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Model comparisons of the reactive burn model SURF in three ASC codes

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Abstract

A study of the SURF reactive burn model was performed in FLAG, PAGOSA and XRAGE. In this study, three different shock-to-detonation transition experiments were modeled in each code. All three codes produced similar model results for all the experiments modeled and at all resolutions. Buildup-to-detonation time, particle velocities and resolution dependence of the models was notably similar between the codes. Given the current PBX 9502 equations of state and SURF calibrations, each code is equally capable of predicting the correct detonation time and distance when impacted by a 1D impactor at pressures ranging from 10-16 GPa, as long as the resolution of the mesh is not too coarse.

Introduction

SURF[1,2,3] is a reactive burn model that attempts to capture shock initiation and detonation propagation in high explosives. SURF is a form of ignition and growth style reactive burn, originally suggested by Lee and Tarver.[4] In the concept of ignition and growth, ignition occurs at hot spot locations and these hot spots grow as they burn. Depending on number of hot spots and how fast they grow, the individual reactions can coalesce into a unified reaction front and ultimately lead to detonation of the explosive. If the number of hot spots is insufficient or if the burn rate is too slow, the reactions will fail to coalesce and ultimately no detonation will occur.

Largely, this view of hot spot coalescence leading to detonation is widely accepted as physically correct. In a heterogeneous explosive like PBX 9502, the response of the HE to shock input can be vastly different. For example, on the low end of the pressure regime, the crystal structure is strong enough to resist pore collapse, and thus no hot spot centers ignite. At exceedingly high pressures, the burn rate should saturate to some plateau that largely matches the reaction zone width. In order to account for the various different responses that PBX 9502 has when shocked, the SURF model implements a piecewise-continuous burn rate that is dependent on the lead shock pressure. Each pressure interval dominates a different detonation phenomenon.

The SURF model includes an algorithm for detecting the lead shock based on the Hugoniot equation for energy. Over the pressure range of interest for this paper (nominally 1 GPa to 40 GPa), the burn rate changes by a factor of 1000. Small zone-to-zone perturbations in the pressure can lead to significant burn rate differences. SURF uses a lead shock detection algorithm to help determine a consistent lead shock pressure. However, this shock detection algorithm differs between the three codes investigated here. Thus, a code-to-code comparison of model results is not informative.

This study will not attempt to name a 'winner' or a 'loser'. We are attempting to ensure the SURF reactive burn model is capable of modeling a simple shock-to-detonation transition experiment within reason. 'Within reason' means the results of any one code should be similar to the results of the other two codes. Thus, running three codes allows us to identify significant differences in the burn model behavior between the codes.

Gas Gun Shock Initiation Experiment

A schematic of the experiment is shown in Figure 1. In these experiments, a Kel-F 81 impactor (shown in cyan) backed by a polycarbonate projectile (shown in gray) is launched out of a two-stage gas gun at a velocity *V*. The impactor collides with an explosive sample of PBX 9502. This collision imparts a shock that moves through the PBX 9502, beginning the initiation process. Electromagnetic particle velocity gauges are embedded in the PBX 9502 sample at various distances from the impact surface. As the shock moves through the explosive, the gauges record the particle velocity of the explosive.

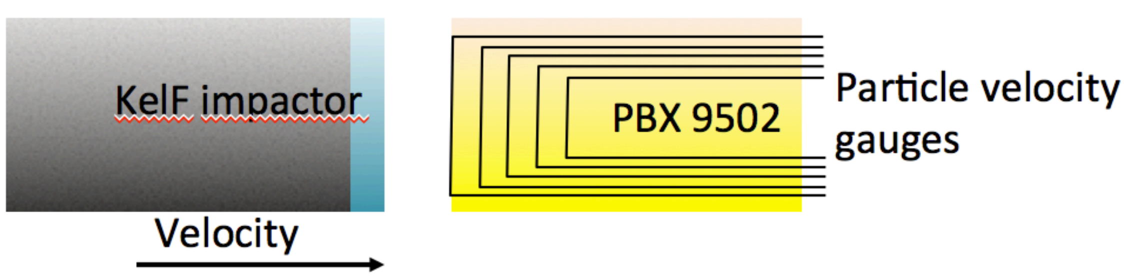

Figure 1: Schematic of embedded gauge experiment.

The velocity of the impactor is chosen such that the pressure in the shock is below the prompt detonation point in PBX 9502, but is high enough to cause chemical reactions to occur. These chemical reactions add energy to the shock front, raising the pressure as the shock traverses the sample. At some distance, the chemical reactions have added enough energy to the shock front to begin the detonation process in the explosive.

Figure 2 shows typical experimental results. Here, the first particle velocity gauge at the far left of the figure represents the impact surface. Note that on impact, the particle velocity jumps from 0 to 1.5 mm/μs and then remains approximately constant throughout the experiment. This is the shock profile obtained from an inert material. As the shock moves through the PBX 9502 from left to right, the shape of the particle velocity profile changes from a largely square wave to progressively more humped. Chemical reactions in the PBX 9502 add energy to the shock front causing increasingly larger velocity excursions above the input shock pressure. At some point in the experiment, there is enough energy from the incident shock (plus ancilliary chemical reactions) to cause the PBX 9502 to detonate. That is shown by the purple peaked velocity profile in Figure 2. Once detonation has been achieved, the detonation proceeds through the rest of the explosive at a nominally constant velocity. Note, the purple trace and the olive green trace are almost identical.

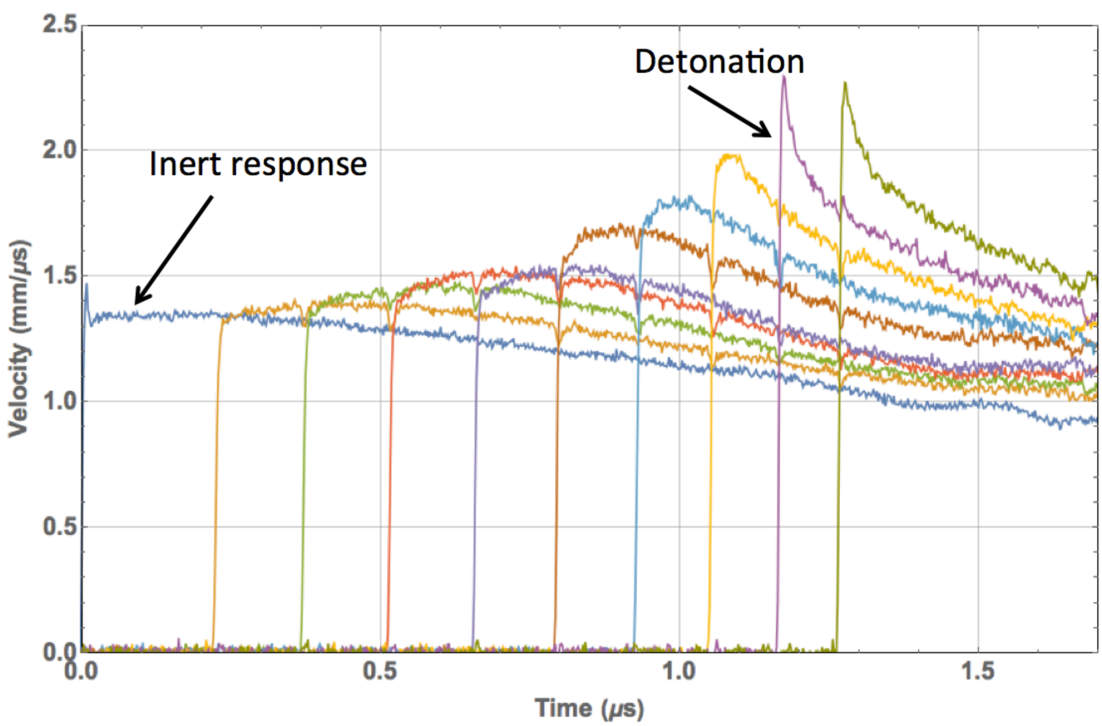

Figure 2: Typical experimental results obtained from a shock initiation experiment.

A detailed description of the shock initiation experiments can be found in Gustavsen et al.[5]

Model

FLAG and PAGOSA each use the same functional form of SURF, but with different calibration parameters. This was the original version of SURF described by Menikoff and Shaw[1]. In this implementation, the shock strength is a piecewise continuous function given by:

$$f(ps) = \begin{cases} 0 & ps \leq p0 \\ f0(ps) - f0(p0) * (1 + B(ps - p0)) & p0 \ < ps \leq p1 \\ f1[1 + df1(1 - \exp(ps - p1))] & p1 < ps \end{cases}$$

where ps is the lead shock pressure determined from the shock front,

$$f0(p) = \exp\,(A + B\,p)$$

$$f1 = fo(p1) - fo(p0)[1 + B(p1 - \ po)]$$

and

$$B2 = \frac{B}{df1} \frac{f0(p1) - f0(p0)}{f1}$$

Finally, the shock strength function *f(ps)* is scaled to get the final burn rate:

$$S = f(ps) * \frac{(p - ps)^n}{p_{scale}}$$

This final burn rate, S, is currently exercised in PAGOSA 17.3 and is not identical to the rate mentioned in the PAGOSA input reference manual. The scaling to get the final burn rate also differs between PAGOSA and FLAG. Since FLAG uses $n = 0$, the different scaling function used by FLAG is not relevant for this analysis. SURF coefficients for the three codes for the same functional form of SURF mentioned above are given in Table 1.

Table 1: SURF coefficients for FLAG and PAGOSA

Parameters	FLAG	PAGOSA	XRAGE (original)
A	-3.1	-3.35	-3.1
B	0.28	0.30	0.28
p0 (GPa)	2.5	2.0	2.5
p1 (GPa)	21.5	20.0	21.5
df1	3.0	2.0	3.0
n	0	5	?
Pscale (GPa)	1	1	1

SURF, as currently implemented in XRAGE, uses the following form for the shock strength function *f(ps):*

$$f(ps) = \begin{cases} 0 & ps \ \leq p0 \\ c_{low}[ps - p0]^{fn_{low}} & p0 < ps \leq p_{low} \\ c \cdot ps^{fn} & p_{low} < ps \leq p1 \\ f(p1)\exp\left[fn \cdot \ln\left(\frac{ps}{p1}\right) \cdot (1 - B2\ln\left(\frac{ps}{p1}\right))\right] & p1 < ps \leq p_{hi} \\ f_{max} & p_{hi} < ps \end{cases}$$

with

$$fn_{low} = (1 - \frac{p0}{p_{low}}) \cdot fn$$

$$c_{low} = c \cdot \left(\frac{p_{low}}{p_{scale}}\right)^{fn} \cdot \left(\frac{p_{scale}}{p_{low} - po}\right)^{fn_{low}}$$

$$B_2 = \frac{1}{2\ln\left(p_{hi}/p1\right)}$$

$$fmax = f(p1) \cdot exp\left[\frac{1}{2}\, fn \ln\left(p_{hi}/p1\right)\right]$$

The parameters associated with this SURF implementation are shown in Table 2.

Table 2. SURF parameters for current implementation in XRAGE.

Parameters	XRAGE
p0 (GPa)	6.0
p_{low} (GPa)	8.0
p1 (GPa)	28.0
p_{hi} (GPa)	60
f_n	4.05
c	4.6×10^{-5}
P_{scale} (GPa)	1.0
n	3.2

Figure 3 shows a comparison of the shock strength function for SURF, as currently implemented and calibrated in the three codes, determined from the forms and calibrations above. The figure is divided into three different regions. The green region ranges from 0 to ~6 GPa and represents pressures which will deaden the PBX 9502. This deadening is the point at which the reaction rate drops precipitously. Note, both FLAG and PAGOSA show the deadening occurring around 2 GPa, whereas, this behavior in XRAGE occurs around 8 GPa. The yellow region represents the shock-to-detonation transition (SDT) pressures that are generally associated with Pop* plots. This pressure region is where dead zone determination or fragment impacts that could cause detonation are located. Within the SDT region, the black dotted box shows the input pressures that were tested and are presented in this paper. The pressures represent the practical extremes for the data acquisition. Beyond ~16 GPa, SDT transition occurs in less than 3 mm; fielding of particle velocity gauges in such a small zone is quite difficult. At pressures lower than ~10 GPa, the SDT distance becomes too large to field in the gas gun. The final region shown in red is the high-pressure region where SDT occurs in distances that are on the order of several hundred microns or less. At these pressures, the hot-spot rate should begin to saturate as the pressures approach the von Neumann pressures of a CJ detonation. For practical purposes, the initation distances at these pressures are all smaller than our typical model zone sizes.

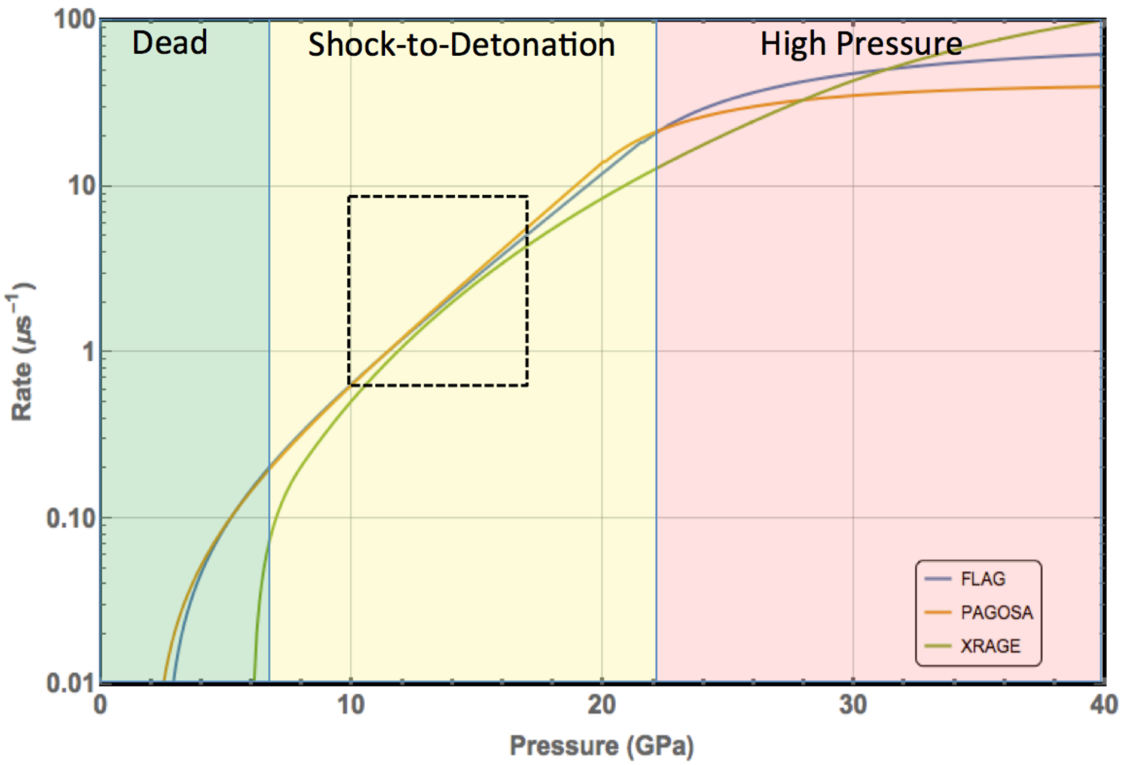

Figure 3: Comparison of SURF's shock strength function in FLAG, PAGOSA, and XRAGE. The region of pressure space explored in this paper is outlined by the dotted box.

One additional noteworthy difference is that each code uses different products and reactants equations of state coupled to the SURF parameters. FLAG uses Davis reactants and Davis products. PAGOSA uses a Mie Gruneisen reactants and JWL products equations of state. XRAGE uses SESAME reactants and SESAME products.

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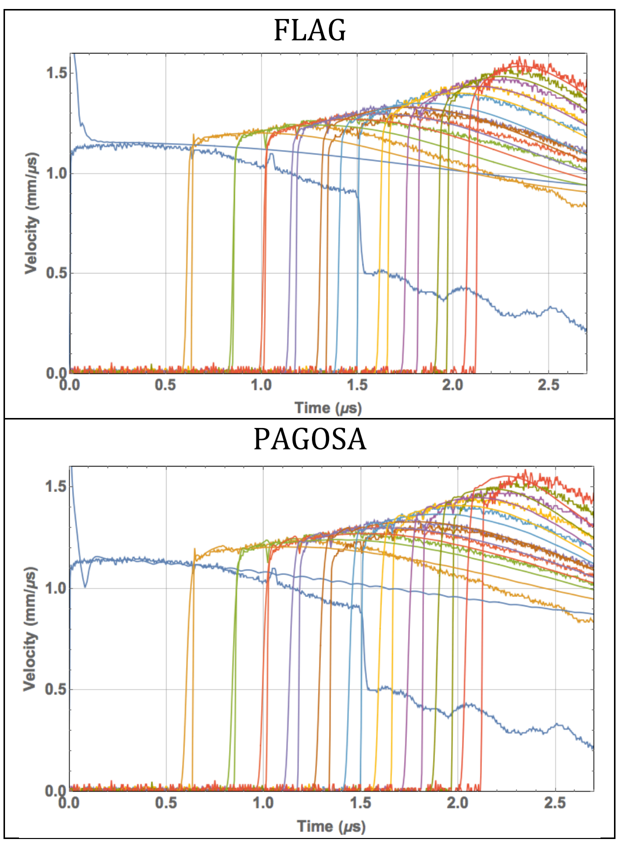
* Pop plots are unrelated to the POP graphing software and are instead named after Alphonse Popolato, one of the first scientists to note a relationship between input pressure and run-to-detonation distance. See Ramsey and Popolato.[6]

The assessment of those equations of state will be the subject of a subsequent WRL publication.[6]

Results

Similar input decks for three shock-to-detonation transition models were generated in all three codes. Each code used 100 μm zone resolution. In XRAGE, the AMR capabilities were turned off in order to ensure the zones were equivalent to the other two codes. Experiment 2S-58 represents one of the lowest input pressures studied. That experiment had an impact pressure of 10.85 GPa and a run-to-detonation distance greater than 15 mm.

Figure 4-Figure 6 show that all three SURF implementations and calibrations can capture the build up to detonation from a planar impact in the 10-16 GPa range. Overall, the models were able to match the particle velocity traces. In all cases, the modeled particle velocity at the impact surface showed little to no reaction. After the impact surface, the tracers all showed a slow increase in velocity as shock-induced reactions in the HE contributed to the particle velocity. Ultimately, all the models showed transition to detonation at roughly the correct probe location and distance.



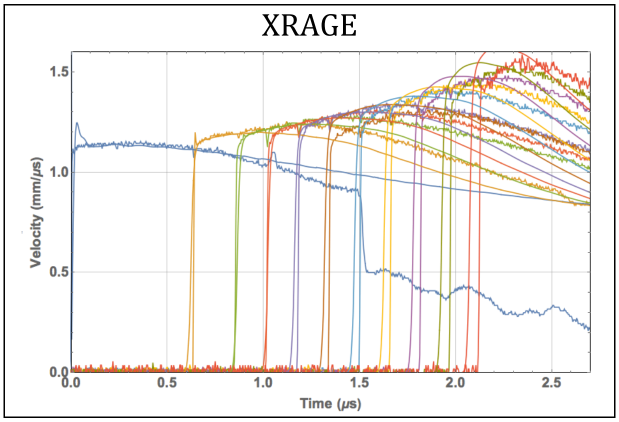
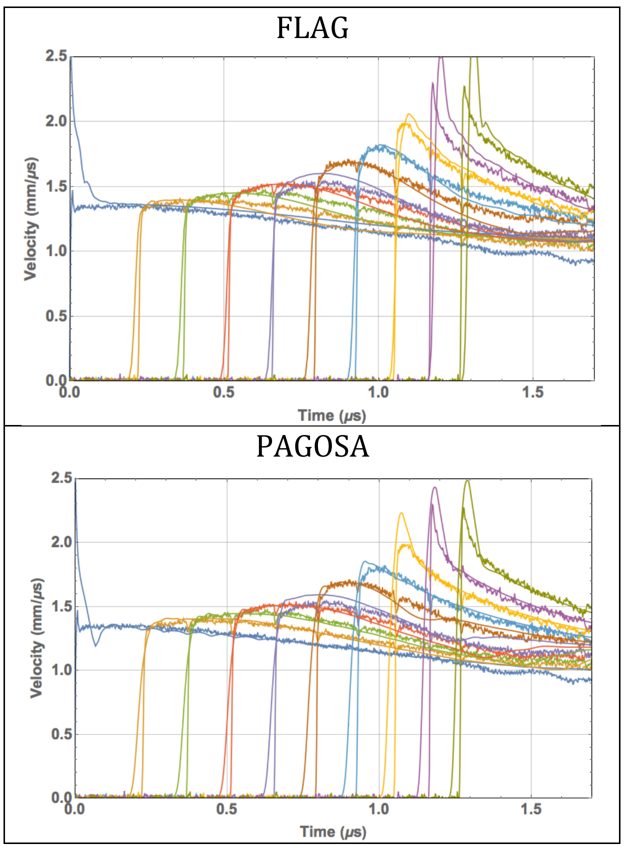


Figure 4: Comparison of SURF results for the lowest pressure experiment 2S-58 (10.85 GPa impact pressure). Gauges are located at 0, 3.1, 4.3, 5.1, 5.8, 6.6, 7.4, 8.2, 9.0, 9.8, and 10.6 mm from the impact surface.



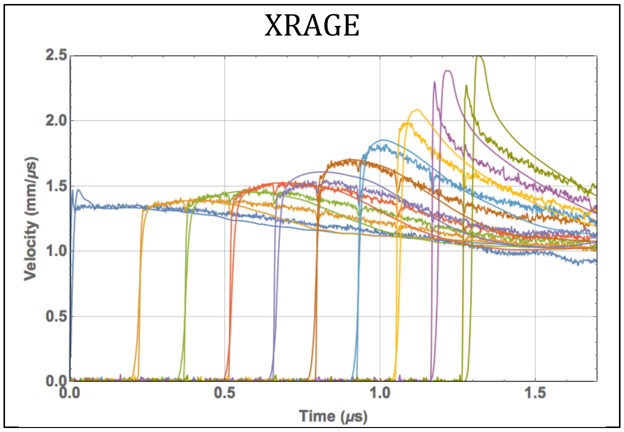
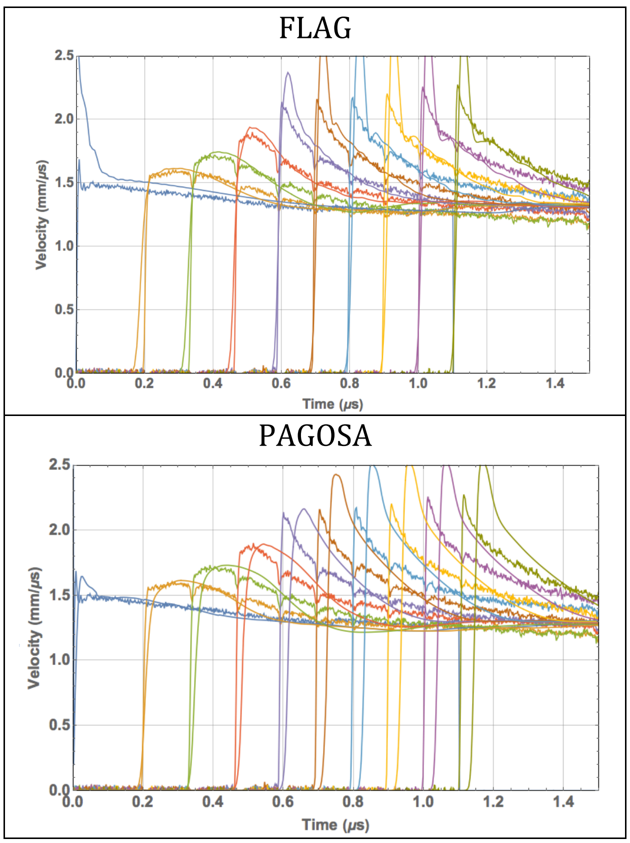


Figure 5: Comparison of SURF results for the mid pressure experiment 2S-118 (13.78 GPa impact pressure). Gauges are located at 0.0, 1.2, 2.0, 2.8, 3.6, 4.3, 5.1, 5.9, 6.7, and 7.5 mm from the impact surface.



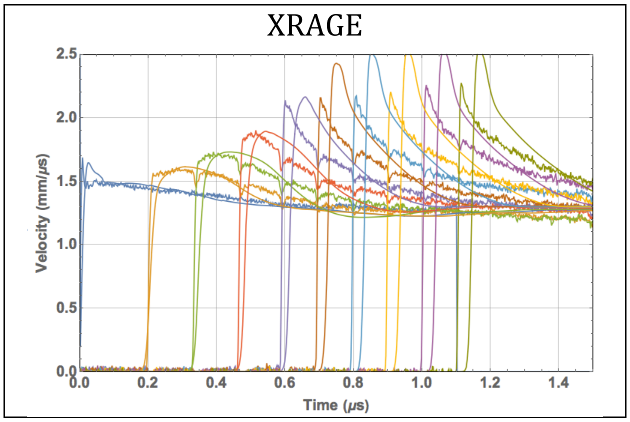


Figure 6: Comparison of SURF results for the highest pressure experiment 2S-85 (16.22 GPa impact pressure). Gauges are located at 0.0, 1.114, 1.93, 2.71, 3.51, 4.29, 5.08, 5.87, 6.66, and 7.46 mm from the impact surface.

All models showed some minor error when determining the detonation distance. The calibrations seem to miss the actual detonation location by ~1 probe (roughly 1mm). Since the detonation wave travels faster than the deflagration wave, missing the actual detonation location will result in a timing offset between shock arrival time when compared to the data. That is largely the cause of the timing shift between data and model seen at the last probe.

The experiments were designed to produce 1D shock behavior. FLAG and XRAGE used 1D models to compare with the experimental results. Additionally, we tested the codes in both 2D and 3D to note any significant deviation in model behavior. FLAG was tested in 1D and 2D. PAGOSA was tested in 2D and 3D (1D models do not exist in PAGOSA). No notable differences in model behavior were found as the dimensionality of the problem was increased. Thus, all three hydrocodes should be capable of predicting SDT behavior in 3D, provided zoning of 100 μm is used. If the zones were larger than 100 μm, SURFs ability to match the particle velocity traces degraded significantly. In large 3D experiments where zone sizes are substantially larger than 100 μm are used, using these calibrations, SURF will likely produce poor results. This will be the subject of a subsequent paper.

It should be noted that all codes used the SURF reactive burn model for PBX 9502. In XRAGE, however, the standard reactive burn model used for PBX 9502 is SURFplus. This model has additional capabilities to account for longer temporal duration carbon clustering reactions. Since none of the other codes have SURFplus, we chose to do a SURF only comparison.

Conclusions

We modeled a series of 1D shock-to-detonation impact experiments in FLAG, PAGOSA and XRAGE using the SURF reactive burn model. Each code has a different implementation of SURF resulting in different code-specific calibrations. With the current implementation and calibrations, all three codes were capable of predicting the SDT transition distance to within +/- 1 mm for shocks in the 10-16 GPa range.

The overall particle velocity profiles behind the detonation front were well matched to the experimental data. Over the input range of nominally 5-20 GPa, SURF should be effective in predicting the transition to detonation scenario as well as assess the presence of dead zones. It should be noted that this work only assessed the build-up to detonation portion of SURF. Subsequent work done on metal after detonation is controlled by the products equation of state. Future work will address how well calibrated the products equation of state is for the various implementations of SURF.

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