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Title: A Preliminary Assessment of the SURF Reactive Burn Model Implementation in FLAG

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A Preliminary Assessment of the SURF Reactive Burn Model Implementation in FLAG

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Abstract

Properly validated and calibrated reactive burn models (RBM) can be useful engineering tools for assessing high explosive performance and safety. Experiments with high explosives are expensive. Inexpensive RBM calculations are increasingly relied on for predictive analysis for performance and safety. This report discusses the validation of Menikoff and Shaw's SURF reactive burn model, which has recently been implemented in the FLAG code. The LANL Gapstick experiment is discussed as is its' utility in reactive burn model validation. Data obtained from pRad for the LT-63 series is also presented along with FLAG simulations using SURF for both PBX 9501 and PBX 9502. Calibration parameters for both explosives are presented.

Introduction

Real high explosive systems have engineering features such as inert interfaces and often consist of multiple layers of HE materials. Consider a modern initiation train which has an electric detonator filled with one HE (PETN) driving a detonation into a second HE (HMX) known as a booster which drives a stronger detonation into a third HE (TATB). Such systems are challenging for existing programmed burn methods but are readily treated with reactive burn methods provided calibration data is available. SURF[1,2] was implemented in FLAG (Matt Bement) to extend its reactive burn modeling capabilities. This report discusses the experimental validation of this implementation. The recently developed LANL Gapstick experiment[8] was used as part of this validation along with other traditional experiments[6] and recent pRad data collected in LT-63.

At this time SURF validation simulation runs in FLAG have been completed conforming to many experimental geometries, for example:

<u>*Embedded gauge gas gun experiments*</u>: Performed by Rick Gustavsen of M-9, Shock and Detonation Physics. Embedded electromagnetic gauges are used to measure the particle velocity in shocked HE generated by a planar flyer. These experiments are 1D owing to the fact that the gauges only record data in an area free from edge release waves. These experiments provide both run-to-detonation (HE pop-plot data) as well as unreacted Hugoniot information. Data exists for many explosives and is available for download from the LANL small-scale database. Variations discussed by Short[6] are also valuable validation tests (double shock, overdriven, short shock). It is important to note that calculations

for 1D shots are possible with extremely fine zone sizes (5 μm typical), which are a requirement for some reactive burn model formulations.

HE cylinder tests: HE cylinder is detonated inside an annealed OFHC Cu tube. PDV or streak is used to record wall expansion. This test is commonly used to calibrate the detonation product Hugoniot. Product Hugoniot calibrations can be obtained through analytic fits[8] or using genetic algorithms. This validation component is being completed with recent experiments with PDV probes recording wall expansion velocity[8,10].

LANL Gapstick experiments: This experiment consists of a repeating array of HE and inert pellets. At each interface a Kynar shock switch is installed. The experiment is detonated from one end and the switch network records wave arrival. As the thickness of the inert pellets is increased the average velocity across each HE pellet is reduced. For variable gap stick experiments the detonation trends slower at first and finally extinguishes past a critical pellet thickness.

LT-63: This series of pRad experiments studies converging shock waves in PBX 9502. The design consists of interior and exterior PBX 9501 charges, which are coupled to a common detonator at the top of the assembly. The interior detonation wave is below the initiation threshold for PBX 9502 therefore the material is pre-shocked when the exterior wave arrives. This is a very challenging test for a reactive burn model. This is currently our only experimental data which uses SURF for two different materials simultaneously.

Gas Gun Experiments

As previously mentioned embedded gauge gun data provide pop-plot data and unreacted equation of state information. Each gun shot represents a point on the pop-plot and possibly the unreacted Hugoniot as well. These experiments are also useful to study a reactive burn models' parameter sensitivity since the particle velocities measured encompass the run-to-detonation with an error on the order of 10 m/s. Highly resolved calculations conforming to these experiments take a few seconds to complete which makes them very useful in algorithm based calibration system. Figure 1 shows an example of typical gas gun data compared to simulation. The overshoot at peak particle velocity is normal and is a consequence of the measurement system clipping the signal at the jump off.

An error calculation function has been written in python to enable a detailed validation study. This python script runs the 1D gas gun shot FLAG input deck and then loads tracer data for plotting. The distance between each point in the simulated particle velocity trace and each point in the corresponding measured particle velocity trace is calculated. This value is then summed up over each gauge location and then summed over all tracers. The output is a numeric 'error' value that reflects how good (or bad) the comparison between model and data for a given set of SURF input parameters. This integrated error value can be used to score a parameter set for comparison against other candidate parameters sets.

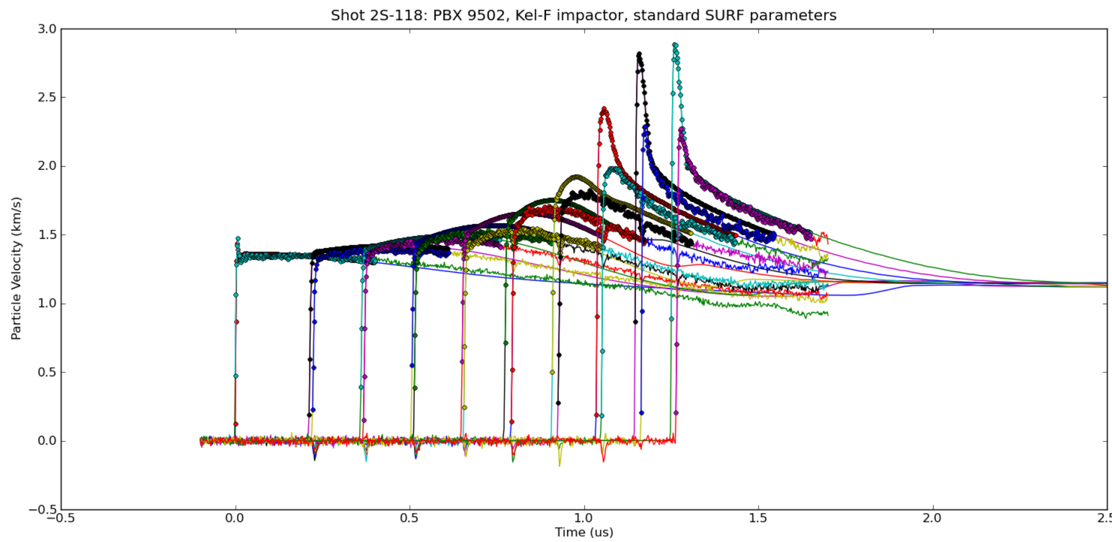

Figure 1 - 2S-118 data compared to values obtained using published SURF parameters. Integrated error is 145.5 for this comparison.

To understand and assess the quality of the SURF parameters for PBX 9502 it is important to know how the calculated error value changes with small, incremental variations in those parameters. The set of values selected represent a single point in Menikoff-Shaw hyperspace (M-S space). A detailed study of M-S space is crucial to properly design calibration algorithms seeking solutions on this field. For example, if M-S space is unimodal (like a hemispherical bowl in 2D) a downhill-simplex method might converge rapidly. However with more complicated solution surfaces downhill-simplex is prone to getting caught in local minima taking a great many iterations to converge (if convergence is attained at all). In figure 1, the published[2] SURF parameters have been ran and comparison made to shot 2S-118[7]. The associated error value for this run is 145.5. Note that in the figure the bold box values on the respective tracer curves are those used for the error calculation. It is also worthwhile to note that an integrated error of < 150 is normal and representative of a 'good' calibration.

Previously it was mentioned that the estimated experimental error in particle velocity is +/- 10 m/s. In Figure 2, the results are shown with projectile velocity at 2.7883 km/s which is 10 m/s less than the value used in Figure 1.

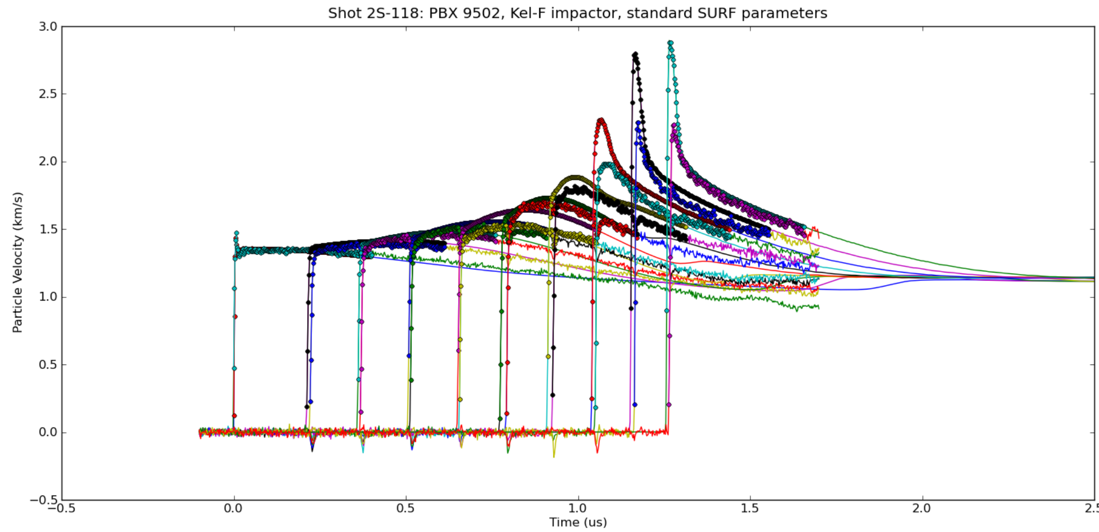

Figure 2 - Sim/Exp comparison at lower impactor velocity range. Integrated error is 136.98 for this run.

The SURF model was ran repeatedly in FLAG for this particular gas gun experiment with parameters varied from the published parameter set by +/- 5% of the author's values. The resulting error value calculated between simulation and experiment are shown in Table 1. From this analysis (and the analysis of the resulting particle velocity traces which are not included) we can infer that small adjustments in the SURF parameter values have small but measurable changes and in most cases the published values are the best. The exceptions are in the P0 and P1 values in which a 5% increase actually led to a better fit to data. This is likely due to a resolution change from that used by the SURF authors. It is worthwhile to point out that the error calculation changes in this brief parameter study are greater than those introduced by changes associated with experimental error.

In an exhaustive examination of available gas gun data (available for download via hed2.lanl.gov) one of the authors (Carver) studied the effect of mesh resolution on pop-plot agreement. It was observed that coarse resolution has a deleterious effect on pop-plot agreement to the extent that low-pressure shock inputs fail to detonate. This result implies that for simulations in which initiation performance is important (e.g. frag impact safety assessments) fine resolution (no larger than 25 μm) should be used.

TABLE 1 – Calculated error values between simulation and experiment for small parameter perturbations.

	-5%	As published	+5%
A	160.0	145.5	154.9
B	172.6	145.5	185.6
P0	145.7	145.5	144.7
P1	150.9	145.5	138.8

One final comment, out of curiosity I ran the case with P0 and P1 at +5% from published values along with a 10 m/s velocity reduction for the Kel-F impactor and the resulting error improved to 129.5, which is the best observed so far. In private communication with Ralph Menikoff he mentioned that he was not surprised that the published parameters were not optimal for FLAG since many other factors affect the reactive burn model performance (hydro, mesh strategy etc) and some amount of adjustment between codes is to be considered natural. Parameter refinement for existing calibrations as well as developing new calibrations for additional HE is an important part of our ongoing activities.

Cylinder Tests

Cylinder test experiments are useful to measure the metal pushing performance of HE. This test (like the gun experiments) are often used in calibration but both are useful in validation as well as a sanity check before proceeding to more complicated experiments. Detailed discussion of cylinder test setup, see Figure 3, and application of data are found in Jackson[9]. Simulations of the Pemberton[10] series in PBX 9502 were completed as part of this work. The FLAG inputs for these simulations as well as the SURF calibrations for PBX 9501 and PBX 9502 are available on xcp-confluence.lanl.gov.

Figure 3 - Cylinder test pre-shot configuration and during detonation (LLNL HE Reference)

Ensight output from a sample FLAG cylinder test simulation is shown in Figure 4. In the pressure profile a ridge is visible following the Taylor wave. At coarse resolution this reflected pressure ridge becomes pronounced and irregular due to increased numerical noise. This on axis noise was found with other reactive burn models as well and is not a flaw in SURF.

In our cylinder test runs the FLAG visar PDV package was used to record surface motion. This package attempts to recreate the line of sight on which the PDV measurement was made. A comparison of PDV data from Pemberton and our simulation is shown in Figure 5. Wall velocity at late time disagrees by 50-100 m/s. In simulations of PBX 9501 cylinder tests Zocher observed that agreement could be improved by increasing the pace of advection in the FLAG run.

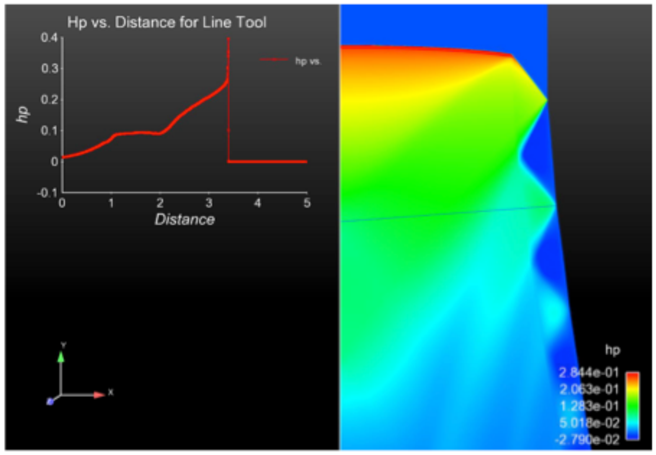

Figure 4 - Pressure field and centerline pressure profile from a PBX 9502 cylinder test simulation. Resolution is 50 μm.

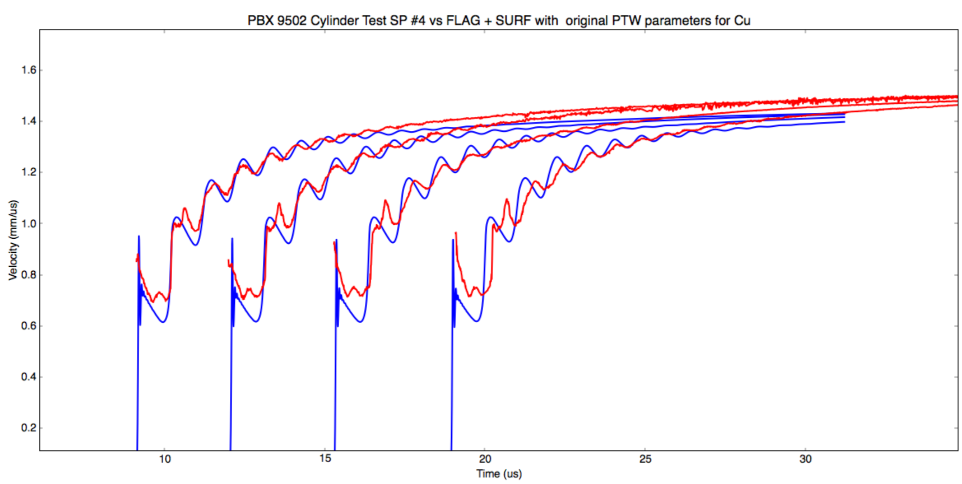

Figure 5 - Comparison between PDV and tracer data for a PBX 9502 cylinder test

The LANL Gapstick

The LANL gap stick is comprised of a succession of gap tests in which the acceptor HE in an upstream gap becomes the donor HE for a downstream gap. Gap stick experiments come in two varieties; constant gap thickness tests and variable gap thickness tests. In the variable gap tests the gap thickness must increase in the direction of flow. Inert gap material was chosen to be Kynar (polyvinylidene fluoride, PVDF) for its good shock impedance match to PBX 9501. An example gapstick test assembly is shown in Figure 6.

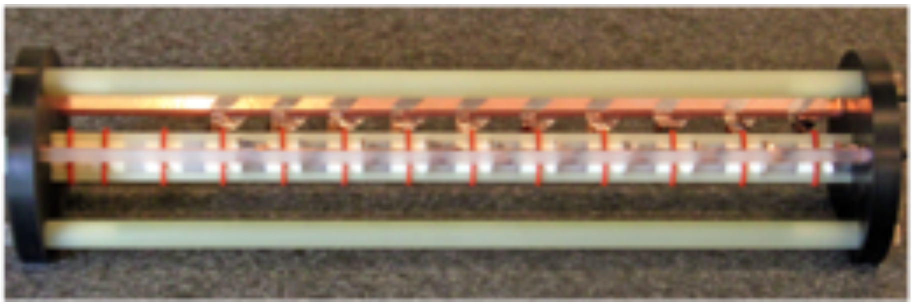

Figure 6 - Test assembly for a PBX 9501 gapstick experiment. The transparent pellets are the Kynar inert gaps and white pellets are ½" by ½" pellets of PBX 9501. Detonator installation is on the left end cap.

Gap stick tests are equipped with Kynar foil shock switches at each HE/gap interface. These switches are connected to a pulse-forming network. When a strong shock or detonation arrives at the foil switch it is shocked into conductivity thereby dumping a capacitor to ground. A pulse emanates from the other side of the capacitor, which is recorded on an oscilloscope. Resolution on the orders of a few ns can be obtained with this setup. For experiments without inert gaps this method is capable of determining detonation velocity to better than 2 m/s[8].

Operationally the gap stick test exercises the initiation behavior of an HE under progressively weaker divergent flow shock wave input conditions. Hill and Preston have obtained data in the HE PBX 9501 thus far and other materials are in consideration for future tests. The gap stick experimental data form an interesting validation test for reactive burn models since they have high time resolution and are inexpensive yet are capable of testing small changes in HE performance. Figure 8 shows a comparison between SURF, WSD, and IGRB simulations using FLAG and ALE3D.

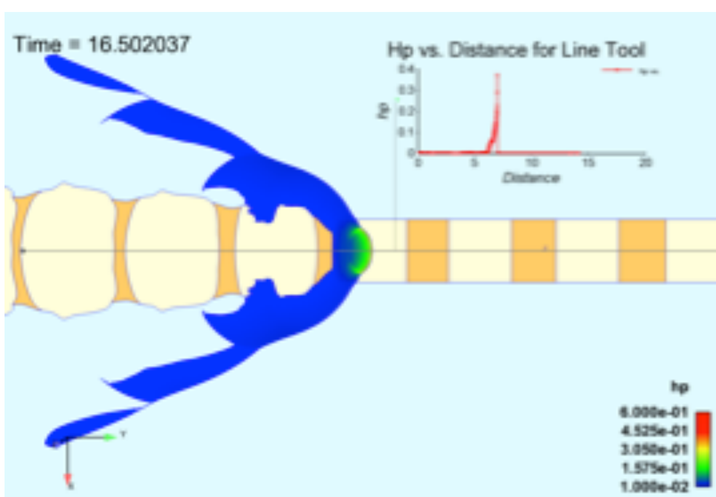

Figure 7 - Ensight output from a FLAG gapstick experiment simulation. Centerline pressure profile is inset at the upper right.

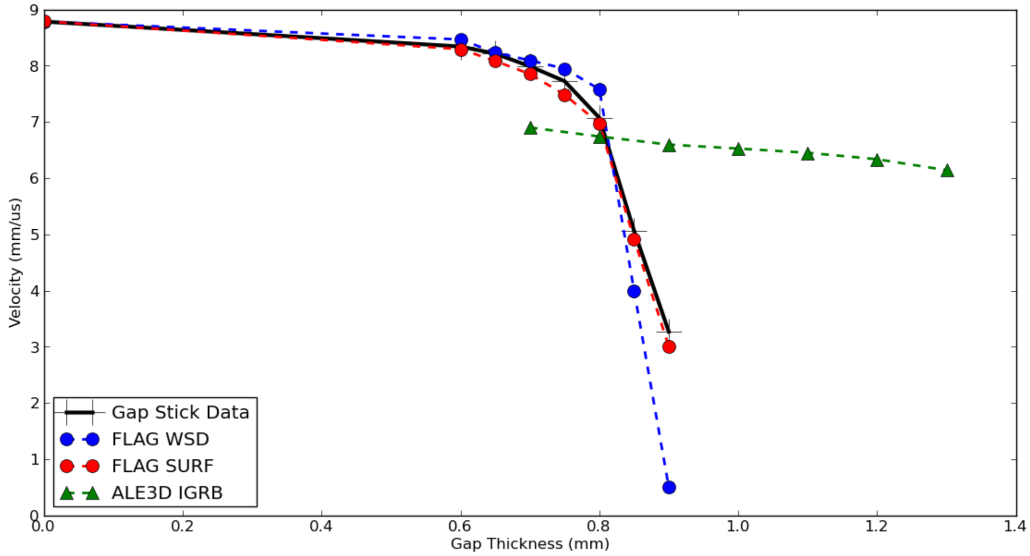

Figure 8 - A comparison between SURF, WSD, and IGRB models.

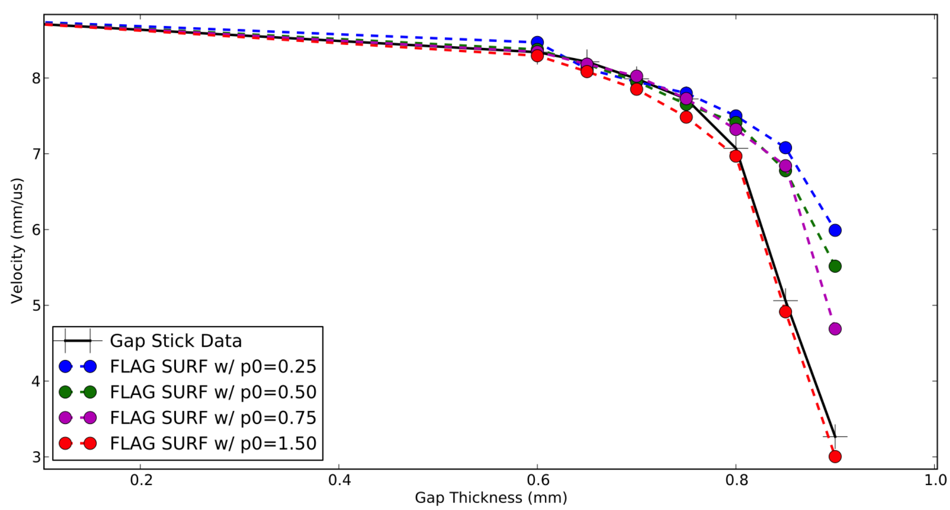

Figure 9 - Effect of small variations in the SURF P_0 parameter.

To assess the sensitivity of the SURF calibration to small variations in parameter value a series of simulations was performed while varying each value. Figure 9 shows the results in variations of the P_0 term. This term sets the reaction threshold and below P_0 no reaction occurs. As P_0 is increased from zero to 1.50 (the published value) performance improves smoothly and then finally agrees well with experiment.

LT-63

This shot series conducted at LANL's Proton Radiography facility was designed to study multi-shock wave interaction effects in PBX 9502. These tests were fielded by Terry Salyer of M-9 working with Greg Chavez in Q-15. This work as not yet been published. The experiment consists of a central cylinder of PBX 9501 surrounding by a layer of PBX 9502 as shown in Figure 10. An outer wrapping of PBX 9501 is added to ensure HE consumption. Both PBX 9501 sections are connected to a single detonator at the top of the fixture. After firing the detonator a detonation passes down the central column. This drives a shock wave radially outward into the PBX 9502 region but it does not initiate due to the low interface pressure from a narrow diameter PBX 9501. The inward travelling shock wave from the outer PBX 9501 region does detonate the PBX 9502 and interesting features are observed where the shocks converge. This experiment drives the HE through a range of performance states from sub-threshold to overdriven detonation and is a challenging problem for reactive burn models.

Simulations have been completed for two of the configurations in the series. Agreement with experiment has been disappointing. In Figure 11 it is clear that the PBX 9502 region is initiating early, a sign that the parameters are too sensitive. Adjustments have been made to the A and B parameters in SURF using pop-plot data (gas gun shots) and additional simulations are being performed to get a better agreement with the data if possible.

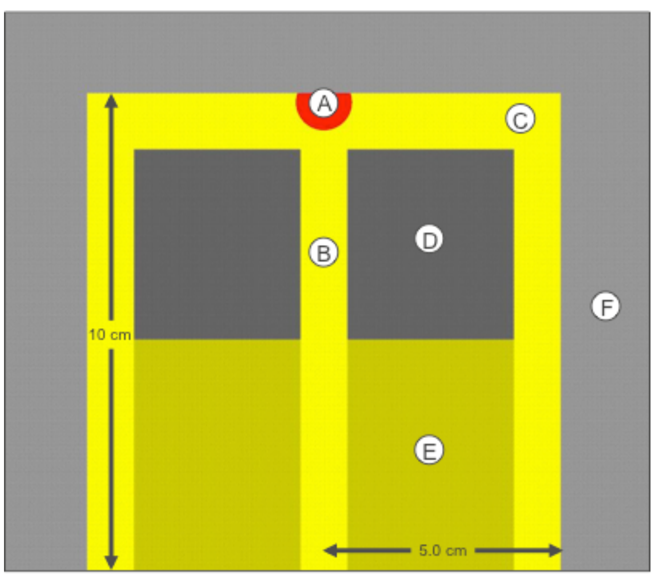

Figure 10 - LT-63 test geometry: part A is the detonator, B and C are PBX 9501, D is Kynar and E is PBX 9502.

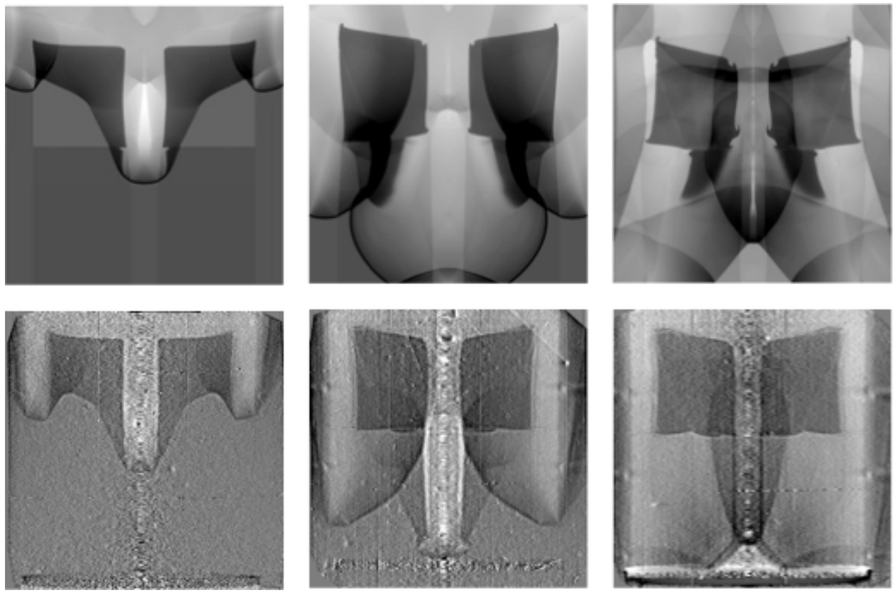

Figure 11 - Simulation (top row) compared to pRad shot 589 results (bottom row).

Conclusions

The FLAG implementation of the SURF reactive burn model has been tested against a variety of experiments and found to be satisfactory for general use provided users respect mesh resolution requirements. As a result of this validation process errors in the implementation have been identified and corrected. SURF in FLAG has been shown to be on par with the older WSD reactive burn model and superior to IGRB for detonation extinction assessments. Validation work remains to be done however particularly for 3D multi-wave systems as well as more complex double shock gas gun experiments.

Additional HE calibrations are needed to broaden the applicability of both FLAG and SURF; this effort would make additional experiments available for use in validation and make FLAG very attractive for a broad class of users. The presented parameters for PBX 9501 and PBX 9502 are available for download from xcp-confluence.lanl.gov.

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