Modelling the effects of temperature-dependent material properties in shear melt layers

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Defence and Security Doctoral Symposium

15-16 November 2016

Thanks to EPSRC and AWE for financial support via an industrial CASE partnership [EP/L505729/1], and to John Curtis and colleagues at AWE for useful scientific discussion.

Overview

- Background
- Low-speed impact modelling
- Shear melt model
- Numerical results
- Conclusions & future work

Background

- Much work focuses on shock detonation of explosive materials or on investigating the constitutive response of explosive materials
- Response of an explosive to low speed impacts is much less well understood
- There have been fatal accidents recorded during routine handling in which explosive samples have ignited. However, existing models suggested ignition would not occur
- Can we identify important ignition mechanisms?

Starobin, A.J. and Dienes, J.K. One-dimensional thermomechanical model for lateral melting and ignition of a thin sheared viscous layer. Combustion Theory and Modelling, 2006

Background

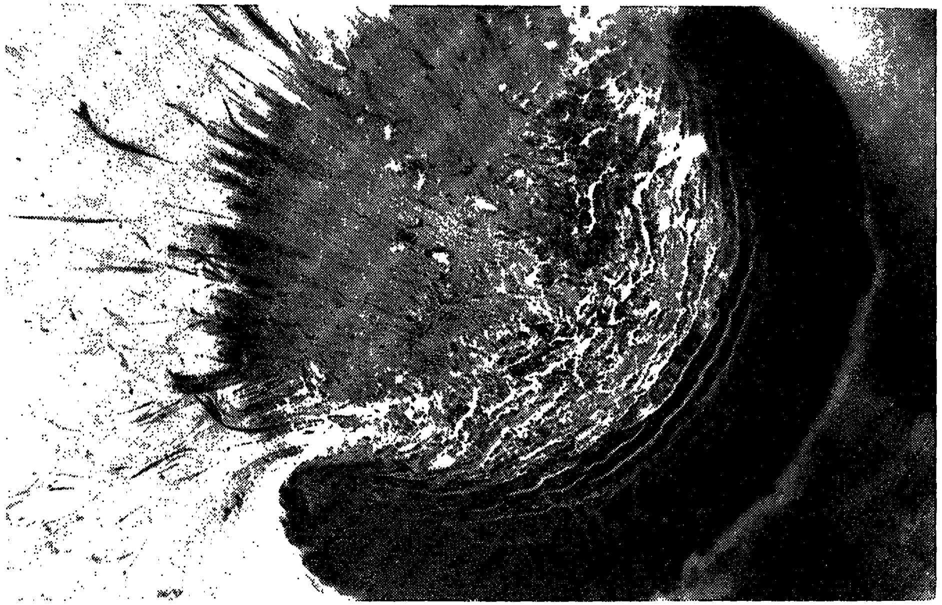
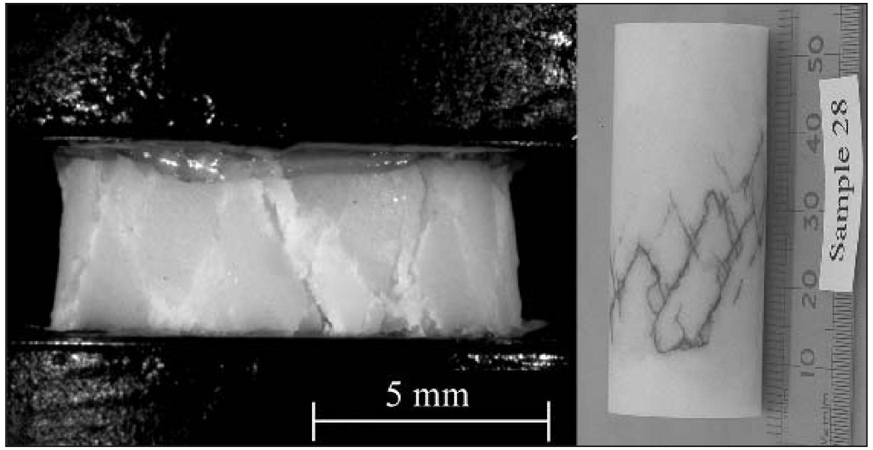


Image from “Hot spot ignition mechanisms for explosives and propellants”, Field et al.

- Focus on low-speed impacts scenarios - “insults”
- Accidental ignition is caused by “hot spots”
- How are these generated?

Background

- Adiabatic compression of trapped gas spaces
- Viscous heating of material rapidly extruded between the impacting surfaces
- Friction between the impacting surfaces, the explosive crystals and/or grit particles in the explosive layer
- Localised adiabatic shear of the material during mechanical failure

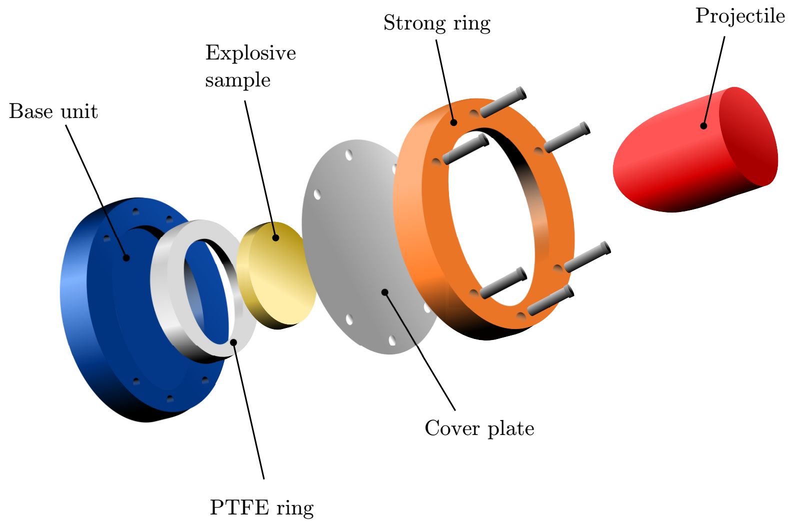


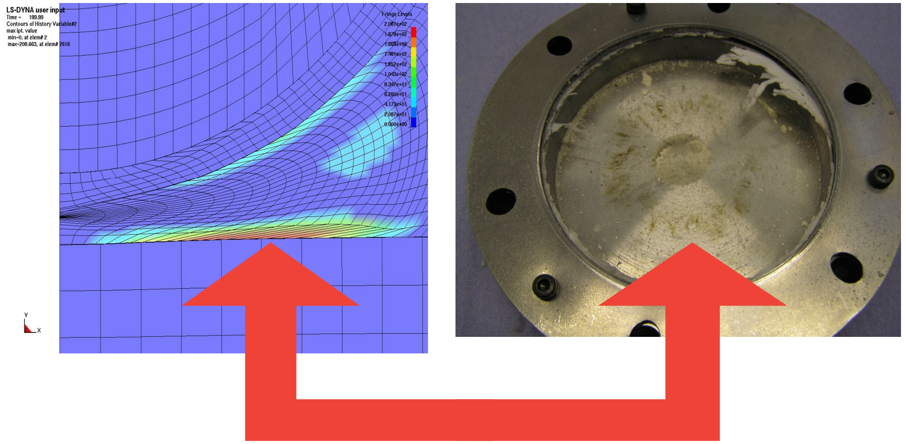
Photograph of shear bands in EDC37 from “Temperature-time response of a polymer bonded explosive in compression (EDC37)”, Williamson et al.

Low Speed Impact Modelling

Steven Test

- Experiments conducted at AWE
- Current LS-Dyna FE model is main approach
- High value of HERMES Ignition Parameter seen near confining walls
- Predicts scorching seen in experiments



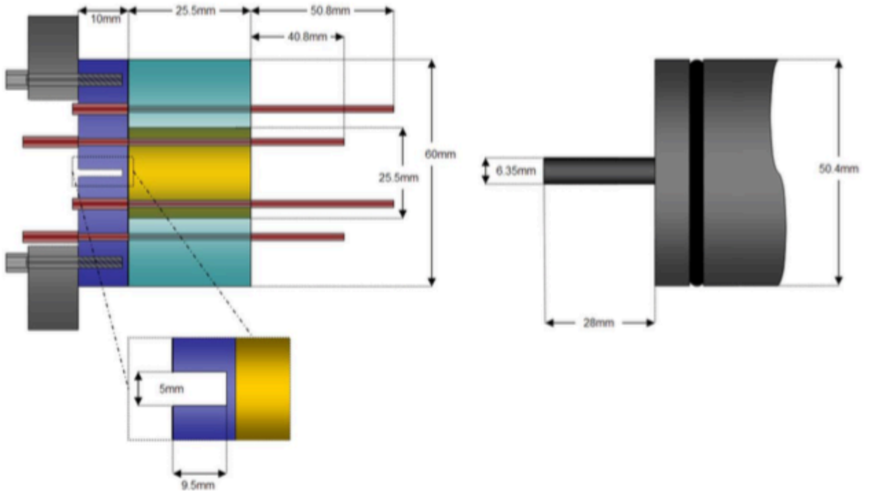


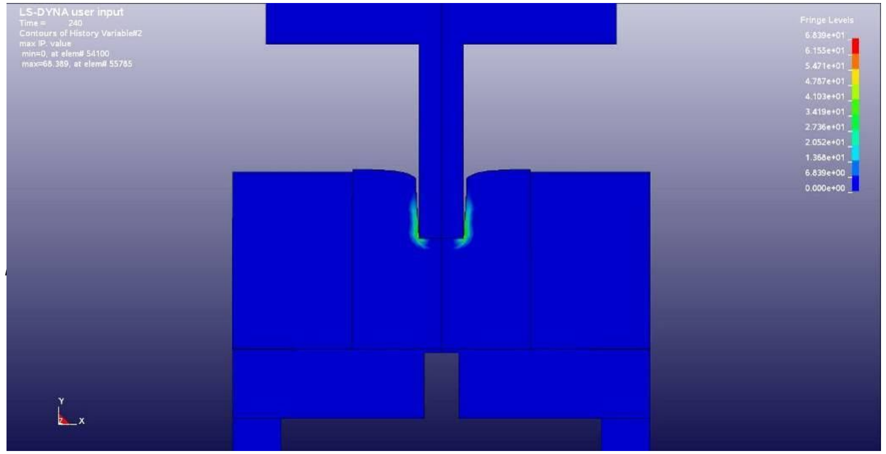
Images courtesy of AWE from CEA Workshop of Explosives, Tours, France

Low Speed Impact Modelling

Spigot Impact

- Localised impact
- High values of HERMES Ignition Parameter at leading edge of spigot
- Impact velocity ranges from 10-40 ms^{-1}





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Simplified Low Speed Impact Modelling

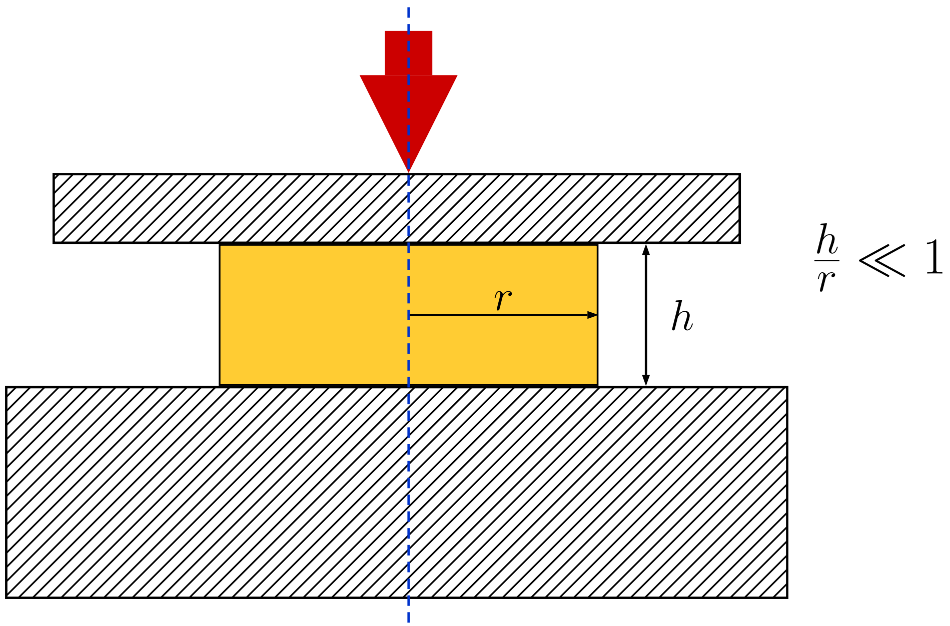
Motivation

- Improve safety during everyday conditions
- Avoid issues associated with numerical models, e.g.
  - severe mesh deformation
  - model break down near walls
- Numerical validation
- Focus on specific mechanisms/gain physical insight

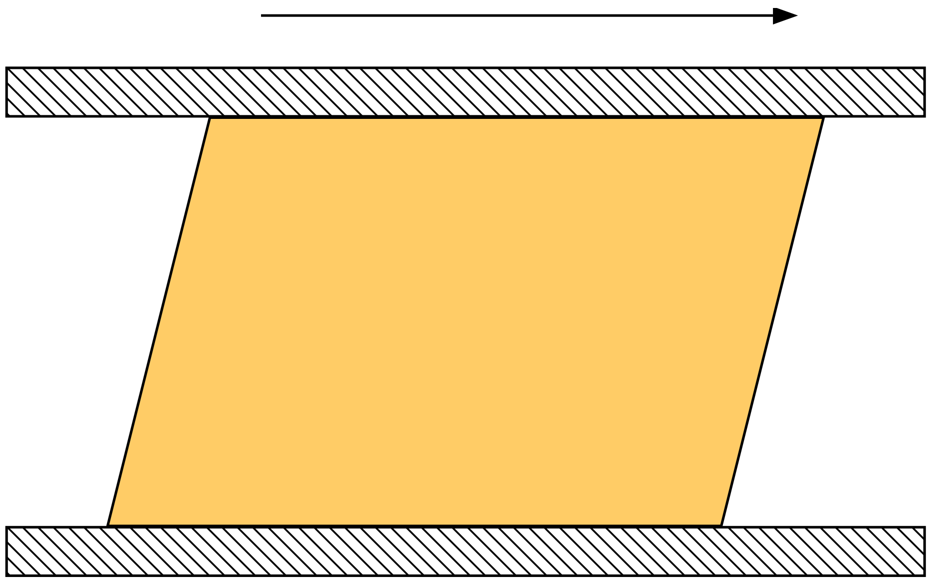
Simplified Low Speed Impact Modelling

Example Geometries

Drop test[i]:



Simple shear[ii]:



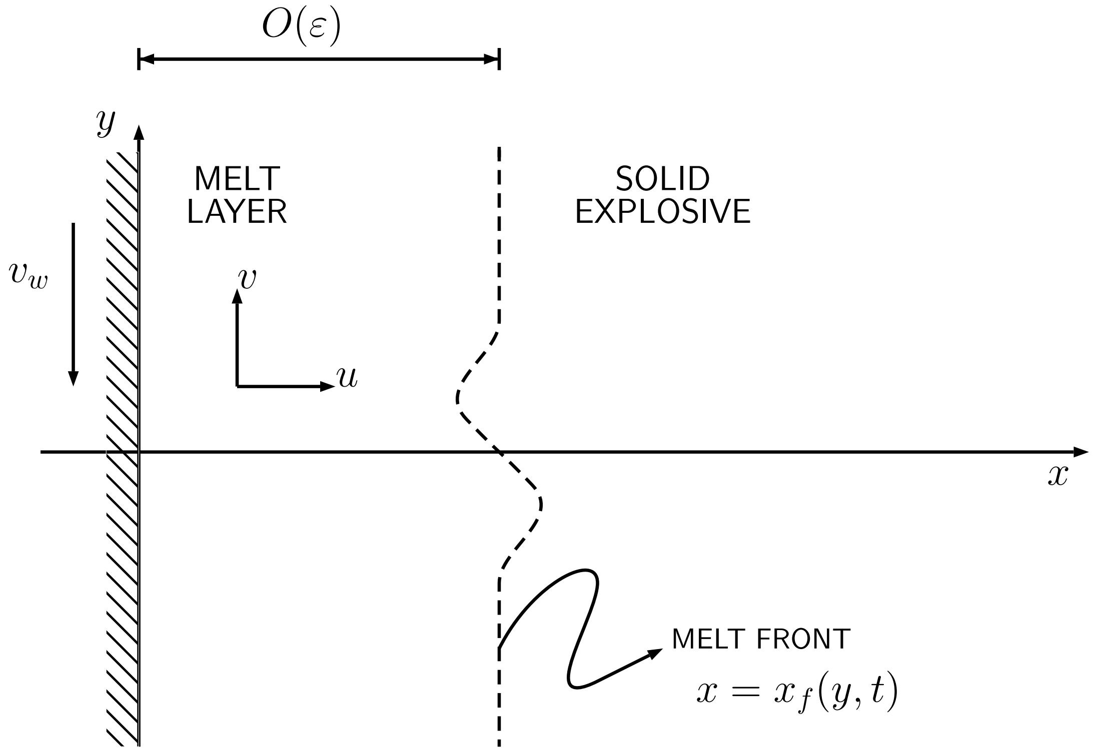
i. J.P. Curtis, A Model of Explosive Ignition due to Pinch, Thirty–Eighth International Pyrotechnics Seminar, Denver, Colorado, USA.
ii. J.P. Curtis, Explosive Ignition due to Adiabatic Shear, 39th International Pyrotechnics Seminar, Valencia, Spain

Shear Melt
Model

- Starobin and Dienes (2006) present 1D model
- 1D model predicts uniform heating and may over predict time to thermal runaway
- Will modelling non-uniformities in material lead to more localised hot spots and/or decreased time to runaway?
- How will temperature dependence of material properties affect the results?

Starobin, A.J. and Dienes, J.K. One-dimensional thermomechanical model for lateral melting and ignition of a thin sheared viscous layer. Combustion Theory and Modelling, 2006

Shear Melt
Model Schematic



(u, v) = velocity components
T = liquid temperature
p = liquid pressure

A solid block of explosive material (HMX) occupies the region $x > 0$. A rigid wall located at $x = 0$ is impulsively moved downward so that at $t = t_0$ a thin melt layer has already formed.

Shear Melt
Model

- Shear is studied in an idealised planar geometry
- Assume temperature dependent specific heat and viscosity
- 2D effects to model non-uniformities in material make up
- Thin melt layer $\Rightarrow$ lateral melting

In melt layer we introduce scalings:

$$x = \varepsilon X, \quad u = \varepsilon U, \quad p = \varepsilon^{-2} P, \quad \varepsilon^2 = \frac{1}{\mathrm{Pe}}.$$

where $\mathrm{Pe} = \frac{\text{advective transport rate}}{\text{diffusive transport rate}}$

Shear Melt

Model Equations

Lubrication equations:

$$\frac{\partial U}{\partial X}+\frac{\partial v}{\partial y}=0,\quad \frac{\partial P}{\partial X}=0,\quad -\frac{\partial P}{\partial y}+\frac{\partial}{\partial X}\left(\mu(T)\frac{\partial v}{\partial X}\right)=0$$

Stefan condition:

$$\frac{\partial X_f}{\partial t}=-\,\mathrm{Ste}\,\frac{\partial T}{\partial X}\bigg|_{X=X_f^-}$$

Energy equation:

$$c(T)\frac{\mathrm{D}T}{\mathrm{Dt}}=\frac{\partial^2 T}{\partial X^2}+\underbrace{\mathrm{Ec}\,\mathrm{Pr}\left(\frac{\partial v}{\partial X}\right)^2}_{\text{Dissipation}}+\underbrace{\hat{\Omega}\hat{A}(1-\alpha)\exp\left(-\frac{\hat{E}}{T}\right)}_{\text{Reaction}}$$

where $\mathrm{Ec}=\frac{\text{advective transport}}{\text{dissipation potential}}$, $\mathrm{Pr}=\frac{\text{viscous diffusion}}{\text{thermal diffusion}}$,
$\hat{\Omega}$ = heat of reaction, $\hat{A}$ = rate constant, and $\hat{E}$ = activation energy.

(U, v) = velocity components
X_f = melt front location
T = liquid temperature
P = liquid pressure
α = reaction extent
$c(T)$ = specific heat
$\mu(T)$ = viscosity

Shear Melt

Temperature-dependent material properties

Specific heat:

$$c(T) = \frac{(\theta_1/T)^2 \exp(\theta_1/T)}{(\exp(\theta_1/T) - 1)^2}$$

Viscosity:

$$\mu(T) = \exp\left(\frac{\theta_2}{T} - \frac{\theta_2}{\theta_3}\right)$$

where $\theta_1 = (1000\,\mathrm{K})/\Delta T$, $\theta_2 = (7800\,\mathrm{K})/\Delta T$ and $\theta_3 = (800\,\mathrm{K})/\Delta T$.

Here ΔT is a typical temperature scale. The non-dimensional specific heat and viscosity are related to their dimensional counterparts through the scalings $c^* = 1034\,\mathrm{J\,kg^{-1}\,K^{-1}}$ and $\mu^* = 5.5 \times 10^{-3}\,\mathrm{kg\,m^{-1}\,s^{-1}}$, respectively.

Austin et. al., Direct numerical simulation of shear localization and decomposition reactions in shock-loaded HMX crystal, Journal of Applied Physics, 2015; Frey, R.B., The initiation of explosive charges by rapid shear, DTIC Document, 1980.

Perturbation scheme

We consider small deviations from a uniform melt layer, i.e. $X=X_f(t)$,

$$[X_f, P](y,t) = [X_{f0}, P_0](t) + \delta[X_{f1}, P_1](y,t) + O(\delta^2),$$
$$[U, v, T, \alpha](\xi, y, t) = [U_0, v_0, T_0, \alpha_0](\xi, t) + \delta[U_1, v_1, T_1, \alpha_1](\xi, y, t) + O(\delta^2),$$
$$[c, \mu](\xi, y, t) = [c_0, \mu_0](\xi, t) + \delta[c_1, \mu_1](\xi, y, t) + O(\delta^2),$$

where $\delta \ll 1$ is a small parameter characterising the disturbance and $\xi = X / X_{f0}$ is the leading order front-fixed coordinate. The function S(y) describes the shape of the disturbance.

Perturbation scheme
Leading order

Integrate directly to find leading order velocity:

$$v_0(\xi, t) = \left(\int_0^1 \frac{1}{\mu_0} \, \mathrm{d}\xi \right)^{-1} \int_0^{\xi} \frac{1}{\mu_0} \, \mathrm{d}\xi - 1.$$

We observe a departure from the linear profile found when assuming constant material properties $\Rightarrow$ spatial dependence in mechanical dissipation.

Perturbation scheme
First order

First order corrections:

$$X_{f1} \sim X_{f1}(t)S(y), \quad U_1 \sim U_1(\xi,t)S'(y), \quad v_1 \sim v_1(\xi,t)S(y),$$
$$\frac{\partial P_1}{\partial y} \sim P_1(t)S(y), T_1 \sim T_1(\xi,t)S(y), \quad \alpha_1 \sim \alpha_1(\xi,t)S(y),$$
$$c_1 \sim c_1(\xi,t)S(y), \quad \mu_1 \sim \mu_1(t)S(y).$$

Gives vertical velocity:

$$v_1(\xi,t) = X_{f0}^2 P_1 \int_0^\xi \frac{\xi'}{\mu_0}\,\mathrm{d}\xi' - \int_0^\xi \frac{\mu_1}{\mu_0}\frac{\partial v_0}{\partial \xi'}\,\mathrm{d}\xi' + d_1(t)\int_0^\xi \frac{1}{\mu_0}\,\mathrm{d}\xi' + d_2(t).$$

Energy Equation

Numerical Solution

Mechanical solutions are substituted into the energy equation, which is solved via an iterative Crank-Nicolson numerical scheme subject to the Stefan condition

$$c(T)\frac{\mathrm{D}T}{\mathrm{D}t} = \frac{1}{X_{f0}^2}\frac{\partial^2 T}{\partial \xi^2} + \mathsf{Ec}\,\mathsf{Pr}\,\frac{1}{X_{f0}^2}\left(\frac{\partial v}{\partial \xi}\right)^2 + \hat{\Omega}\frac{\partial \alpha}{\partial t}$$

$$\frac{\partial \alpha}{\partial t} = \hat{A}(1-\alpha)\exp\left(-\frac{\hat{E}}{T}\right)$$

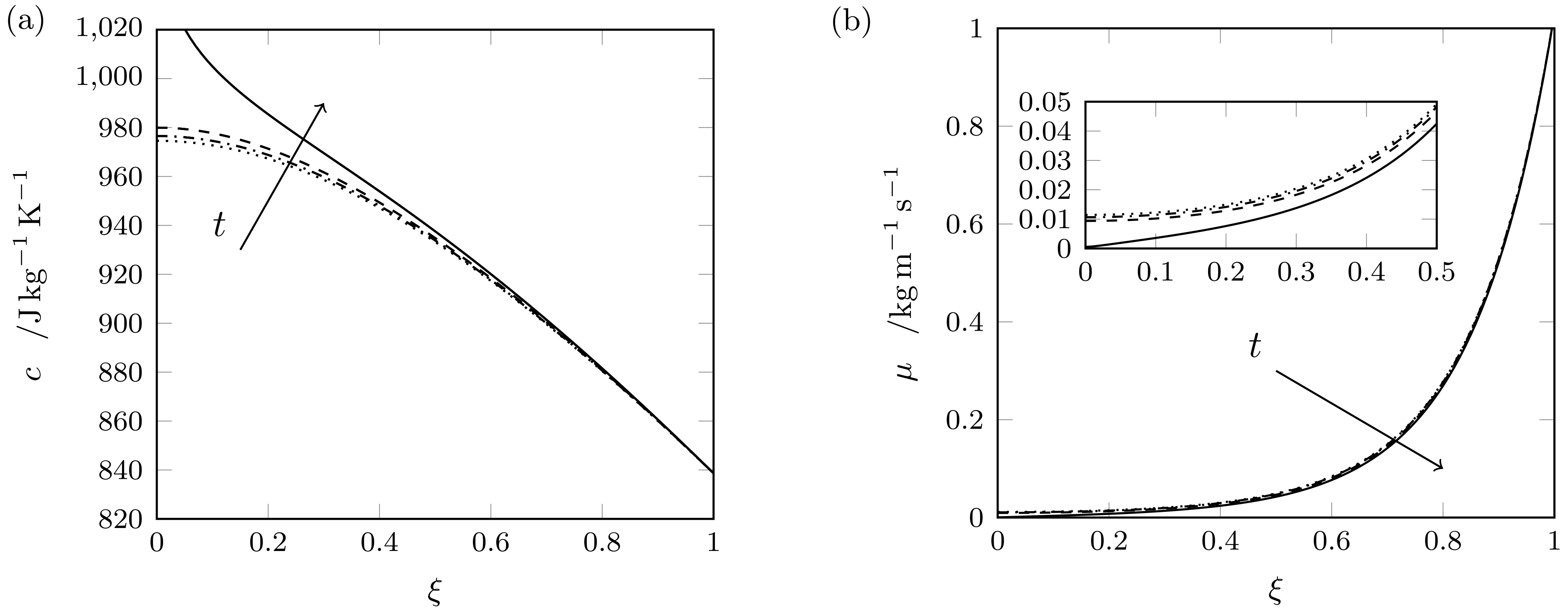
$$\frac{\partial X_f}{\partial t} + \mathsf{Ste}\,\frac{1}{X_f}\frac{\partial T}{\partial \xi}\bigg|_{\xi=1^-} = 0$$

Numerical Results
Material properties

Explosive Property	HMX
Activation Energy E	$2.2 \times 10^5\,\mathrm{J\,mol^{-1}}$
Heat of Reaction Ω	$5.02 \times 10^6\,\mathrm{J\,kg^{-1}}$
Molar Gas Constant R	$8.314\,\mathrm{J\,kg^{-1}\,K^{-1}}$
Pre-Exponential Const. A	$5.011\,872\,336 \times 10^{19}\,\mathrm{s^{-1}}$
Density ρ	$1860\,\mathrm{kg\,m^{-3}}$
Reference Viscosity μ^*	$5.5 \times 10^{-3}\,\mathrm{kg\,m^{-1}\,s^{-1}}$
Latent Heat L	$2.08 \times 10^5\,\mathrm{J\,kg^{-1}}$
Melting Temperature T_m	$520.6\,\mathrm{K}$
Reference Specific Heat c^*	$1034\,\mathrm{J\,kg^{-1}\,K^{-1}}$
Thermal Conductivity κ	$0.404\,\mathrm{W\,m^{-1}\,K^{-1}}$

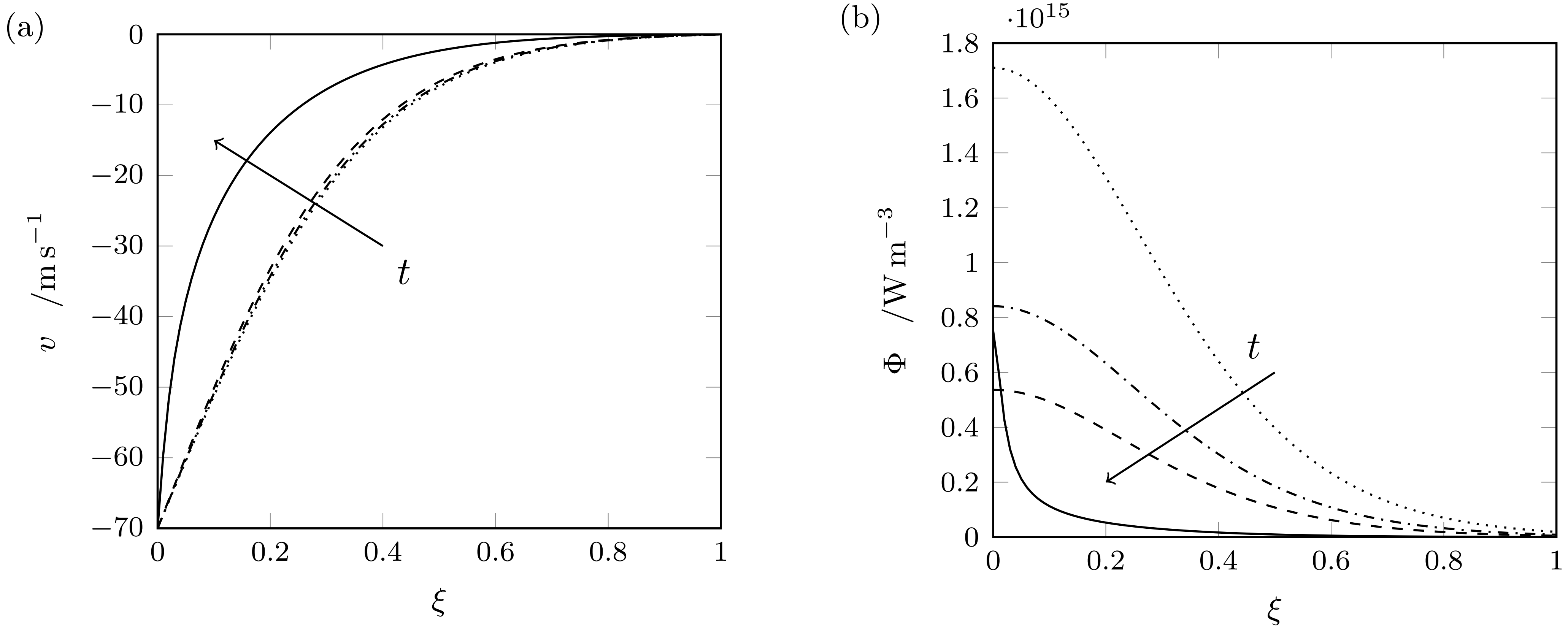
Material properties for HMX taken from Curtis (2013), Menikoff and Sewell (2002) and Starobin and Dienes (2006).

Numerical Results



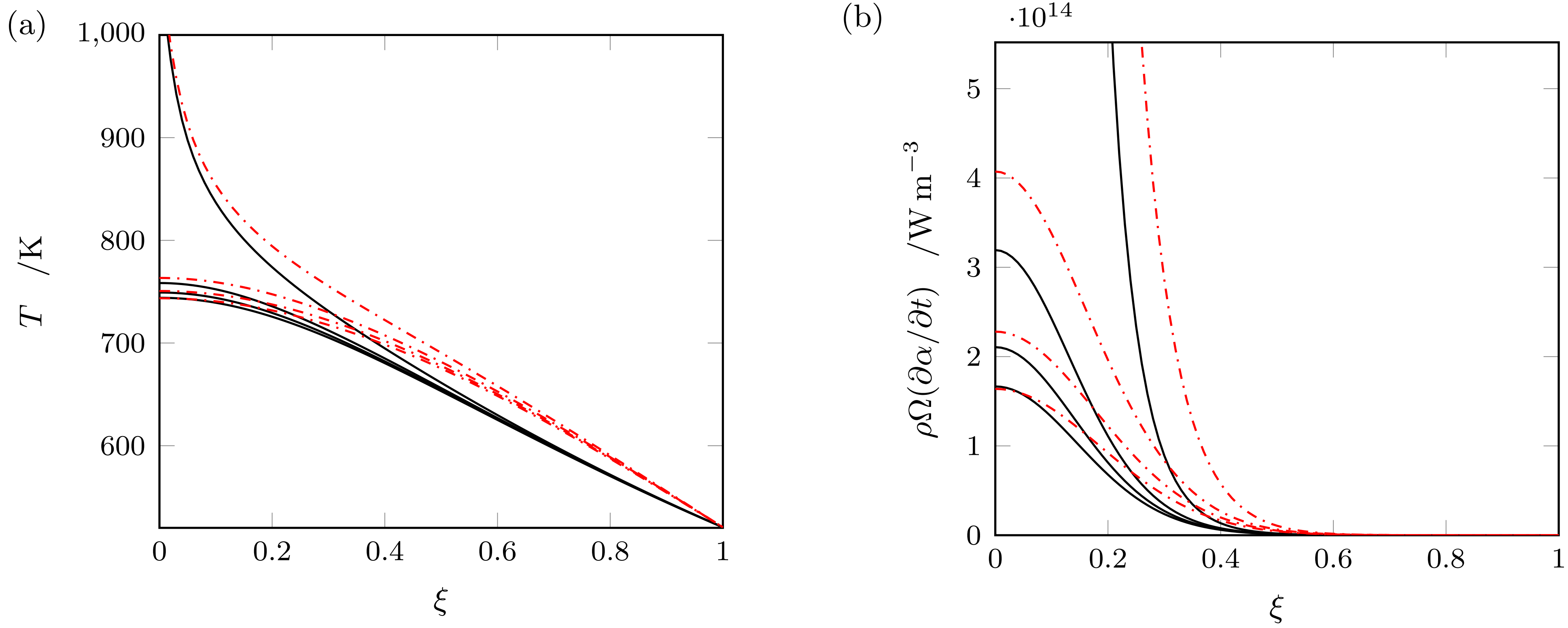
(a) The dimensional specific heat c across the melt layer at times t = 501, 992, 1483 and 1974 ns. (b) The dimensional viscosity μ across the melt layer shown at the same times.

Numerical Results



(a) The vertical velocity profile across the melt layer at times t = 501, 992, 1483 and 1974 ns. (b) The power density of the viscous dissipation term as a function of $\xi = X/X_{f0}$, the front-fixed coordinate across melt layer, shown at the same times.

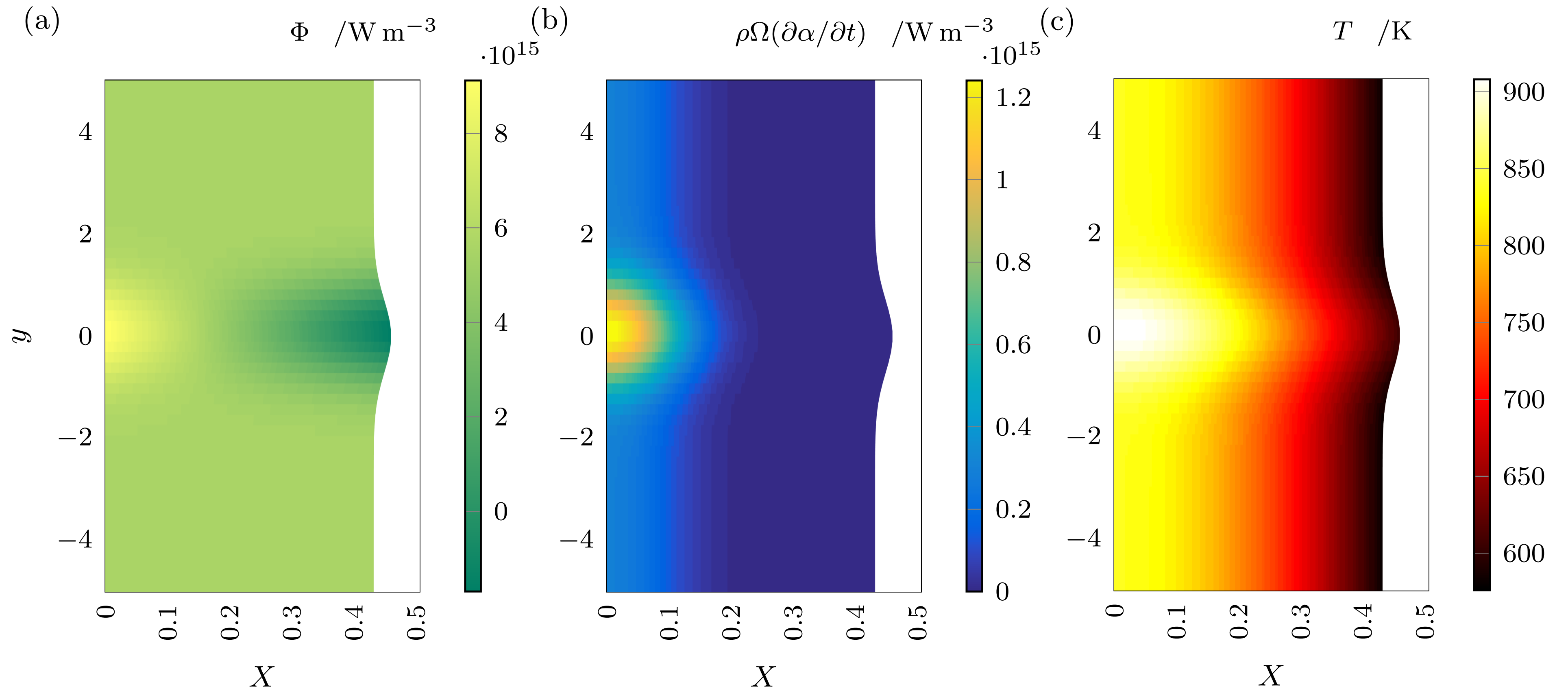
Numerical Results



(a) The temperature across the melt layer, and (b) the power density of the Arrhenius source term in the constant material properties case (red) and with temperature dependent material properties (black). The plots show snapshots at approximately 25%, 50%, 75% and 100% of the time to thermal runaway. For the constant material properties simulation this corresponds to times t = 228, 446, 664 and 882 ns, and for the temperature dependent simulation the corresponding times are t = 501, 992, 1483 and 1974 ns.

Numerical Results

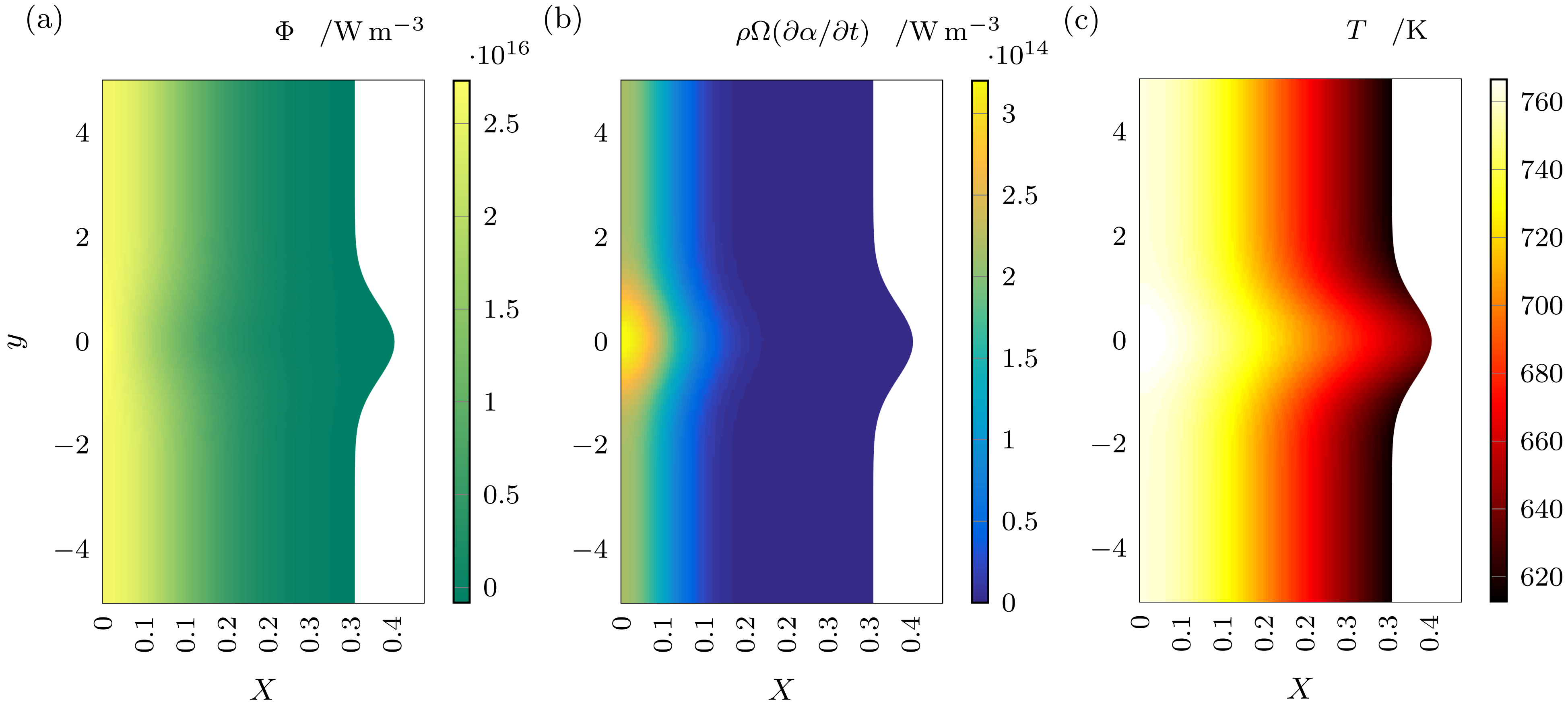
Constant material properties



Snapshot of results from the constant material properties model showing: (a) Power density of mechanical dissipation source term (Wm^{-3}); (b) power density of Arrhenius source term (Wm^{-3}); and (c) dimensional temperature (K) for a sample of HMX.

Numerical Results

Temperature dependent material properties



Snapshot of results from the temperature dependent material properties model showing: (a) Power density of mechanical dissipation source term (Wm^{-3}); (b) power density of Arrhenius source term (Wm^{-3}); and (c) dimensional temperature (K) for a sample of HMX.

Conclusions

- Modelling 2D effects gives rise to temperature localisation
- The asymptotic approach allows locations of potential hot spot generation caused by mechanical dissipation to be determined
- Previously identified hot spot mechanisms persist when the assumption of constant material properties is relaxed

Future Work

- Continue study of temperature/pressure dependent material properties
- Model initiation of melt layer
- Account for heat loss to the wall
- Presence of grit on the wall
- More realistic chemistry
- Shear bands
- Void collapse

Acknowledgements

- John Curtis and colleagues at AWE
- Richard Purvis (UEA)

This work was supported by the UK's Engineering and Physical Sciences Research Council and the Atomic Weapons Establishment via an industrial CASE partnership [EP/L505729/1].