calculations of realistic accident situations to be made.

The mechanisms are in place to do calculations of realistic experiments such as that shown in Fig. 24. However, many of the parameters needed to complete the calculations are unknown and must be estimated. Until independent data on items such as the strength, thermal properties, or viscosity of HE are known, this approach to modeling HE initiation cannot be realistically tested.

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APPENDIX

The appendix contains a listing of the main routines added to MESA-2D to perform the shear band calculations. In addition to these routines, modifications were made to the MESA-2D subroutines that calculate yield strength and that advect cell variables. Four cell variables associated with the shear band model were advected in the same manner as energy: shear band temperature (tsb), shear band size (sbs), heat flux for the temperature distribution model (qsb), and fraction of HE reacted in a cell (fherx).

```
      subroutine muserb

c-----------------------------------------------------------------------
c     user initialization routine
c-----------------------------------------------------------------------

*call basic
*call burn
*call str
*call strength
*call eos
c     jfk shear band model3
*call shband
*call fylnames

c     jfk shear band model3
c
c     check ispare2 to ispare5 for setting limits on shear band model
c     ispare2 and ispare3 set limits on radial direction
c     ispare4 and ispare5 set limits on axial direction
c     if zero, set to whole mesh
      if(ispare2 .eq. 0 .and. ispare3 .eq. 0) then
         ispare2 = 1
         ispare3 = ncr
      endif
      if(ispare4 .eq. 0 .and. ispare5 .eq. 0) then
         ispare4 = 1
         ispare5 = ncz
      endif
c
c     check ispare8 - if 0 use msband, if 1 use msband1
      if(ispare8 .lt. 0) ispare8 = 0
c     check for existing file with shear band data
c     if isparel .lt. 0, look for shear band data file called sbandata
      if(isparel .lt. 0) then
         isparel = iabs(isparel)
         open(unit=15,file='sbandata',status='old',err=20,iostat=ios)
         read(15,*) ncinp
         if(ncinp .ne. nc) go to 30
```

```
         read(15,10) (tsb(i,1),i=1,nc)
         read(15,10) (sbs(i,1),i=1,nc)
         read(15,10) (qsb(i,1),i=1,nc)
         read(15,10) (fherx(i,1),i=1,nc)
   10    format(1p10e15.6)
         close(15)
      else
c     zero shear band temperatures and total plastic work at start of calc
         do 50 i=1,nc
         tsb(i,1) = 0.0
         qsb(i,1) = 0.0
         plwo(i,1) = 0.0
         qpold(i,1) = 0.0
         fherx(i,1) = 0.0
   50    continue
      endif

c     open file to write shear band  data
      fyl(15) = 'sbnd_'//suf
      open(unit=15,file=fyl(15),status='unknown',err=22,iostat=ios)

      write(15,55) title
   55 format(a)

      write(15,57)
   57 format(/' data are:'/
     &        ' line 1: t,isb,i,j,tsb,tcell,sbs,qsb,denr,plwk,plst'/
     &        ' line 2: t,$2,i,j,dplwx,dvswx,fren,tred,tadhe,tadm,',
     &        'fherx')

      go to 9999

   20 write(*,21)
   21 format(' shear band data file (shbandata) not found')
      call crash(' missing shear band data file')
      go to 9999

   22 write(*,23)
   23 format(' problem opening shear band data file to write data')
      call crash(' problem opening shear band data file to write data')
      go to 9999

   30 write(*,31) ncinp,nc
   31 format(' ncinp = ',i5,' is not equal to nc = ',i5)
      call crash(' mismatch on shear band data dimension')

 9999 continue
      end


      subroutine muser

c-----------------------------------------------------------------------
c     user routine
c-----------------------------------------------------------------------

*call basic
*call burn
*call str
*call strength
```

```
*call eos
c     jfk shear band model3
*call shband
      dimension il(13),jl(13)
c
      common /tdmod/  fac1(4),fac2(4),fac3(4),facdelt,mmm
c
c     set up order to get cells to average plastic work
      data il /0,0,1,0,-1,1,1,-1,-1,2,0,-2,0/
      data jl /0,-1,0,1,0,-1,1,-1,1,0,-2,0,2/

c     jfk shear band model3
c
c     use ispare and rspare to input general data
c     ispare1 = material number of shear band material
c     ispare2 and ispare3 = lower and upper i cell index limits for sb model
c     ispare4 and ispare5 = lower and upper j cell index limits for sb model
c     ispare6 = print interval to shear band file - print every ispare6 time
        steps
c     ispare7 = control of velocity of a specific material
c               0 = do not change material velocities
c               .gt. 0 then
c                     set r vel of mat ispare7 to rspare1
c                     set z vel of mat ispare7 to rspare2
c     rspare1 = r velocity
c     rspare2 = z velocity
c     rspare3 = value of artificial viscosity above which to skip shear band
        calc
c     ispare8 = shear band model control
c             = 0 = use temp distribution model (call msband)
c             = 1 = use grady-kipp model (call msband1)
c     ispare9 = number of surrounding cells to average for plastic work
c               use 1, 5, 9, or 13
c
c     use strcon variables to input data
c     strcon(8,m) = d(melt temp)/d(pressure) (dmdd)
c     strcon(9,m) = heat capacity (cv)
c     strcon(10,m) = thermal diffusivity (thdiff)
c     strcon(11,m) = minimum yield strength (ymin)
c     strcon(12,m) = thermal conductivity (xk)
c     strcon(13,m) to strcon(16,m) = 4 constants in viscosity correlation
c                                  = avis, bvis, cvis, dvis
c     strcon(17,m) = time to start shear band model (tstart)
c     strcon(18,m) = heat of melting (qmelt)
c     strcon(19,m) = pre-exponential factor in he heat release relation (qz)
c     strcon(20,m) = activation energy/gas constant in he heat rel. relation
        (eor)
c      strcon(21,m) = max number of times to call subroutine react before
        quitting

c     set data print control
      if(ispare6 .le. 0) then
         iprtmod = 10
      else
         iprtmod = ispare6
      endif
      iprt = mod(istep,iprtmod)

      if(ispare1 .le. 0) go to 9999
```

```
c     set up initial parameters for shear band model 3
      m = isparel
c     check if time to start yet
      tstart = strcon(17,m)
      if(t .lt. tstart) go to 9999
      dmdd = strcon(8,m)
      cv = strcon(9,m)
      thdiff = strcon(10,m)
      xk = strcon(12,m)
      am = strcon(4,m)
      if(ideos(m) .eq. 9 .or. ideos(m) .eq. 13) then
         tmelt = strcon(5,m)
         troom = strcon(6,m)
      else
         tmelt = strcon(5,m)/cv
         troom = strcon(6,m)/cv
      endif
      if(tmelt .le. 1.0e-9) tmelt = 1.0e-9
      if(troom .lt. 0.0) troom = 0.0
      dtm = tmelt - troom + zeps
      if(dtm .gt. 25.0) then
         dtlim = dtm
      else
         dtlim = 25.0
      endif
c     coefficients for viscosity correlation
      avis = strcon(13,m)
      bvis = strcon(14,m)
      cvis = strcon(15,m)
      dvis = strcon(16,m)
c     heat of melting
      qmelt = strcon(18,m)
      if(qmelt .lt. 0.0) qmelt = 0.0
      if(dvis .le. 0.0) dvis = 1.0e+20
      if(xk .le. 0.0) then
         write(*,20)
   20    format(' thermal cond of shear band material .le. 0')
         call crash(' thermal cond of shear band material .le. 0')
      endif
c     set constants for he energy release correlation
      qz = strcon(19,m)
      eor = strcon(20,m)
      ictmax = ispare9
      if(ictmax .lt. 1) ictmax = 1
      if(ictmax .gt. 13) ictmax = 13
c
      artvislim = rspare3
      if(artvislim .le. 0.0) artvislim = 1.0e+99
      if(artvislim .lt. 1.0e-10) artvislim = 1.0e-10
c     set tsbmax, isbmax, and jsbmax to 0
      tsbmax = 0.0
      isbmax = 0
      jsbmax = 0
c
      if(strcon(21,m) .gt. 1.0) then
         maxreact = ifix(1.000001*strcon(21,m))
      else
         maxreact = 100000
      endif
c
```

```
      iquit = 0
c
c     get list of cells with material m
      call wheneq(nc,lf,1,m,ix,nx)

c     loop on cells
      do 50 l = 1,nx
      n = ix(l)

      if(lf(n,1) .gt. 0 .and. q(n,1) .lt. artvislim) then

         j = (n-1)/ncr + 1
         i = n - (j-1)*ncr
c     check limits for application of shear band model - skip if outside
         if(i .lt. ispare2 .or. i .gt. ispare3) go to 50
         if(j .lt. ispare4 .or. j .gt. ispare5) go to 50
c     calc average cell size
         cellsize = sqrt(cdr(i)*cdz(j))
c     if(sbs(n,1) = 0, set it to cellsize - usually at first time through
         if(sbs(n,1) .le. 0.0) sbs(n,1) = cellsize

         if(ideos(m).eq.9 .or. ideos(m).eq.13) then
            tcell = th(n,1)
         else
            tcell = (e(n,1)/cv)
         endif
         if(tsb(n,1) .eq. 0.0) tsb(n,1) = tcell
c     dplwx is the rate at which plastic work is generated in the shear band
c     assume 1/2 the plastic work goes in each direction from the shear band
c     skip first time to eliminate problems with restart
c     zero dplwx if tsb from last time .gt. tmelt
         if(tsb(n,1) .lt. tmelt) then
            if(plwo(n,1) .gt. 0.0) then
               if(ictmax .gt. 1) then
                  isum = 0
                  dplwx = 0.0
                  sumvol = 0.0
                  do 25 ict = 1,ictmax
                     ii = min(max(1,i+il(ict)),ncr)
                     jj = min(max(1,j+jl(ict)),ncz)
                     nn = ncr*(jj-1) + ii
                     if(lf(nn,1) .eq. m .and. plwo(nn,1) .gt. 0.0) then
                        dplwx = dplwx + 0.5*(plwk(nn,1)-plwo(nn,1))
     &                                 *vol(nn,1)
                        sumvol = sumvol + vol(nn,1)
                        isum = isum + 1
                     endif
                     if(isum .ge. 9) go to 27
   25                continue
   27                if(sumvol .gt. 0.0) then
                        dplwx = dplwx/(sumvol*dth)
                     else
                        dplwx = 1.0e-10
                     endif
                  else
                     dplwx = 0.5*(plwk(n,1)-plwo(n,1))/dth
                  endif
               else
                  dplwx = 1.0e-10
               endif
```

```
            else
               dplwx = 0.0
            endif
            if(dplwx .lt. 0.0) dplwx = 0.0
c        dplwx is plastic work rate in mbar-cc/microsec-cc
         if(sbs(n,1) .gt. 0.0) then
            dplwx = dplwx*d(n,1)*cellsize/sbs(n,1)
         else
            dplwx = dplwx*d(n,1)
         endif
c
c        only begin to calc viscous energy dissapation if temp is near tmelt
c        dvswx is the rate at which viscous shear energy is dissapated
c        assume 1/2 the energy goes in each direction from the shear band
c        calc velocity gradients needed
c        nn is the equivalent to n that would give the correct i and j
c           for nvr rather than ncr as the first dimension
c        (nn,1) = (i,j),  (nn+1,1) = (i+1,j),  (nn+nvr,1) = (i,j+1)
c        (nn+nvr+1,1) = (i+1,j+1)
         if(tsb(n,1) .gt. 0.90*tmelt) then
            nn = n + j - 1
c        vgrad is velocity gradient in shear in units of 1/microsec
            vgrad=(uz(nn+1,1)+uz(nn+nvr+1,1)-uz(nn,1)-uz(nn+nvr,1))/cdr(i)
     &           +(ur(nn+nvr,1)+ur(nn+nvr+1,1)-ur(nn,1)-ur(nn+1,1))/cdz(j)
c        scale vgrad to shear band width
            if(sbs(n,1) .gt. 0.0) vgrad = vgrad*cellsize/sbs(n,1)
c        set tsb in kelvins for viscosity calculation
            if(ideos(m).eq.9 .or. ideos(m).eq.13) then
               tsbk = tsb(n,1)
            else
               tsbk = tsb(n,1) + 300.0
            endif
c        pvisc is pressure to use in viscosity correlation - limit to 20 kbar
            pvisc = max(0.0,min(0.02,p(n,1)))
c        visc is viscosity units of mbar-microsec
            visc = avis*exp((bvis/tsbk) - cvis)*exp(pvisc/dvis)
c        dvswx is viscous heating in shear band in units of mbar-cc/microsec-cc
            dvswx = 0.5*visc*((0.5*vgrad)**2)
c        phase in viscous heating from 0.9*tmelt to tmelt
c        fren is fraction of viscous heating to add to shear band energy
            if(tsb(n,1) .lt. tmelt) then
               fren = 10.0*((tsb(n,1)/tmelt) - 0.9)
            else
               fren = 1.0
            endif
         else
            dvswx = 0.0
            fren = 0.0
         endif

c        calc energy dissapation rate for shear band
c        units of denr and denrn are mbar-cc/microsec-cc
         denrn = dplwx + (fren*dvswx)
c        average of last and this value if tsb .lt. tmelt
         if(tsb(n,1) .lt. tmelt) then
            denr = 0.5*(denrn + qpold(n,1))
         else
            denr = denrn
         endif
         if(denr .lt. 0.0) denr = 0.0
```

```
c     save current value of denrn
      qpold(n,1) = denrn

c     only go into shear band model if cell is undergoing plastic work
c     and shear band stability criterion is met
c     isb = 0 means shear band has not yet formed
c     isb = 1 means shear band growth active
c     isb = 2 means no plastic work or dyde is positive, but allow decay
c             of existing temperature distribution
         if(strt(n,1) .gt. 0.0 .and. dyde(n,1) .lt. 0.0 .and.
     &      denr .gt. 0.0) then
            isb = 1
c     qsb = is the integrated heat flux for temp dist model
            qsb(n,1) = qsb(n,1) + (dth*denr)
c     calc qp and qpint as energy/(area time) = mbar-cc/microsec-cm**2
c     for use in temperature distribution model (sub msband)
c     need to change for grady-kipp model (sub msbandl)
c     qp = denr*(shear band vol)/(shear band area)
c        = denr*sbs*cellarea/cellarea = denr*sbs
            qp = denr*sbs(n,1)
            qpint = qsb(n,1)*sbs(n,1)
         elseif(tsb(n,1) .gt. 1.001*tcell) then
            isb = 2
            qp = 0.0
            qpint = 0.0
         else
            isb = 0
            qp = 0.0
            qpint = 0.0
            tsb(n,1) = tcell
            go to 50
         endif
c     calc delt if nothing done
         delto = tsb(n,1) - tcell
         if(delto .lt. 0.0) delto = 0.0

         if(ispare8 .eq. 0) then

c     calc shear band size and temperature from heat flux on a central
c     plane using integral method
            call msband(isb,thdiff,xk,qp,qpint,sbs(n,1),sbsn
     &           ,dth,delto,deltn)

         elseif(ispare8 .eq. 1) then

            tstar = (tsb(n,1) - troom)/(tmelt - troom)
            tstar = max(0.0, min(1.0,tstar))
            fmelt = 1.0 - tstar**max(0.01,am)
            if(fmelt .gt. 0.0 .and. tstar .gt. 0.0) then
               dydt = am*(1.0-fmelt)/(fmelt*dtm*tstar)
               ysh = ysv(n,1)/1.732050808
            else
               dydt = 1.0e-12
               ysh = 1.0e-6
            endif
c     units of denrgk are mbar-cc/microsec-g
         denrgk = denr/(sbs(n,1)*d(n,1))

c     calc shear band size and temperature using grady & kipp model
            call msbandl(d(n,1),cv,thdiff,ysh,dydt,strt(n,1),sbs(n,1),
```

```
     &          sbsn,denrgk,dth,cellsize,delto,deltn)

          else

             sbsn = cellsize
             deltn = 0.0
          endif

c      check if temp is in or above melting range
c      limit temperatrue rise to account for heat of melting
c      assume melting takes place over range from 0.99*tmelt to 1.01*tmelt
c
          tm1 = 0.99*tmelt
          tm2 = 1.01*tmelt
          qm1 = cv*tm1
          qm2 = (cv*tm2) + qmelt
          dqm = qm2 - qm1
          if(tsb(n,1) .le. tm1) then
             qold = cv*tsb(n,1)
          elseif(tsb(n,1) .gt. tm1 .and. tsb(n,1) .lt. tm2) then
             qold = qm1 + ((tm2-tsb(n,1))*dqm/(tm2-tm1))
          else
             qold = qm2 + (cv*(tsb(n,1) - tm2))
          endif
c
          qnew = qold + cv*(deltn - delto)
c
          if(qnew .gt. qm1 .and. qnew .lt. qm2) then
             deltn = ((qnew-qm1)*(tm2-tm1)/dqm) + tm1 - tcell
          elseif(qnew .ge. qm2) then
             deltn = tm2 + ((qnew-qm2)/cv) - tcell
          endif
c
c      damp change in temperature near tmelt of for large deltn
c
          tsbn = tcell + deltn
          if(tsb(n,1) .gt. 0.7*tmelt .or. tsbn .gt. 0.7*tmelt
     1       .or. deltn .gt. 0.1*dtlim) then
             if(deltn .ge. delto .and. delto .gt. 0.0) then
                rfac = (deltn/delto) - 1.0
             elseif( deltn .lt. delto .and. deltn .gt. 0.0) then
                rfac = (delto/deltn) - 1.0
             elseif( delto .eq. 0.0 .and. deltn .gt. 0.1*dtlim) then
                rfac = (deltn/0.1*dtlim) - 1.0
             else
                rfac = 0.0
             endif
          else
             rfac = 0.0
          endif
          deltn = delto + ((deltn - delto)/(1.0+rfac))
c
c      calc new shear band temp and shear band size
c
          if(deltn .gt. 0.0) then
             tsb(n,1) = tcell + deltn
          else
             tsb(n,1) = tcell
          endif
c      limit shear band size to cell width
```

```
         if(sbsn .lt. cellsize) then
            sbs(n,l) = sbsn
         else
            sbs(n,l) = cellsize
         endif
c
c     check for heat release from shear band material
c
      if(qz .gt. 0.0 .and. tsb(n,l) .gt. 1.0001*tcell) then
c
c     set cell temp in k
         if(ideos(m).eq.9 .or. ideos(m).eq.13) then
            tcellk = tcell
         else
            tcellk = tcell + 300.0
         endif
c
c     frank-kamenetskii induction period model

         t2eor = tcellk*tcellk/eor
         tredfk = deltn/(t2eor*facdelt)
         if(tredfk .gt. 1.0) then
            tadhe = (cv*t2eor/qz)*exp(eor/tcellk)
            tq = (d(n,l)*cv/(2.3921*xk))*((sbsn/fac3(mmm))**2)
            gamma = tadhe/tq
            if(denr .gt. 0.0) then
c     denr is in mbar-cc/microsec-cc in the shear band
               tadm = cv*t2eor*d(n,l)/denr
               betta = tadhe/tadm
            else
               tadm = 1.0e+99
               betta = 0.0
            endif
            betalim = gamma*(alog(gamma) - 1.0)
            if(betta .gt. betalim .and. tredfk .gt. alog(gamma)) then
               call integ(betta,gamma,value)
               tind = tadhe*value
               fherx(n,l) = fherx(n,l) + (dth/tind)
               if(fherx(n,l) .gt. 1.0) fherx(n,l) = 1.0
               if(fherx(n,l) .gt. 0.9) call react(maxreact,iquit)
            endif
         else
            tadhe = 1.0e+99
            tadm = 1.0e+99
         endif
c
      endif

c     write data to file
            if(iprt .eq. 0) then
               write(15,40) t,isb,i,j,tsb(n,1),tcell
     &            ,sbs(n,l),qsb(n,l),denr,plwk(n,l),plst(n,l)
               write(15,41) t,i,j,dplwx,dvswx,fren,tredfk,tadhe
     &             ,tadm,fherx(n,l)
            endif
   40       format(1pe13.5,3i5,1p7e13.5)
   41       format(1pe13.5,"   $2",2i5,1p7e13.5)

c
c     check for maximum tsb and save data
```

```
         if(tsb(n,1) .gt. tsbmax) then
            tsbmax = tsb(n,1)
            isbmax = i
            jsbmax = j
         endif

      endif

   50 continue
c
c     print max data if set
      if(isbmax .gt. 0) write(15,55) t,isbmax,jsbmax,tsbmax
   55 format(1pe13.5,"   $4",2i5,1pe13.5)

c     update saved plastic work
      do 70 i=1,nc
      plwo(i,1) = plwk(i,1)
   70 continue
c
      if(iquit .eq. 1) then
         call mxit('maximum react calls')
         call crash('job terminated with max calls to react')
      endif

 9999 continue
      end


      subroutine musere

c-----------------------------------------------------------------------
c     user wrap-up routine
c-----------------------------------------------------------------------

*call basic
*call burn
*call str
*call strength
*call eos
c     jfk shear band model3
*call shband
*call fylnames

c     jfk shear band model3
c     write shear band temperature and size to file
      write(15,8)
    8 format(/' restart data for file sbandata')
      write(15,*) nc,t
      write(15,10) (tsb(i,1),i=1,nc)
      write(15,10) (sbs(i,1),i=1,nc)
      write(15,10) (qsb(i,1),i=1,nc)
      write(15,10) (fherx(i,1),i=1,nc)
   10 format(1p10e15.6)
      close(15)
      go to 9999

 9999 continue
      end
```

```
      subroutine mvelusr (uu, vv)

c=======================================================================
c     This empty subroutine is provided for the user to write special
c     code for non-standard velocities (at the boundary, etc.).
c=======================================================================

*call basic
*call lagcom
*call str
*call strength
*call eos

      dimension uu(nvr,nvz), vv(nvr,nvz)

c     set boundary velocities for shear band problem
c     only if ispare7 .gt. 0
      if(ispare7 .gt. 0) then
         do 50 j = 1,ncz
         do 49 i = 1,ncr
            if(lf(i,j) .eq. ispare7) then
               uu(i,j) = rspare1
               uu(i,j+1) = rspare1
               uu(i+1,j) = rspare1
               uu(i+1,j+1) = rspare1
               vv(i,j) = rspare2
               vv(i,j+1) = rspare2
               vv(i+1,j) = rspare2
               vv(i+1,j+1) = rspare2
            endif
   49    continue
   50    continue
      endif

 9999 continue
      end


      subroutine msband(isb,thdiff,xk,qp,qpint,sbso,sbsn
     &      ,dth,delto,deltn)

c     sub to calculate shear band temperature distribution
c     and size from temperatures
c     assume polynomial distribution with integral method of
c     approximating temperature distribution from time varying
c     heat flux at a surface into an infinite medium
c     m is the order of the polynomial
c     set up for m = 1, 2, 3, or 4 only

      common /tdmod/  fac1(4),fac2(4),fac3(4),facdelt,m

c     m is the order of the polynomial approx to the temp distribution
c     fac1 = m
c     fac2 = m*(m+1)
c     fac3 = 2*(1 - (0.5**(1/m)))
      data fac1 / 1.0, 2.0, 3.0, 4.0 /
      data fac2 / 2.0, 6.0, 12.0, 20.0 /
      data fac3 / 1.0, 0.5857, 0.4126, 0.3182 /
      data m / 3 /
```

```
c     facdelt = fraction of total delt to return
      data facdelt / 0.75 /

c     calculate scale length
c     this is the penetration depth of the temperature pulse
c     into an infinite medium
      delsbs2 = fac2(m)*thdiff*dth
      sbsx = sbso/fac3(m)
      if(isb .eq. 1) then
         sbs1 = sqrt(fac2(m)*thdiff*qpint/qp)
      else
         sbs1 = 0.0
      endif
      sbs2 = sqrt((sbsx**2) + delsbs2)
      if(sbs2 .gt. 0.0 .and. sbs1 .gt. sbs2) sbs1 = sbs2
c
c     calculated temperature at center of shear band
      delt1 = qp*sbs1/(fac1(m)*xk)
      if(sbs2 .gt. 0.0) then
         delt2 = delto*sbsx/(sbs2*facdelt)
      else
         delt2 = 0.0
      endif
c
c     decide which result to use
      if (delt1 .gt. delt2) then
         deltn = facdelt*delt1
         sbsn = fac3(m)*sbs1
      else
         deltn = facdelt*delt2
         sbsn = fac3(m)*sbs2
      endif

      return
      end

      subroutine msband1(d,cv,thdiff,ysh,dydt,strt,sbso,sbsn,denr,
     &   dth,cellsize,delto,deltn)

c     sub to calc shear band size and temperature using grady & kipp model

      if(ysh .gt. 0.0 .and. dydt .gt. 0.0 .and. strt .gt. 0.0) then

         sbsn = 9.0*(d**3)*cv*cv*(thdiff**3)/((ysh**3)*dydt*dydt*strt)
         sbsn = sbsn**0.25
         if(sbsn .lt. 1.0e-6) sbsn = 1.0e-6
      elseif(delto .gt. 0.0 .and. strt .le. 0.0
     &      .and. sbso .gt. 0.0) then
         sbsn = sbso
      else
         sbsn = cellsize
      endif

      deltn = 0.0
      if(cv .gt. 0.0) then
c     units of denr are mbar-cc/microsec-g
c     units of cv are mbar-cc/g-k
         dtpw = denr*dth/cv
         if(sbsn .gt. 0.0) then
            fac = 4.0*thdiff*dth/(sbsn*sbsn)
```

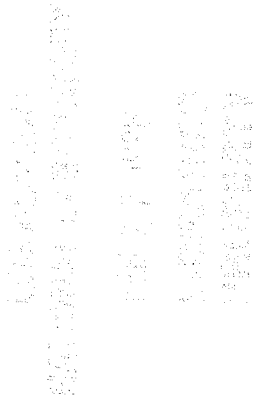
```
         else
            fac = 1.0e+9
         endif

         delt = (dtpw - (fac*delto))/(1.0 + fac)
         deltn = delto + delt
      endif

      return
      end


      subroutine integ(b,g,v)
c
c     sub to integrate induction time integral
c
      sum = 0.0
      if(g .gt. 3.5) then
         tlimg = 4.0*alog(g)
      else
         tlimg = 5.0
      endif
      if(b .gt. 1.0) then
         tlimb = alog(b)
      else
         tlimb = 0.0
      endif
      if(tlimg .gt. tlimb) then
         tlim = tlimg
      else
         tlim = tlimb
      endif
      del = tlim/float(100)
      do 25 i=1,101
         t = float(i-1)*del
         sum = sum + (1.0/(exp(t) + b - (g*t)))
   25 continue
      v = sum
      return
      end


      subroutine react(max,iquit)
c
c     subroutine to stop if icnt .gt. max
c
      data icnt / 0 /
c
      icnt = icnt + 1
      if(icnt .le. max) then
         iquit = 0
      else
         iquit = 1
      endif
c
      return
      end
```



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