Mesoscale Reaction Modeling of Granular Beds of Explosives Subject to Impact

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Abstract

A temperature and pressure dependent model for combustion of a representative explosive, octahydro-1,3,5,7-tetranitro-1,3,5,7-tetrazocine (HMX), has been implemented in the massively parallel Uintah Computational Framework and applied to mesoscale simulations of granular beds. The work underscores the importance of high pressure gases trapped in pores between grains. Further experimentation may lead to better understanding of deflagration-to-detonation transition, which has caused a number of accidental explosions. Results will help in the design of accurate sub-grid scale models applicable on the macroscale.

Methods

Material Models

An elastic-plastic constitutive model [1,2] with added melting temperature and specific heat models was used [3,4].

$$T_m = T_{m0}(1+av) \qquad C_v(T) = \frac{T^3}{aT^3+bT^2+cT+d}$$

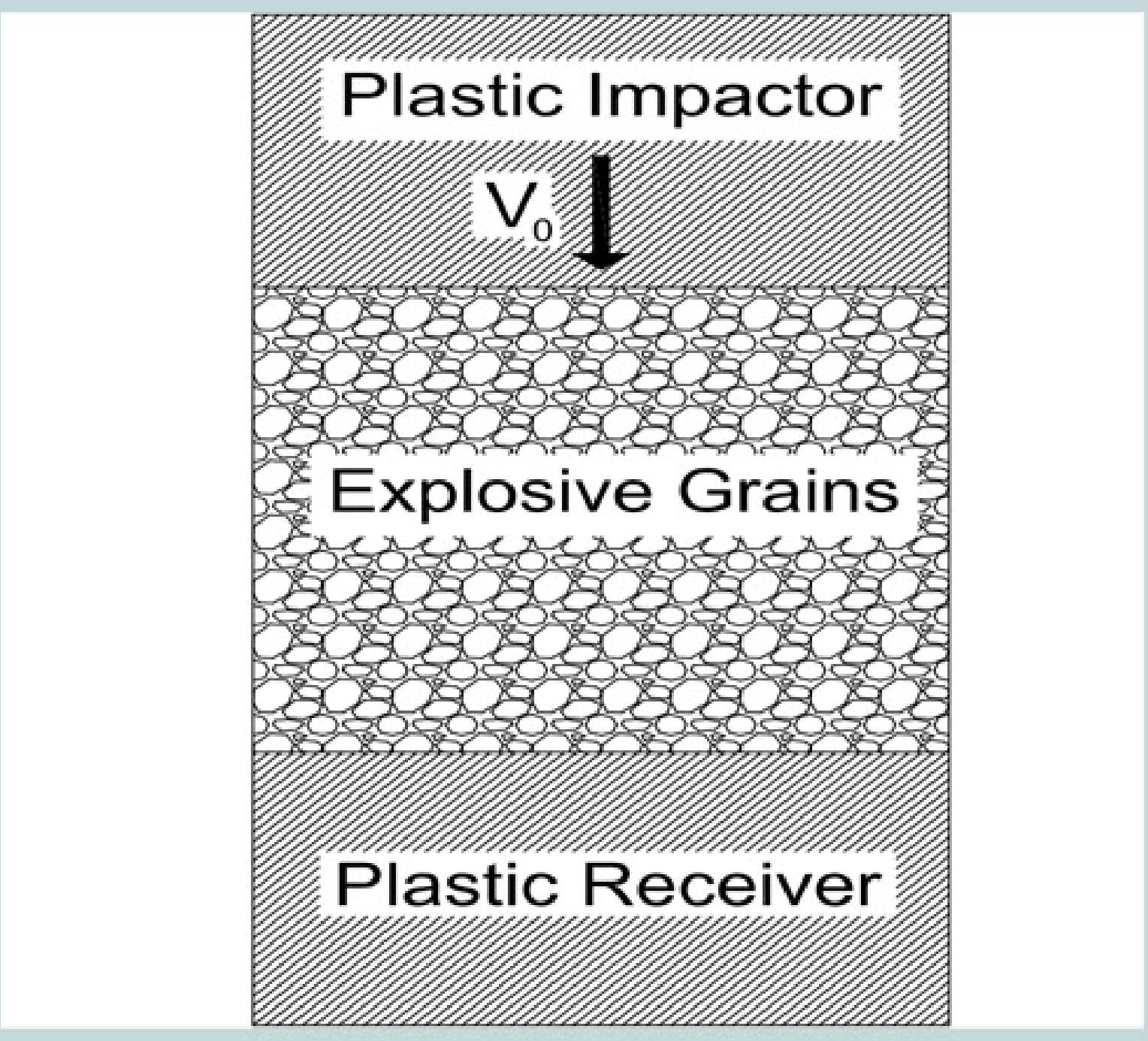
Reaction Models

A temperature dependent induction time model [5], and a temperature and pressure dependent burn model were used [6].

$$t_{adb} = \left[\frac{T^2C_v}{T_aQ}\right]\frac{e^{\frac{T_a}{T}}}{k} \qquad m^2 = \frac{A_cRT_s^2k_c\rho_c e^{-E_c/RT_s}}{E_c\left[C_p(T_s-T_0)-Q_c/2\right]}$$

Simulation Setup

The computational methods Material Point Method (MPM) and MPM-Implicit Continuous Eulerian (MPMICE) were utilized [7,8]. Random cylinder packing from experimental distribution [9,10] were impacted at different velocities (Scheme 1). The effect of input stress was examined (Figure 1).



Scheme 1. Experimental setup where V varies from 150 and 700 m/s.

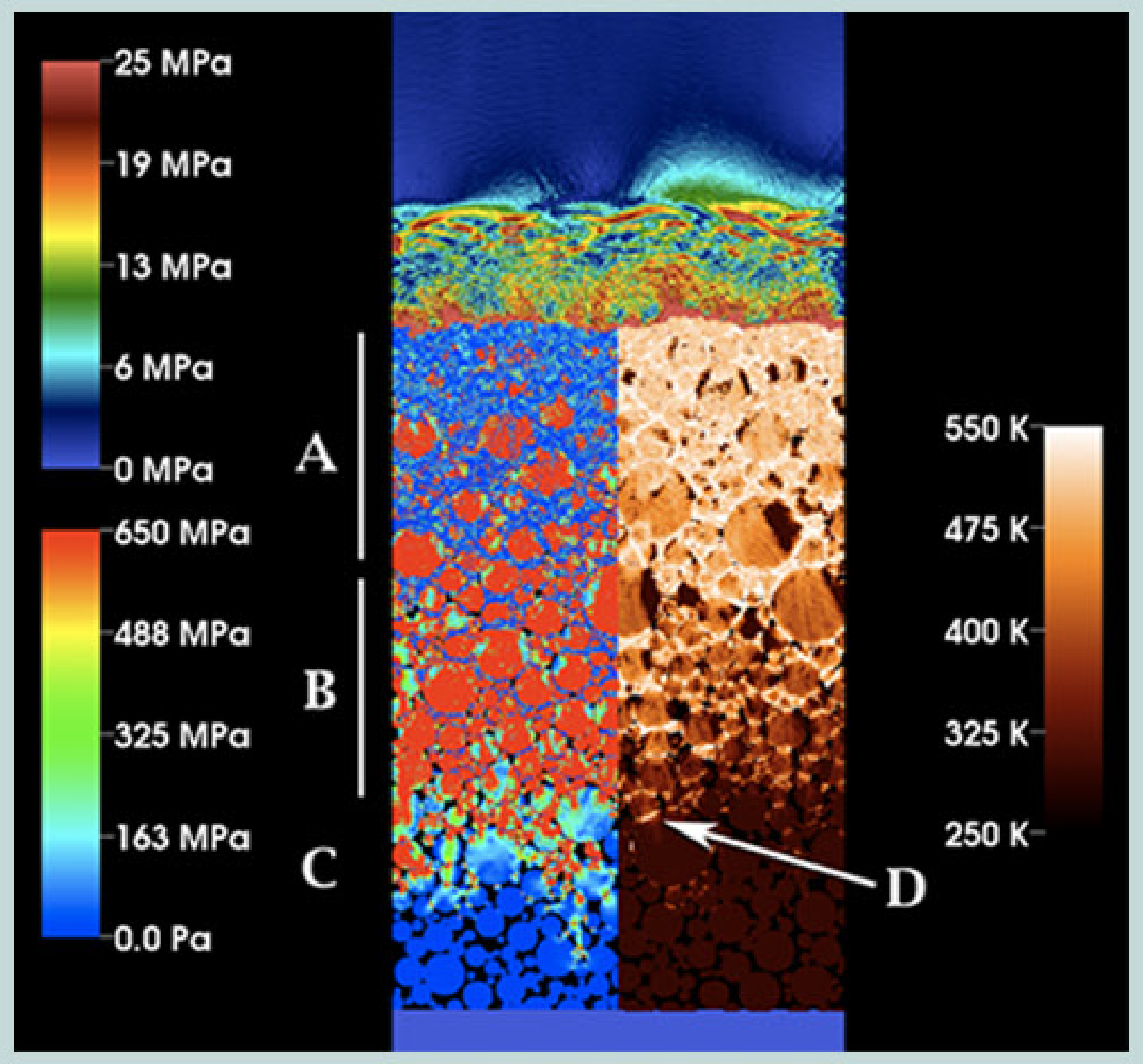


Figure 1. A granular explosive impacted at 288 m/s. Stress (left) and temperature (right). Features: A) plastic flow, B) compaction, C) stress fingers, D) friction hot-spots

Constitutive Model Validation

Single crystal experiments [13] used to validate the bulk material response (Figure 2).

Stress and velocity profiles [11] reproduce the major features of experiments (Figure 3,4).

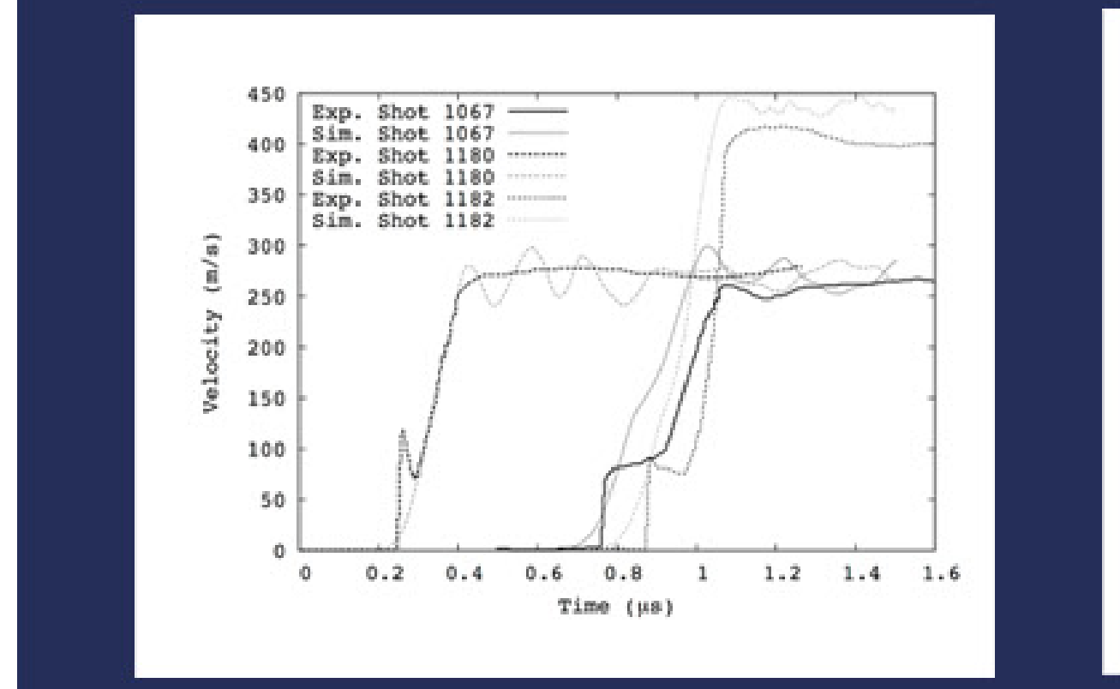


Figure 2. Single crystals of HMX impacted at different velocities.

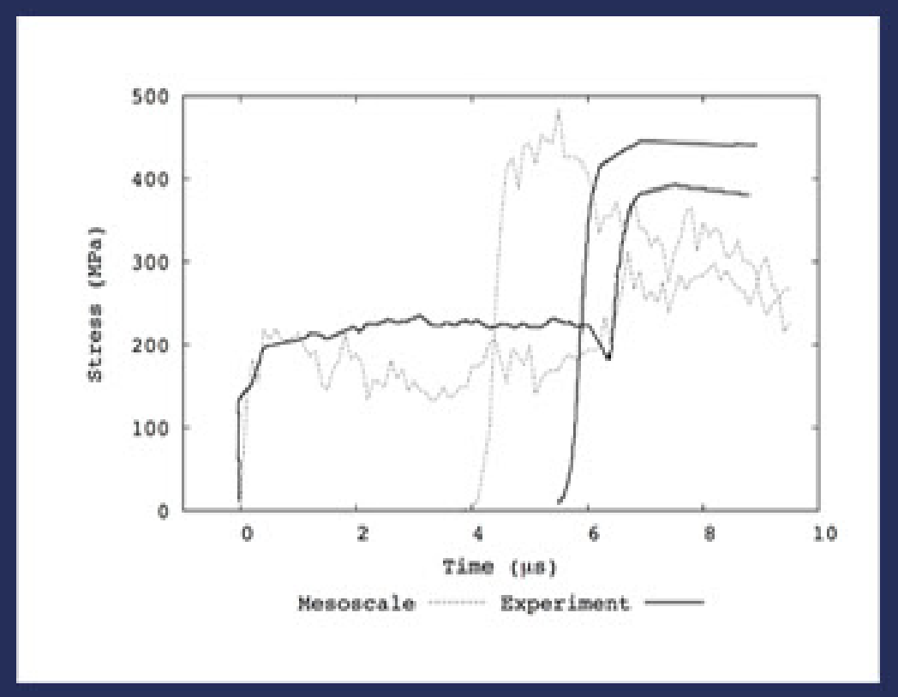


Figure 3. Stress traces at the top (left) and bottom (right) of the granular bed.

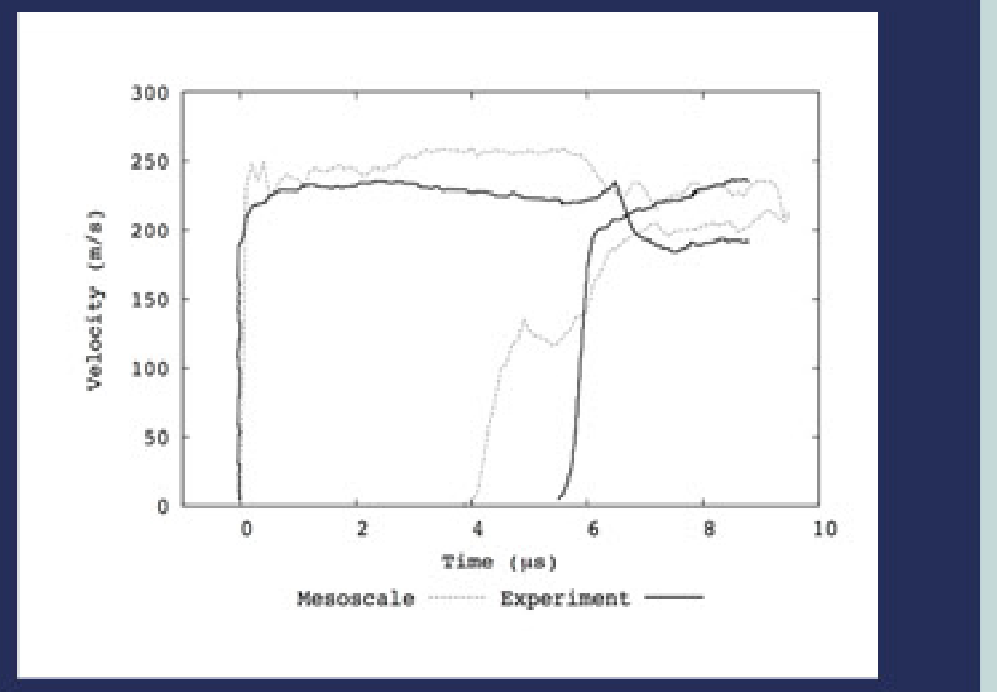


Figure 4. Velocity traces at the top (left) and bottom (right) of the granular bed.

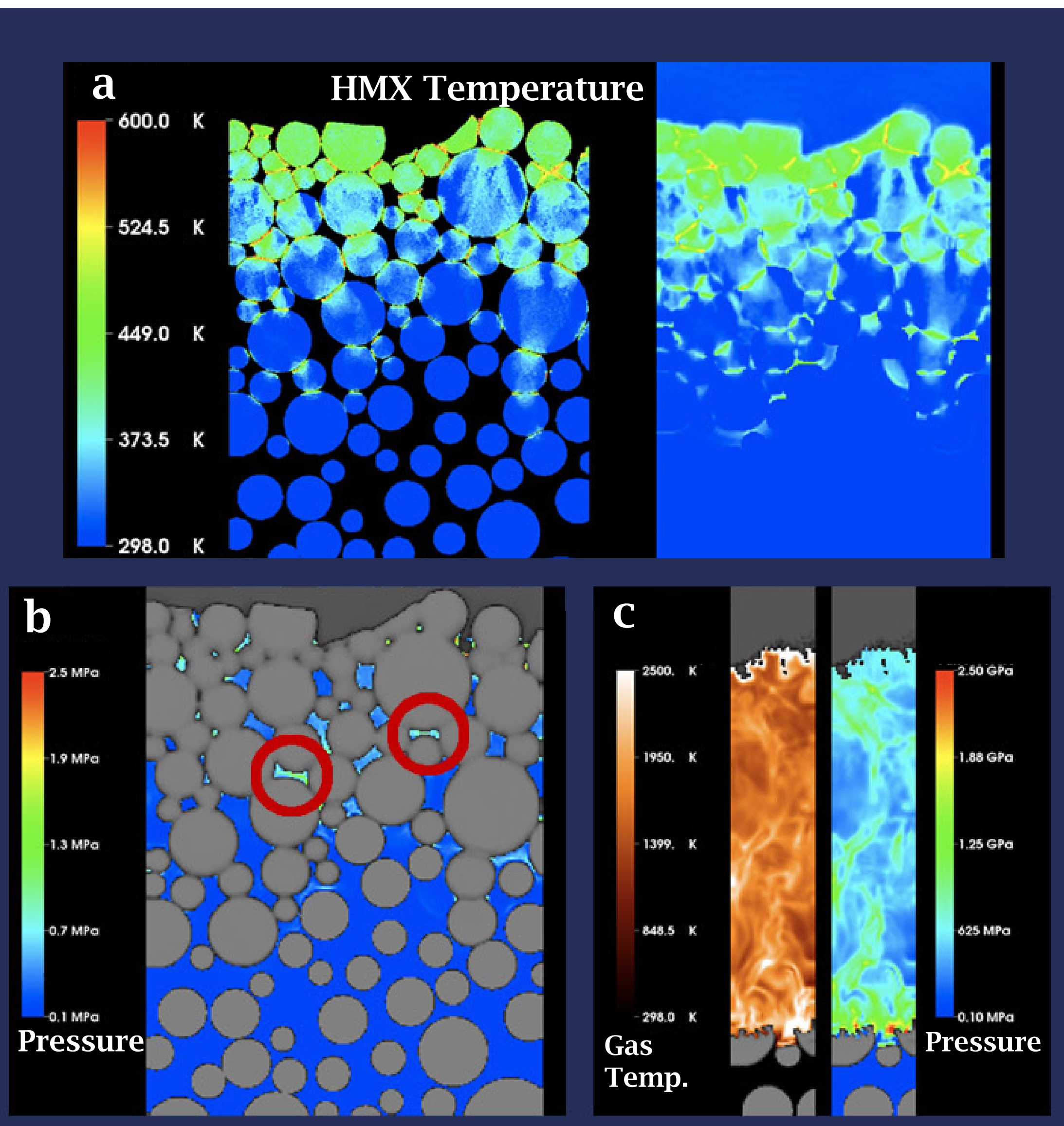


Figure 5.

a) MPM and MPMICE temperature comparison.

b) Gases trapped in pores

c) Temperature and pressures ~1.15 microseconds post 696 m/s impact.

Solid and Gas Results

Temperatures differ negligibly for MPM and MPMICE (Figure 5a). MPMICE allows pressurization of gases trapped in 10 to 100 micron pores (Figure 5b). Reaction occurs in the 696 m/s experiment similar pressure and velocity at impactor boundary (Figure 5c). Temperature profiles for different density beds over compared favorably with other simulated results [14] (Figure 6). Reaction begins in a pore for the 696 m/s impact experiment is shown (Figure 7).

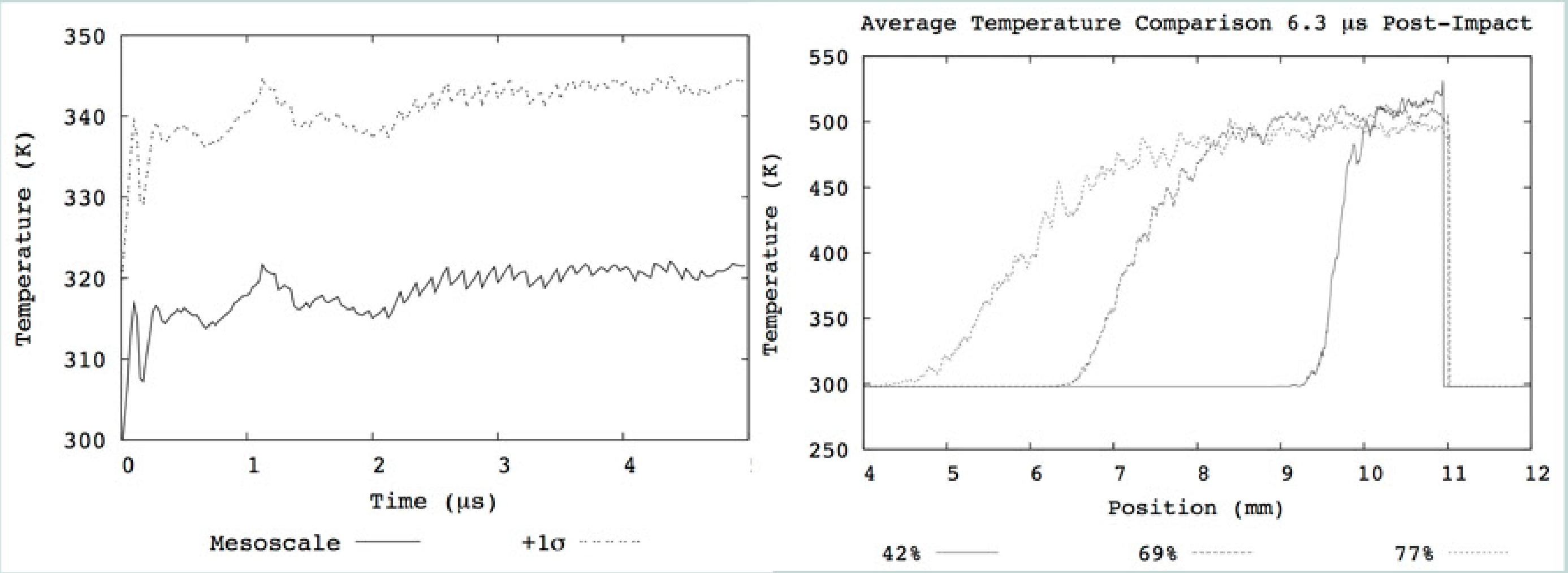


Figure 6. Mass average temperature at 288 m/s impact surface (left). Mass average temperature for 3 different density packings (right).

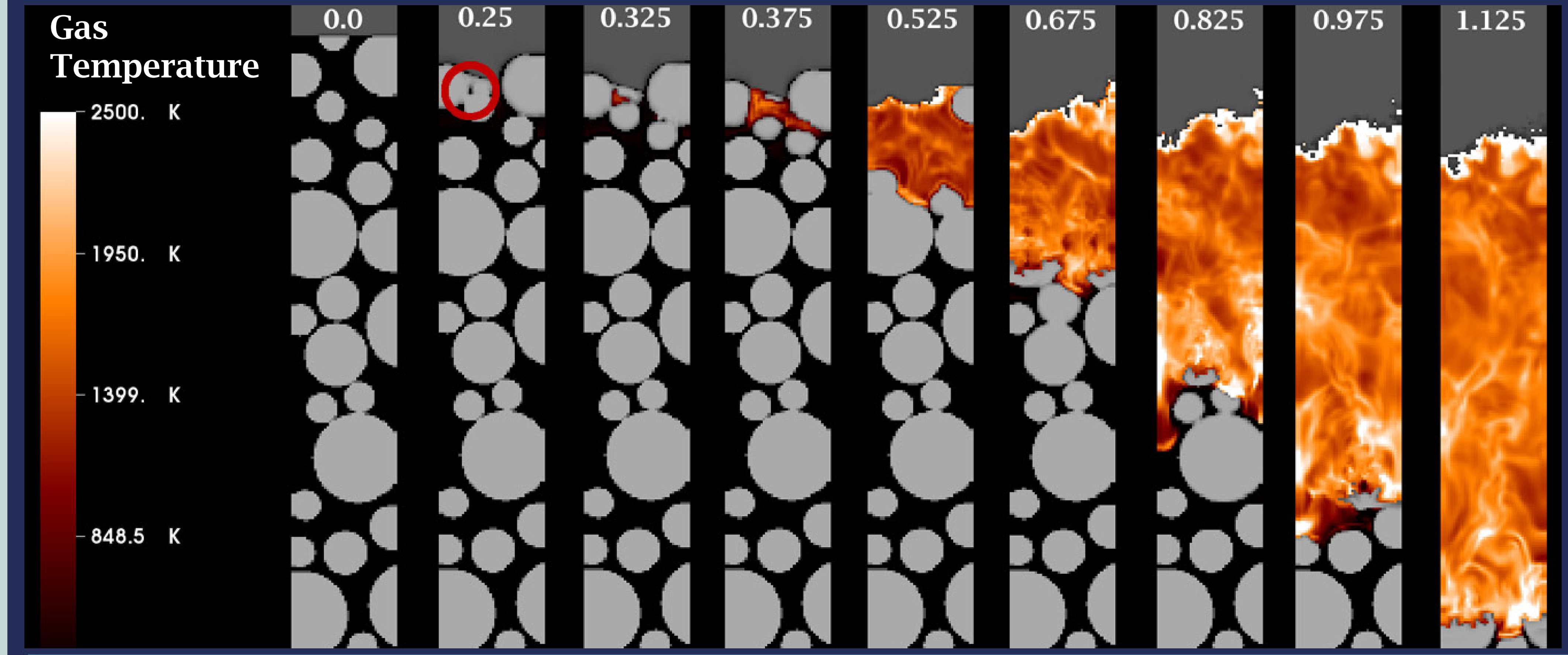


Figure 7. A sequence of images for a 65% density HMX bed impacted at 696 m/s undergoing reaction. The gas pore where reaction begins is indicated with the red circle. Reaction beings close to the interface and between the flyer and the explosive, as in the experiments [11]. Pressures at the flyer surface are similar to those of the experiments. Time after impact in microseconds is indicated above each frame.

Conclusions and Future Work

1) Induction time is required to limit reaction in non-reactive experiments.
2) High pressure gases trapped in pores play a key role.
3) Simple kinetic modeling can help elucidate mechanism of deflagration-to-detonation transition.
4) Optically obtained microstructures (figure 8) will be used to study surface area and pore size effects on reaction rate.

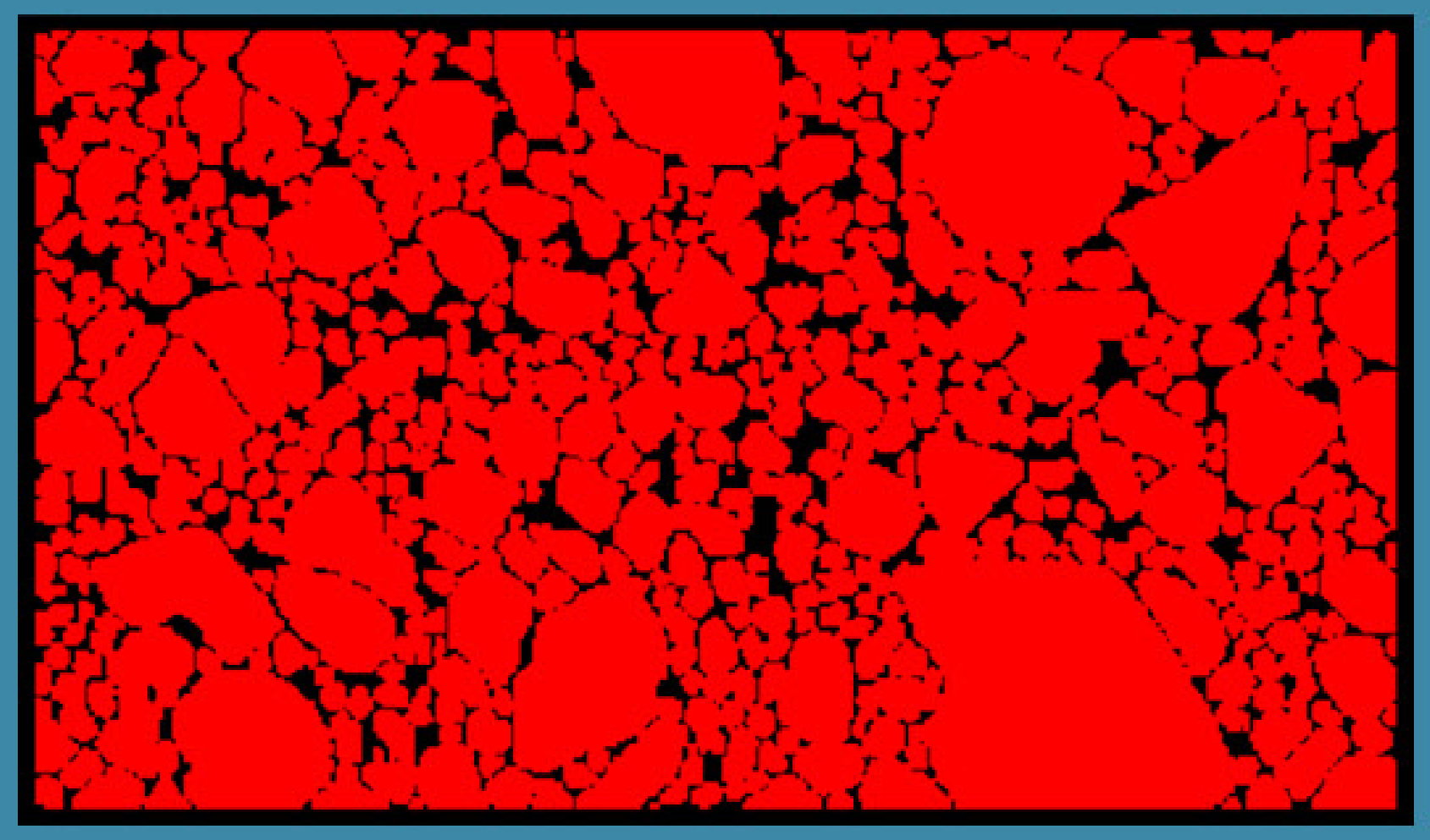


Figure 8. Digitized version of optically acquired HMX microstructure by Benson et al. [2]

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References

1. Steinberg, D.J., Cochran, S.G. and M.W. Guinan. A constitutive model for metals applicable at high strain rate. *J. Appl. Phys.*, 51 (1980) 1498.
2. Benson, D.J. and P. Conley. Eulerian finite-element simulations of experimentally acquired HMX microstructures. *Modelling Simul. Mater. Sci. Eng.*, 7 (1999) 333-354.
3. Menioff, R. and T.D. Sewell. Constituent Properties of HMX Needed for Meso-Scale Simulations. *Combust. Theory Model.*, 6 (2002) 103-125.
4. Sewell, T.D. and R. Menikoff. Complete Equation of State for Beta-HMX and Implications for Initiation. *Shock Compression of Condensed Matter*, (2003) 157-160.
5. Menikoff, R. Detonation Wave Profile in PBX-9501. *Shock Compression of Condensed Matter*, (2005).
6. Ward, M.J., Son, S.F. and M.Q. Brewster. Steady Deflagration of HMX With Simple Kinetics: A Gas Phase Chain Reaction Model. *Combust. Flame.*, 114 (1998) 556-568.
7. Kashiwa, B. A multimaterial formalism. Technical Report LA-UR-94-771, Los Alamos National Laboratory, Las Alamos, NM, 1994.
8. Guilkey, J., Harman, T., Kashiwa, B. and J. Schmidt. An eulerian-lagrangian approach for simulating large deformation fluid structure interaction problems, part 1: Algorithm development. *Fluid Structure Interactions II*, Cadiz, Spain, 2003. WIT Press.
9. Gustavsen, R.L., Sheffield, S.A. and R.R. Alcon. Low Pressure Shock Initiation of Porous HMX for Two Grain Size Distributions and Two Densities. *Shock Compression of Condensed Matter*, (1995).
10. Bardenhagen, S.G., Roessig, K.M., Byutner, O., Guilkey, J.E., Bedrov, D. and G.D. Smith. Direct Numerical Simulation of Weak Shocks in Granular Material. *12th Int. Det. Symp.* (2002).
11. Sheffield, S.A., Gustavsen, R.L. and R.R. Alcon. Shock Initiation Studies of Low Density HMX Using Electromagnetic Particle Velocity and PVDF Stress Gauges. *10th Int. Det. Symp.* (1993).
12. Dick, J.J. Stress-Time Profiles in Low Density HMX. *Combust. Flame.*, 69 (1987) 257-262.
13. Dick, J.J., Hooks, D.E., Menikoff, R. and Martinez, A.R. Elastic-plastic wave profiles in cyclotetramethylene tetranitramine crystals. *J. Appl. Phys.*, 96 (2004) 374.
14. Panchadhara, R. and K.A. Gonthier. Mesoscale analysis of volumetric and surface dissipation in granular explosive induced by uniaxial deformation waves. *Shock Waves*, 21 (2011) 43-61.