LA-UR-16-24389

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Intended for: Report

Issued: 2017-01-31 (rev.2)

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Analysis of historical and recent PBX 9404 cylinder tests using FLAG

By

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X Theoretical Design-Primary Physics (XTD-PRI)

Abstract

Cylinder test experiments using aged PBX-9404 were recently conducted. When compared to similar historical tests using the same materials, but different diagnostics, the data indicate that PBX 9404 imparts less energy to surrounding copper. The purpose of this work was to simulate historical and recent cylinder tests using the Lagrangian hydrodynamics code, FLAG, and identify any differences in the energetic behavior of the material. Nine experiments spanning approximately 4.5 decades were simulated, and radial wall expansions and velocities were compared. Equation-of-state parameters were adjusted to obtain reasonable matches with experimental data. Pressure-volume isentropes were integrated, and resultant energies at specific volume expansions were compared. FLAG simulations matched to experimental data indicate energetic changes of approximately -0.57% to -0.78% per decade.

Introduction

The release of energy by detonating high explosives (HE) is a complex process, and the energy itself is difficult to quantify. With the nuclear weapons complex, cylinder tests have historically been used to infer energy release of high explosives and to calibrate the equations-of-state (EOSs) used by hydrodynamic codes that model HE detonation. A cylinder test comprises a stack of 0.5 or 1.0-inch diameter cylindrical pellets confined within a 0.10-inch thick copper confiner. The cylinder, usually 12.0 inches long, is detonated at one end, and the detonation products perform work on the surrounding copper, causing it to expand in the radial and axial directions.

Historically, this wall expansion was measured using the streak camera diagnostic, in which the cylinder was located in between a light source and the camera with a thin aperture oriented perpendicular to the cylinder axis. Within the camera is a mirror that rotates and projects the image from the aperture to a curved strip of film. The cylinder casts a shadow viewed by the aperture, and during detonation, the expanding copper wall increases the width of the shadow on the film as the mirror rotates. The width of the shadow is then used to measure the wall expansion as a function of time. These linear wall expansion data were time-differentiated to produce wall velocities in the radial direction. Limitations of the data typically reported from streak diagnostics are its low temporal and spatial resolutions, which are usually based on the shadow's position relative to the images of regularly-spaced fiducials that produce wall expansions markers along the film.

Recently, photon doppler velocimetry (PDV) has replaced streak camera measurements. PDV uses a single-wavelength laser aimed at the copper surface. As the wall accelerates, the reflected laser light is frequency-shifted and recombined with the source frequency. The differences in frequency result in an interference pattern with a "beat frequency" that is related to the velocity of the moving copper surface. Measuring and resolving this beat frequency using fast electronics produces a velocity record of the copper wall.

Description of experiments

Jackson [1] conducted two cylinder test experiments in 2015. A summary of the key geometric details for the historical and recent experiments is provided in Table I.

Wall expansion and velocity data using streak diagnostics for the three early experiments, circa 1967 and 1973, (K260235, K260237, and K260273) are recorded in the compilation of LLNL cylinder test data by McMurphy [2], and include 50 data points between wall expansion values of 0.2 mm and 32.0 mm. Los Alamos experiments conducted in the 1960s for shots C4526 and C4527 include 81 and 82 data points (streak), respectively, for wall expansion only. Experiments 8-1292 and 8-1293, performed at LANL in the early 2000s used PDV (8-1292) and both streak and PDV (8-1293) diagnostic methods, with the laser oriented 7° normal to the copper. The most recent tests by Jackson used only PDV diagnostics with lasers oriented normal to the copper.

Table I shows that the K- and C-series experiments were conducted with slightly thicker copper walls (approximately 2.59 mm) compared to the later experiments (approximately 2.54 mm). Minor variations in HE density and radius are evident in Table I, but as shown in Table II, the standard deviation of these are much smaller than the deviation in copper wall thickness.

Description of FLAG models

The LANL radiation hydrodynamics code, FLAG (ver 3.6.Alpha.15), was used to model the experiments listed in Table I. FLAG includes an extensive HE modeling capability allowing multiple options for describing solid and gaseous equations of state (EOS), strength of materials, detonics, and diagnostic methods. Table III lists simulation considerations used in this study. Given the narrow variations in HE density and radii over the series of experiments, only copper wall thickness was varied in this study. Additionally, EOSs are specific for given density. While minor variations in HE density will produce different results, density variations were not considered in this study due to its minimal variance across the series of experiments.

Although geometries may be specified with the FLAG input file, a separate LANL mesh-generating code, Ingen (ver 2.7.2), was used to create boundaries and the Lagrangian mesh for all experiments. Visualization and inspection of FLAG output was performed using Ensight (ver 10.1.6).

As with any model, assumptions are required to allow for accurate computation of physical processes within the constraints of computational resources, times required for the simulation, and limitations of numerical methods. In this study, the goal was to simulate 9 cylinder experiments spanning approximately 5 decades. Two materials are required: PBX 9404 high explosive, and annealed copper.

PBX 9404 is a plastic-bonded sensitive high explosive developed in the 1960s comprising primarily HMX (94%), and bonding and plasticizer agents nitrocellulose (NC) (3%) and tris-beta-chloroethylphosphate (CEF)(3%). Typical HE modeling applications within XTD division use two EOSs, one for the unreacted HE, and one for the gaseous explosive products. In this study, we apply the Grüneisen and Jones-Wilkins-Lee (JWL) EOSs to the reactants and gaseous produces respectively.

The copper confiner was also simulated with a Grüneisen EOS and a Preston-Tonks-Wallace (PTW) material strength model as described [3,4]. Table III lists the parameters used for the HE reactant and copper Grüneisen EOSs. Table IV presents the PTW parameters used to model copper strength.

Upon detonation, HE is converted from reactants to gaseous products at the so-called Chapman-Jouget, or "CJ" state, the pressure, temperature, and density at which the HE ignites. The physical state of these products is described by product EOSs, which for this case, is the JWL. The isentropic form of the EOS is shown in Eq. 1,

$$P(V) = Ae^{-R_1 V} + Be^{-R_2 V} + \frac{C}{V^{(1+\omega)}} \quad [1]$$

where A, B, C, R_1, and R_2, and ω are parameters that are typically fit to cylinder test data, and V represents the inverse of relative compression, V = v/v_0, where $v_0 = 1/\rho_0$ and $v = 1/\rho$. In FLAG, the JWL isentrope is specified by setting A, B, R_1, and R_2, and ω, and by setting the "heenergy" variable.

Burning of the HE is simulated using the Lund model, in which the detonation times at each node within the HE are pre-computed from the distance from the initial detonation point(s) and the detonation speed. The detonation point for this work is set to the center of the HE base surface.

Table I. PBX-9404 cylinder test geometries and HE ages.

Lab	Identifier	ρ_o (g/cc)	Detonation velocity (mm/µs)		ID (mm)	OD (mm)	HE Radius (mm)	Cu Thickness (mm)	PDV Probe Angle (deg)	Diagnostic	Age (Years)
LLNL	K260235	1.845	8.782	± 0.009	25.43	30.617	12.715	2.5935		Streak	< 3
LLNL	K260237	1.845	8.665		25.427	30.618	12.7135	2.5955		Streak	< 3
LLNL	K260273	1.843	8.783	± 0.059	25.433	30.648	12.7165	2.6075		Streak	< 3
LANL	C4526	1.847	8.787	± 0.001	25.43	30.62	12.715	2.595		Streak	3.5
LANL	C4527	1.847	8.783	± 0.001	25.43	30.62	12.715	2.595		Streak	3.5
LANL	8-1292	1.845	8.791	± 0.005	25.41	30.5	12.705	2.545	7 deg	PDV	37.5
LANL	8-1293	1.845	8.787	± 0.003	25.41	30.48	12.705	2.535	7 deg	Both	37.5
LANL	8-1874	1.845	8.81	± 0.005	25.41	30.48	12.705	2.535	normal	PDV	>46
LANL	8-1875	1.845	8.802	± 0.004	25.41	30.48	12.705	2.535	normal	PDV	>46

Table II. Variations in HE density, radius, and copper wall thickness.

	HE density (g/cc)	HE radius (mm)	Cu-Thickness (mm)
min	1.843	12.705	2.535
mean	1.8452	12.711	2.571
max	1.847	12.717	2.608
stdev	0.0012	0.0106	0.0744

Table III. Grüneisen parameters for PBX 9404 and copper.

Parameter	PBX 9404	Copper	Description
r0	1.843	8.94	reference density
g0	0.7989	2.02	Grüneisen gamma at reference density
a	0	0.47	internally overriden by FLAG
s1	1.737	1.489	Grüneisen coefficent s1
s2	0	0	Grüneisen coefficent s2
s3	0	0	Grüneisen coefficent s3
c	0.2339	0.394	bulk sound speed at reference density
cv	2.99E-06	3.84E-06	constant specific heat
tzero	300	294	zero-energy reference temperature

Table IV. PTW strength parameters for copper.

Parameter	Value	Description
r	0	rate smoothing parameter
theta0	0.025	Initial strain hardening rate
p	3	Constant modifying Voce' hardening law
kappa	0.17	temperature dependence material constant
gamma	8.00E-06	strain-rate dependence material constant
alpha	0.447	shear modulus constant
g_0	0.525	shear modulus at 0K
tm	1356	melting temperature
am	1.06E-22	average mass per atom
s0	0.0092	maximum saturation stress
sinf	0.0022	minimum saturation stress
y0	1.00E-04	maximum yield stress at 0K
y1	0.094	yield stress material constant
y2	0.575	yield stress material constant
yinf	1.00E-04	minimum yield stress
beta	0.25	yield stress material constant

The historical experimental data for PBX 9404 cylinder tests are tables describing radial wall expansion and radial wall velocities as a function of time, as streak data (early experiments) and PDV (recent experiments). To obtain output data that closely resembles the experimental data, the FLAG output function "VISAR_PDV" was applied to the simulation. Points in space relative to the cylinder were selected to approximate the positions of the experimental PDVs used in shots 8-1874 and 8-1875, and are shown in Fig. 1.

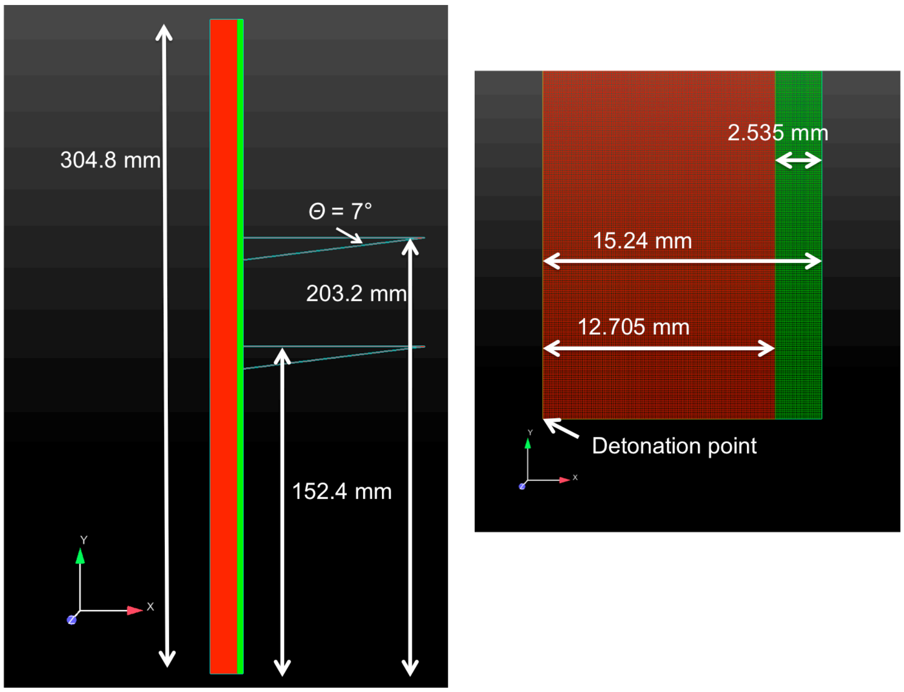

Figure 1. FLAG geometry of shot 8-1874.

The VISAR_PDV in FLAG simulates the PDV laser's position and detection of an interface, and therefore requires (a) a spatial coordinates, (b) direction, and (c) an interface to monitor. For this simulation, the spatial coordinates mimic the axial position of the PDV lasers in shots 8-1874 and 8-1875. PDVs were also oriented with directions normal to the copper boundary, and with a 7° tilt to simulate the orientation of the PDV lasers in shot 8-1293.

VISAR_PDV output reports the magnitude of the velocity of the desired interface along the specified laser direction vector, and the coordinates of the intersection of the direction vector at the specified interface at a user specified frequency, in this case which was set to 0.1 μsec.

In addition to VISAR_PDV output, this simulation also included tracer particles located on the copper outer boundary. While VISAR_PDV tracks the velocity and coordinates of an interface along a specified vector, any number of tracer particles may be positioned anywhere throughout the volume. Their coordinates, also reported at a frequency of 0.1 μsec, can be used to track the Lagrangian "flow" of material, and are also convenient for examining the shapes of surfaces.

Shot 8-1874 was used as the reference experiment for this study. A 100 μm/zone mesh was created using the geometries described in Table I using Ingen. Given the cylindrical symmetry of this problem, each experiment was modeled as a half-cylinder, with the minimum x-axis representing the axis of the cylinder, as shown in Fig. 1. To prevent mesh tangling, the bottom and top of the cylinder were modeled as fixed boundaries, allowing material flow in the radial direction only. In addition, a slide-line boundary was introduced between the HE and copper to prevent the mesh from tangling as a result of shearing along the interface as the detonation progressed axially along the cylinder.

Methods & Results

FLAG was run for shot 8-1874 iteratively, each time adjusting the A, B, R_1, R_2, and heenergy variables. The JWL is a thermodynamically-consistent relationship between pressure and volume, and the parameters are closely tied to detonation properties, as described by the CJ state. Briefly, the CJ state derives from the jump condition, in which during a detonation, a material instantaneously changes from an inert state at a given pressure and volume (P_0,V_0), to a compressed new state (P, V) at which point the detonation gaseous products following a new pressure-volume relationship. In P-V space, the line connecting (P_0,V_0) to (P, V) is the Rayleigh line, and (P,V) represents the CJ state, denoted by (P_{cj}, V_{cj}). The Rayleigh line is tangent to the detonation product P-V isentrope, described by the JWL.

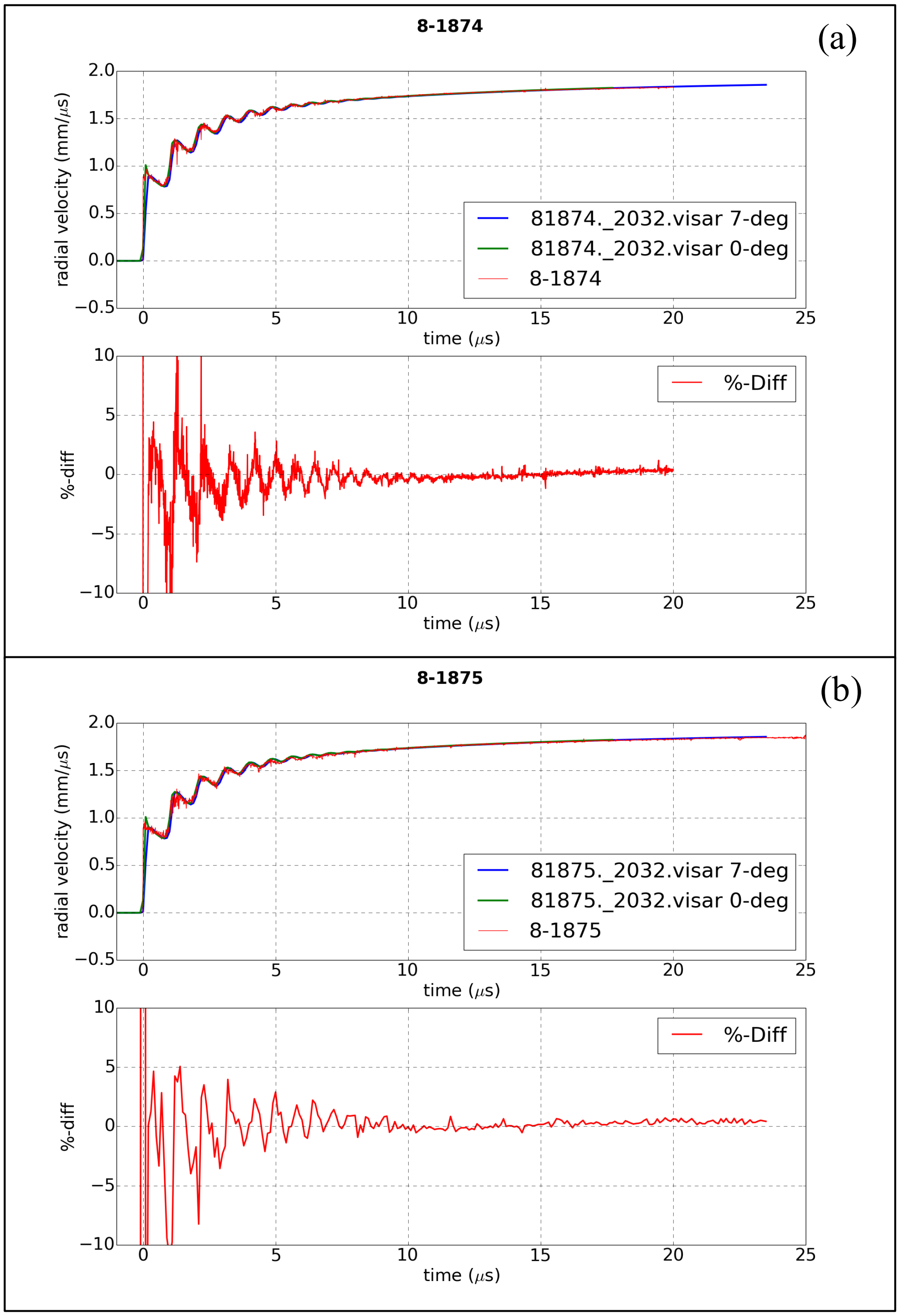

Figure 2. FLAG simulations (blue and green curves) and PDV measurement data for shots 8-1874 (a) and 8-1875 (b) with JWL EOS parameters obtained via iteration. Percent-differences are also shown.

The detonation speed, D_{cj}, P_{cj}, and V_{cj} are all interrelated to each other, and to the JWL parameters. Thus, changing any of the parameters will change the CJ state. Therefore, care must be taken to alter the parameters in a way that preserves the thermodynamically consistent nature of the JWL, while also producing pressure distributions capable of producing the desired wall motion.

Following each iteration, the PDV wall velocities were compared to the measured data until a reasonable match was obtained. Fig. 2 shows the FLAG 8-1874 and 8-1875 wall velocities compared to experiment after JWL parameters were determined.

The JWL parameters that were found to match shot 8-1874 were then applied to the other 7 experiments, and for each experiment (except for 8-1875, which as found to be sufficiently close to 8-1874), the process of JWL parameter alteration was repeated.

For the K- and C-series shots, for which the streak camera was the primary diagnostic, the raw data are the wall expansion measurements as a function of time. For these shots, wall expansion data were compared during the iterative JWL adjustments. Wall expansion data for shot K-260235 with the JWL matched to 8-1874 are shown in Fig. 3a. This figure indicates that cylinder wall in the FLAG simulation is expanding a lower rate than measured by experiment. In Fig. 3b, the JWL was adjusted to achieve a wall motion very similar to experiment.

Equation 1 is the isentropic form of the JWL. FLAG's implementation of the JWL precludes the use of the "C" parameter, and instead implements the "heenergy" variable. As previously mentioned, the interrelated nature of the JWL parameters required a method to translate the FLAG parameters to the parameters of Eq. 1, thereby allowing for Eq. 1 to be integrated according to Eq. 2, to determine the energy for each shot [5].

$$\mathrm{E} = -\int_{V_{cj}}^{\infty} P(V)dV \qquad [2]$$

A Mathematica script was written by T. Aslam to solve the system of equations to compute "C" and the CJ state parameters from the FLAG-adjusted JWL parameters. Additionally, a Python subroutine written by G. Maskaly was used to verify computation of the CJ state. Lastly, as an additional check, pressure-volume distributions were extracted for each experiment using Ensight, and JWL parameters (except for ω, which was held constant at 0.28) were fit to the data via linear regression. Figure 4 shows the isentrope and corresponding JWL parameter fits for shot C4526. Table V presents the FLAG and fit JWL parameters, in addition to the CJ state for for all experiments.

Given the complete parameters needed for the JWL, a Python script was written to integrate each experiment's JWL between each experiment's V_{cj} and upper limits ranging between $1.0 \leq V/V_0 \leq 10.0$, subtracting the mechanical energy used to compress the explosive to the CJ state. An example of the integration and subtraction schema is presented in Fig. 5 for shot 8-1874.

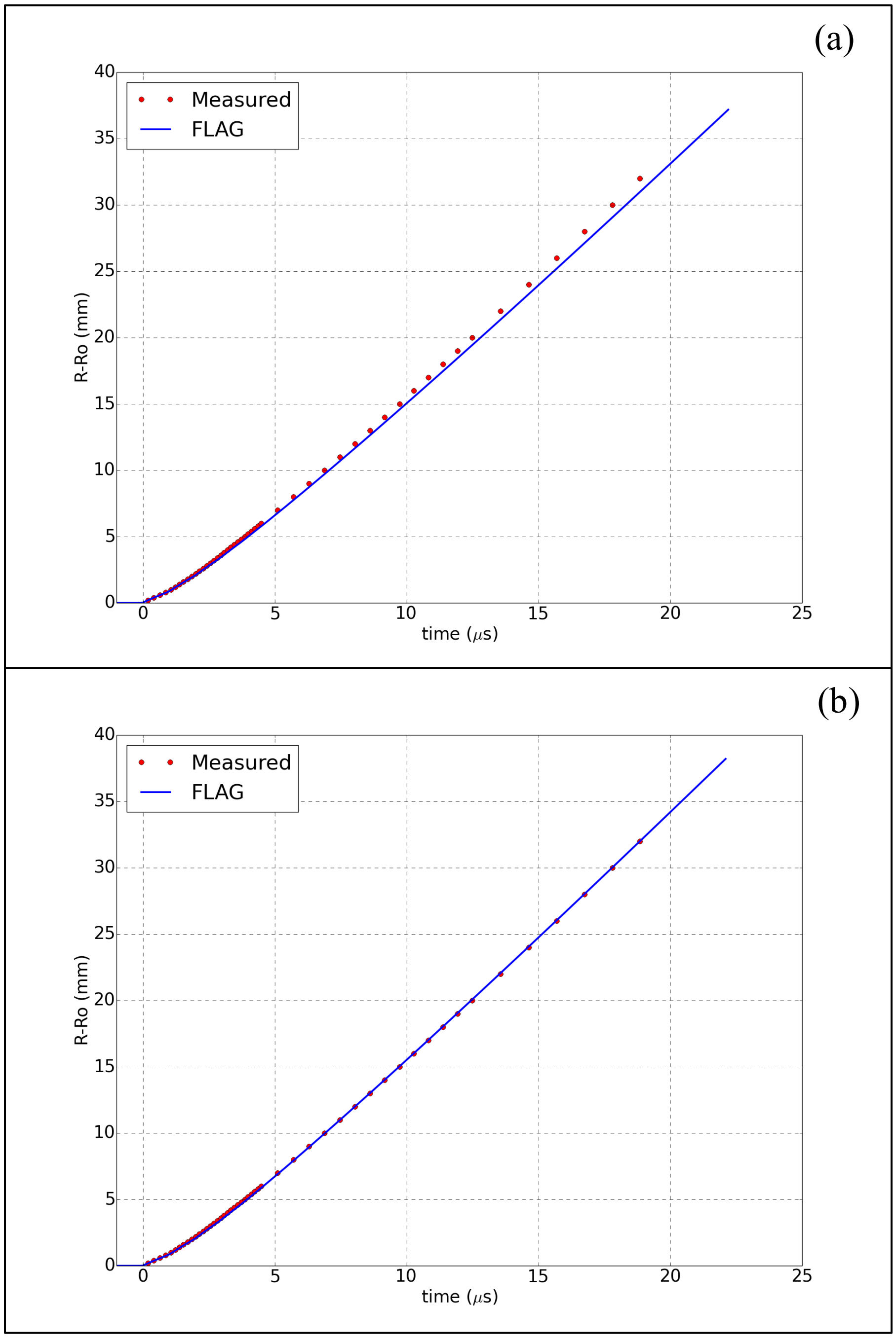

Figure 3. The JWL used to match shot 8-1874 is applied to shot K-260235 (a), and then adjusted (b) to match the measured data.

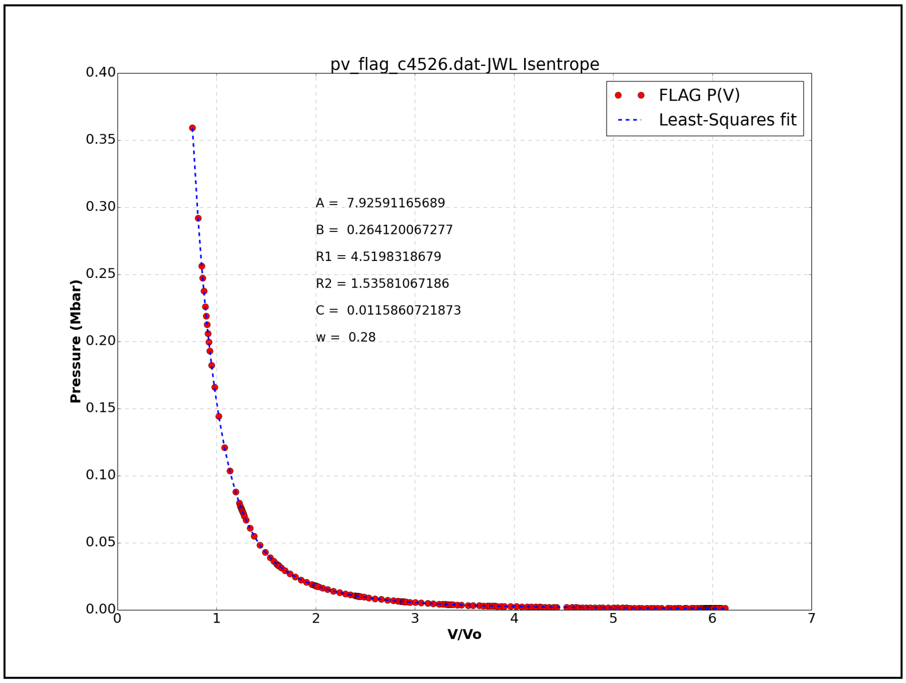

Figure 4. Pressure-volume distribution from FLAG for shot C4526, and corresponding JWL parameter fit.

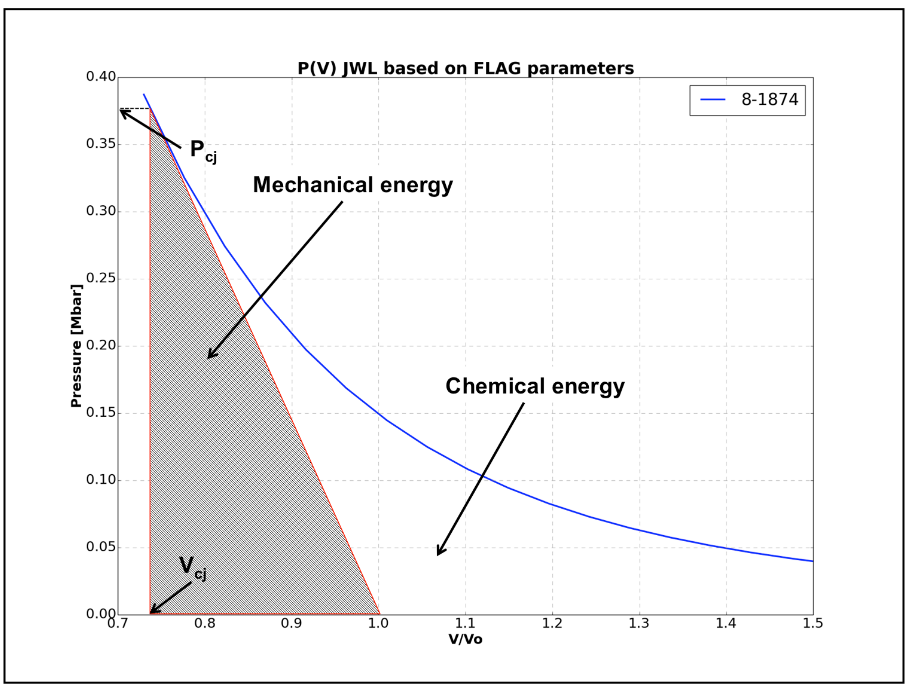

Figure 5. Isentrope, CJ state, and energies for shot 8-1874.

The shaded triangle represents the mechanical energy required to compress the HE from initial density (V/V_0 = 1.0) to the CJ state. The total energy under the curve is described in Eq. 2.

Subtracting the area in the shaded triangle yields the chemical energy of the HE, according to Eq. 3[6].

$$E_{chem} = -\int_{V_{cj}}^{\infty} P(V)dV - \tfrac{1}{2}P_{cj}(1-V_{cj}) \qquad [3]$$

By computing Eq.3 for each experiment, replacing the upper limit of infinity to expansions between $1.0 \leq V/V_0 \leq 10.0$, one obtains the integrated energies shown in Fig. 6. By plotting the energy values as a function of approximate age at V/V_0 = 1.9, 6.0, and 8.0 (the red dashed lines in Fig. 6), and normalizing a linear fit, one obtains Fig. 7, which shows the relative change in energy as a function of age. Approximate energy changes of -0.78%, -0.67%, and -0.57% per decade are evident at expansions of V/V_0 = 1.9, 6.0, and 8.0, respectively.

Discussion

As pointed out by Jackson, the early K-series data exhibits a larger measurement variance compared to later experiments. Little information is known about the lots and ages of the materials used for these shots, and the copper wall thicknesses were slightly larger than standard. More information is known about the C-series shots, and the variation between these data is much less. The temporal resolution of the streak measurements is lower than that obtained using more modern techniques. Using the early data as the *de facto* standard for matching FLAG EOS parameters therefore ignores any measurement uncertainties present in those experiments.

Within the FLAG simulations, uncertainties are associated with (a) characterization of the material properties chosen for PBX 9404 and annealed copper, (b) choice of detonation physics models, (c) choice of the EOSs describing the states of the reactants and products, and (d) numerical approximations used for hydrodynamic computations, including zone resolution, fixed boundaries, slide lines.

Many plastic-bonded high explosives are formulated as powders, then processed with coatings, and formed into billets so the material may then be further processed (e.g., machined, or pressed) for various applications. The processed material is therefore heterogeneous at the micrometer level, containing grains of various sizes, voids, and different materials, despite having a nominal mass density. These heterogeneities lead to local hotspots and jetting that may change the behavior of the HE during detonation. In this study, we ignore heterogeneities within PBX 9404, and assume both the HE and the copper are homogeneous and of uniform density. Although minor differences in density of < 0.22% were measured between the experiments (Table I), offline FLAG simulations including these effects show minimal effect on the wall motion (<1%), and were therefore not included. With these assumptions, the program burn detonation model used was considered reasonable for this study. In future analyses, use of more sophisticated models such as reactive burn, and detonation-shock-dynamics that account for local composition and shock front curvature, is recommended to determine if these techniques suggest similar HE trends.

In this study, adjustment of the JWL parameters was a manual and therefore inefficient process. Figures in Appendix A show that, in general, the manually-edited JWLs produce wall expansions within < 0.2 mm of measurements (for K- and C-series shots) and velocities <1% in the incompressible wall motion regions > 5-7 μsec. It is therefore possible that an automated approach to searching the JWL parameter space might produce wall motions with smaller differences from measurements.

Differences in zone resolution were not investigated in this study. It is possible that increasing resolution may more accurately simulate the curvature of the detonation front as it performs work on the copper wall. However, offline-simulations of self-similar planar HE detonation waves, both supported and unsupported, do not indicate improvements in the shape of the shock front as the resolution increases above 4000 zones per cm [7].

Conclusion

FLAG simulations were performed for 9 PBX 9404 cylinder tests conducted between 1964 and 2015. To match historical cylinder test experimental data the gaseous products EOSs within FLAG simulations were manually altered, resulting in EOSs that were directly evaluated via integration. These simulations accounted for copper strength, consistent with the widely-used PTW model for copper, used program burn and Lund detonic models, and were computed with a resolution of 100 μm/zone. Integrated JWLs indicate energy changes of -0.78%, -0.67%, and -0.57% per decade at expansions of V/V_0 = 1.9, 6.0, and 8.0, respectively.

Acknowledgements

The authors wish to thank Tariq Aslam (Shock and Detonation Physics group, M-9) for insightful conversations during this project and for assistance with CJ state computations.

Table V. JWL and CJ state parameters used in FLAG, and as determined using CJ state solves and linear regression fits.

		k260235	k260237	k260273	c4526	c4527	8-1292	8-1293	8-1874
FLAG	A	9.290371175	7.3	8.5	7.6	7.6	7.696566552	7.696566552	7.696566552
	B	0.275	0.235	0.205	0.245	0.25	0.204099805	0.204099805	0.204099805
	R1	4.85	4.45	4.6	4.45	4.455	4.455	4.455	4.455
	R2	1.45	1.45	1.49	1.5	1.5	1.485	1.485	1.485
	ω	0.28	0.28	0.28	0.28	0.28	0.28	0.28	0.28
	D_{cj}	0.877034084	0.874845749	0.885378155	0.891475972	0.89117665	0.882937339	0.882937339	0.882937339
	heenergy	0.063548562	0.059576777	0.065534455	0.060900705	0.061893652	0.063548562	0.06321758	0.061893652
Fit to P(V)	A	10.21752626	6.648845595	8.259777879	7.925911657	7.81019032	8.393983234	8.337457264	7.819673474
	B	0.299819948	0.200846307	0.195287843	0.264120067	0.263150268	0.242960778	0.240236135	0.21138129
	C	0.012480244	0.009939248	0.015930541	0.011586072	0.01178257	0.014747634	0.0145685	0.013645811
	R1	4.992261003	4.295040489	4.554285112	4.519831868	4.501276479	4.598790534	4.588017952	4.480596846
	R2	1.494012284	1.374204831	1.466901121	1.535810672	1.524485294	1.569319715	1.563934994	1.501967496
	ω	0.28	0.28	0.28	0.28	0.28	0.28	0.28	0.28
T.Aslam	C	0.0121624	0.0105829	0.0160396	0.0104397	0.0117067	0.0144121	0.0142473	0.0135872
	V_{cj}	0.739125935	0.729475987	0.740436308	0.729706362	0.730401173	0.734702735	0.734783827	0.735113724
	P_{cj}	0.369817	0.381587	0.373556	0.396183	0.394611	0.381549	0.381187	0.379736
	D_{cj}	0.877033	0.874845	0.883675	0.891801	0.891176	0.883377	0.883094	0.881958
G. Maskaly	V_{cj}	0.739140625	0.729492188	0.74046875	0.731054688	0.730390625	0.7346875	0.734765625	0.735078125
	P_{cj}	0.369797334	0.381564002	0.373508353	0.392609554	0.394627574	0.381570894	0.381214042	0.379786334
	D_{cj}	0.877033122	0.87484502	0.883675191	0.889991328	0.891176142	0.883377017	0.883093875	0.881958376

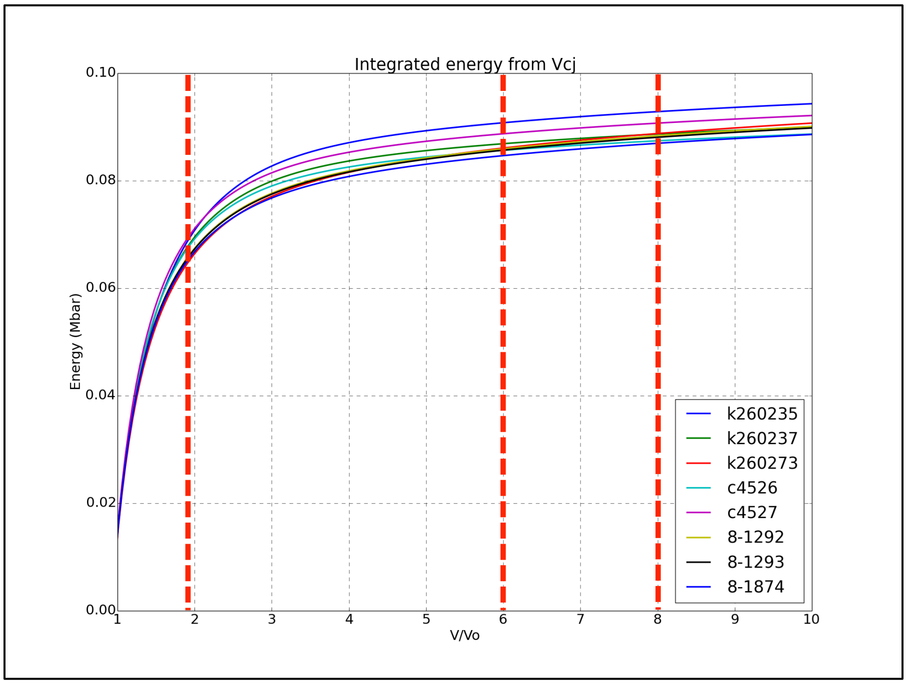

Figure 6. Energies obtained by integrating each experiment's JWL between V_{cj} and V/V_0 between 1.0 and 10.0. Vertical lines at V/V_0 = 1.9, 6.0, and 8.0 are indicated.

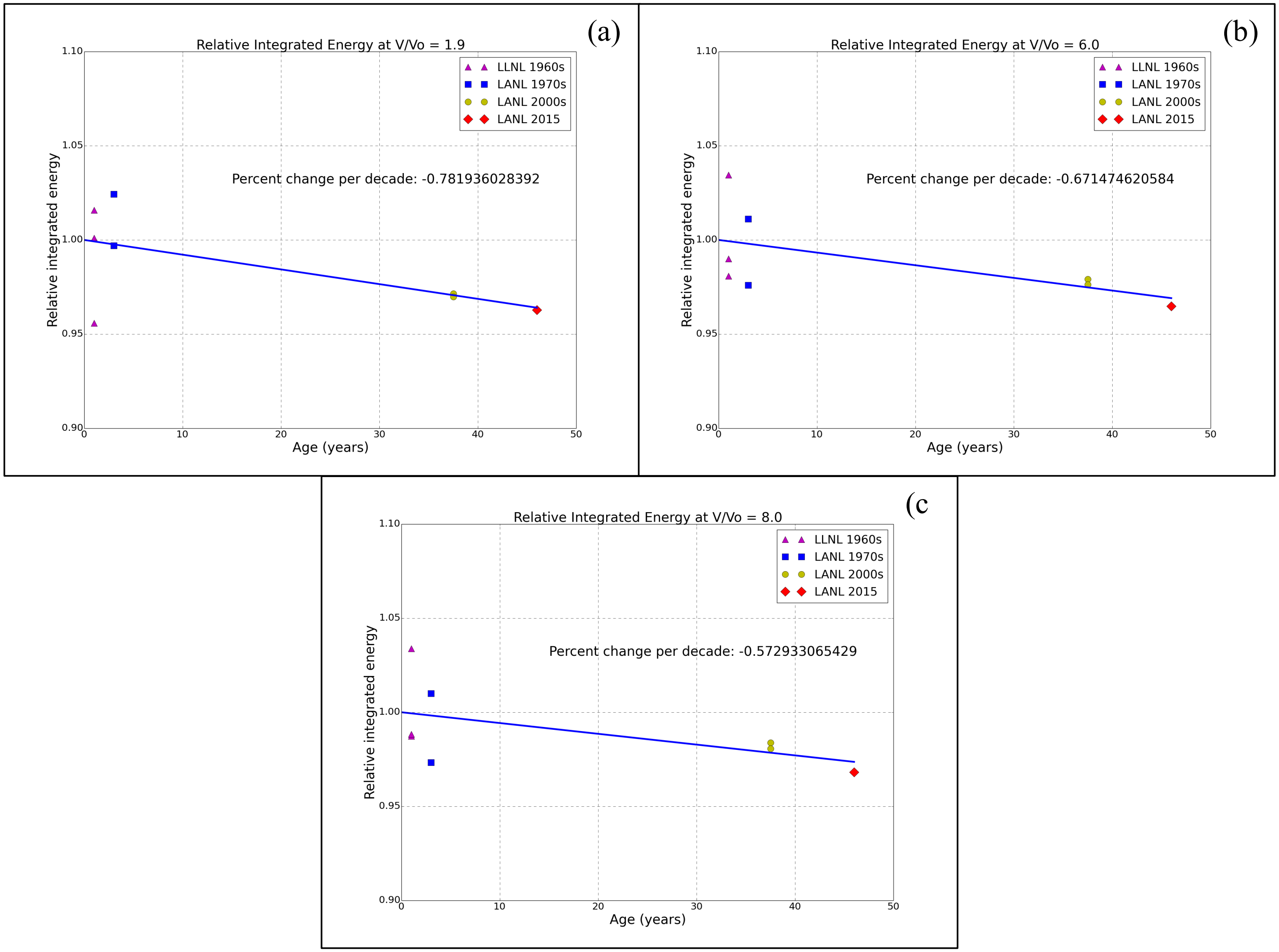

Figure 7. Energy changes for PBX 9404 for V/V_0 = 1.9, 6.0, and 8.0

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Appendix A.
Wall expansion and velocity profiles

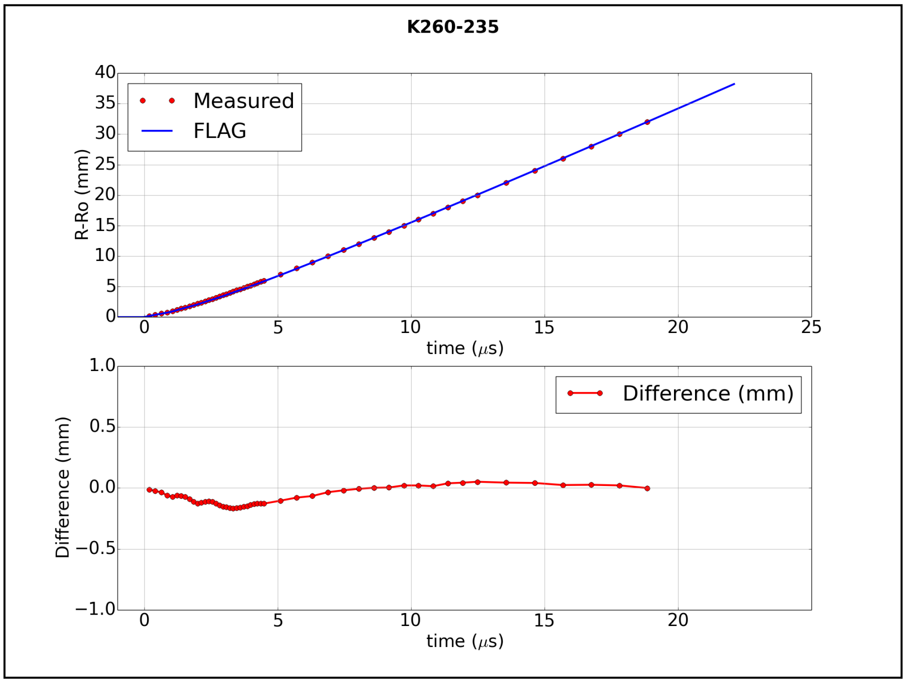

Figure A.1. Wall expansion, FLAG vs. measured, for shot K-260235

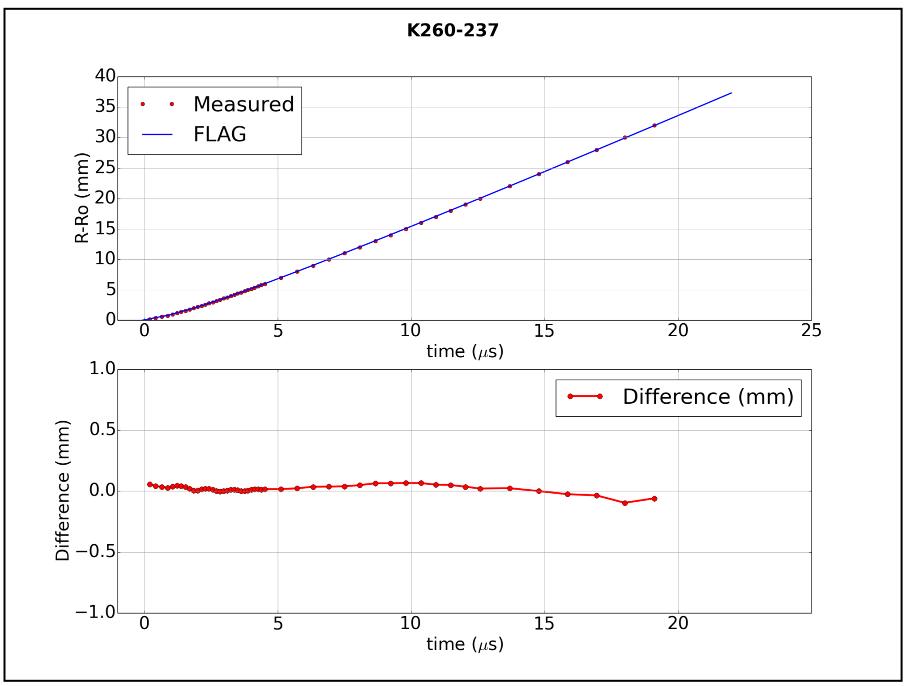

Figure A.2. Wall expansion, FLAG vs. measured, for shot K-260237

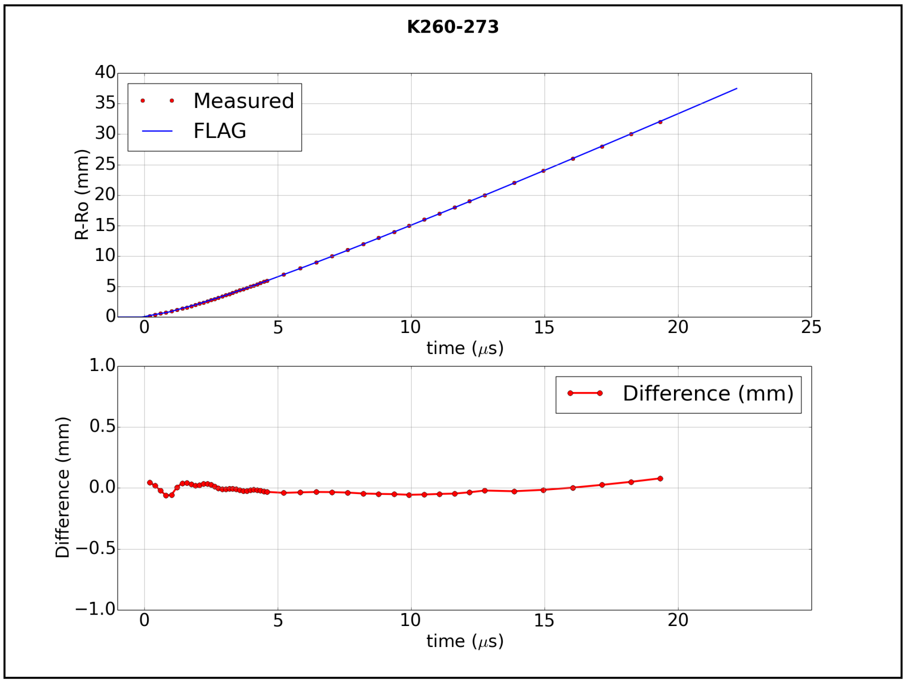

Figure A.3. Wall expansion, FLAG vs. measured, for shot K-260273

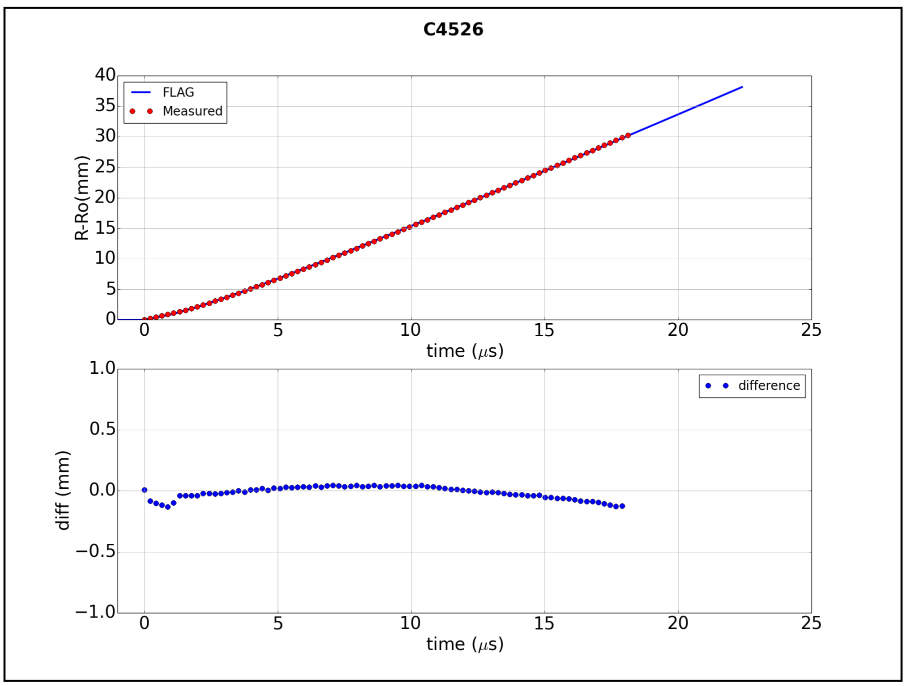

Figure A.4. Wall expansion, FLAG vs. measured, for shot C4526

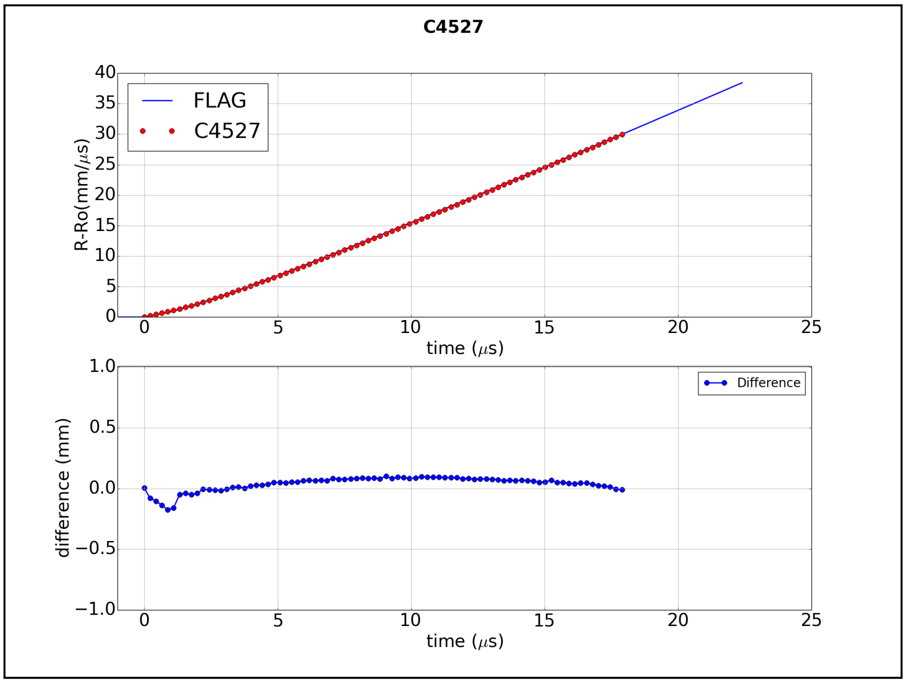

Figure A.5. Wall expansion, FLAG vs. measured, for shot C4527

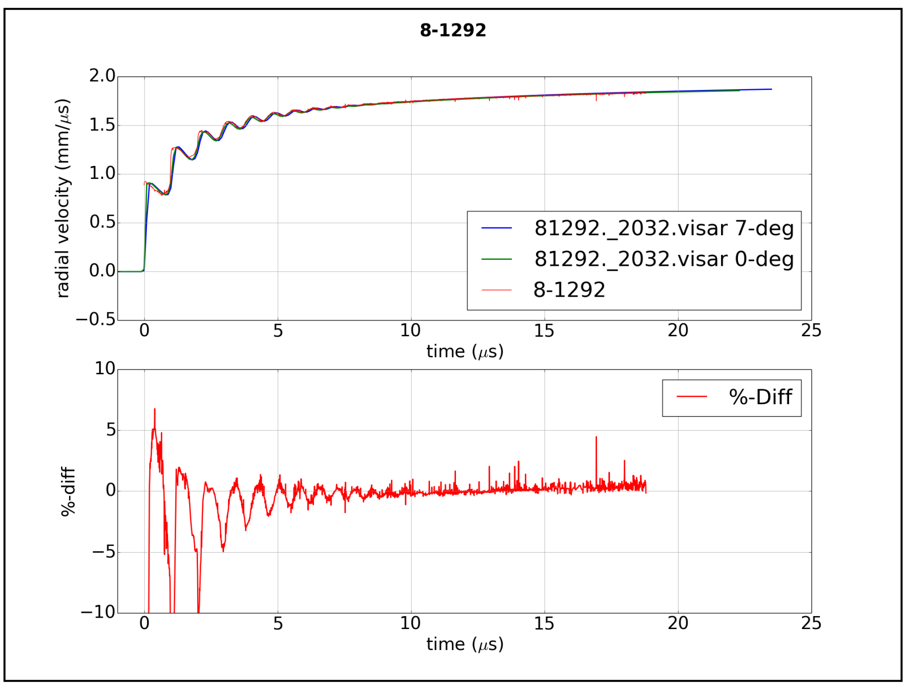

Figure A.6. Radial wall velocity, FLAG vs. measured, for shot 8-1892

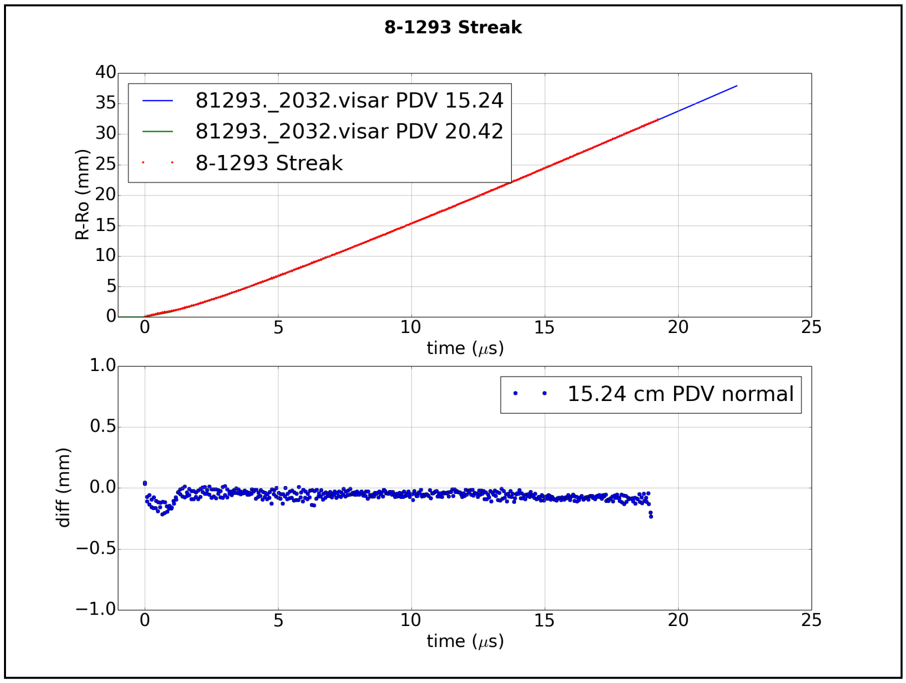

Figure A.7. Wall expansion, FLAG vs. measured, for shot 8-1293

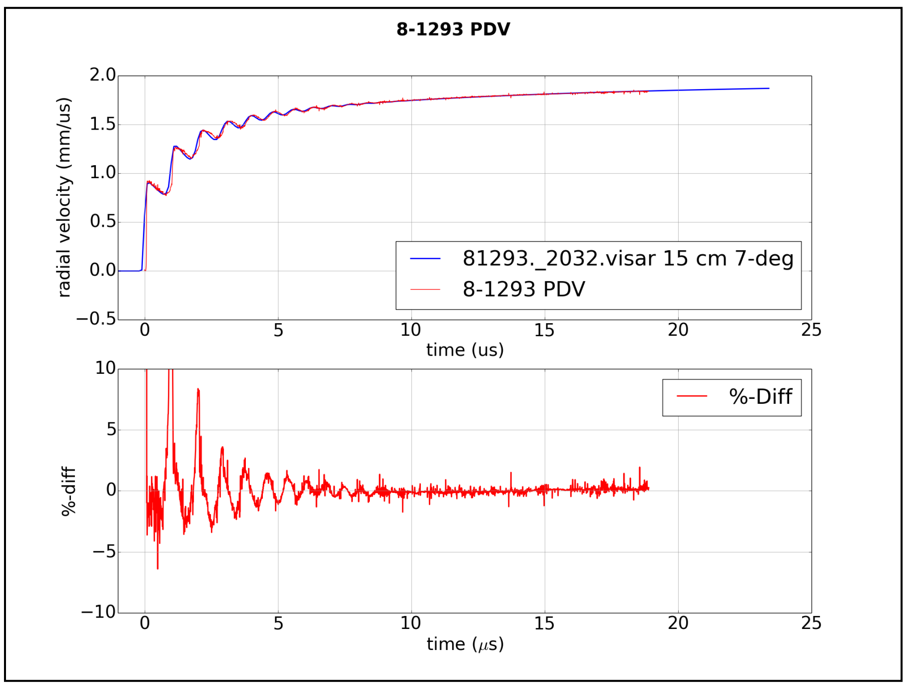

Figure A.8. Radial wall velocity, FLAG vs. measured, for shot 8-1893

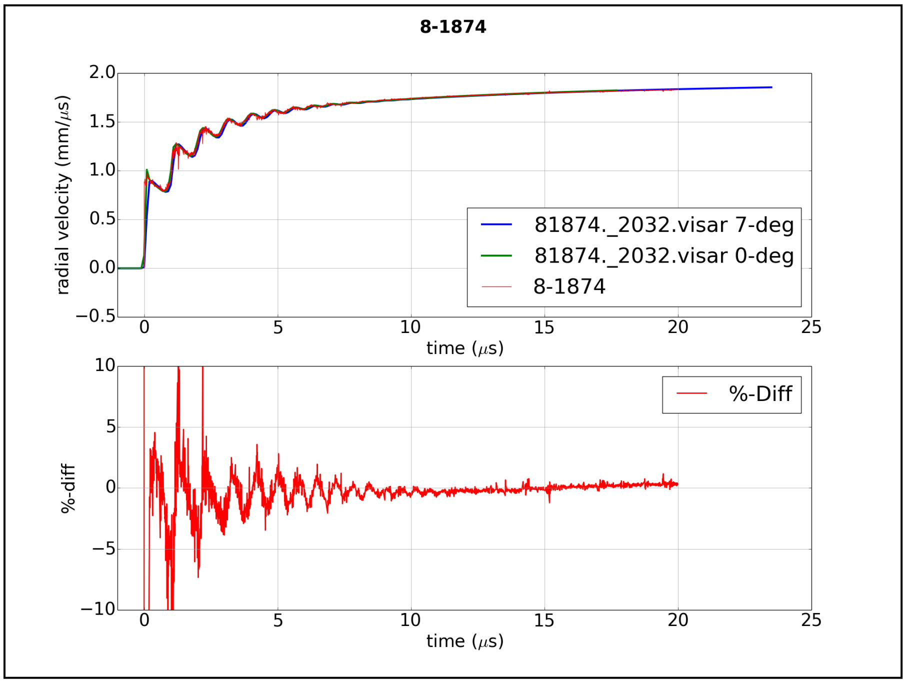

Figure A.9. Radial wall velocity, FLAG vs. measured, for shot 8-1874

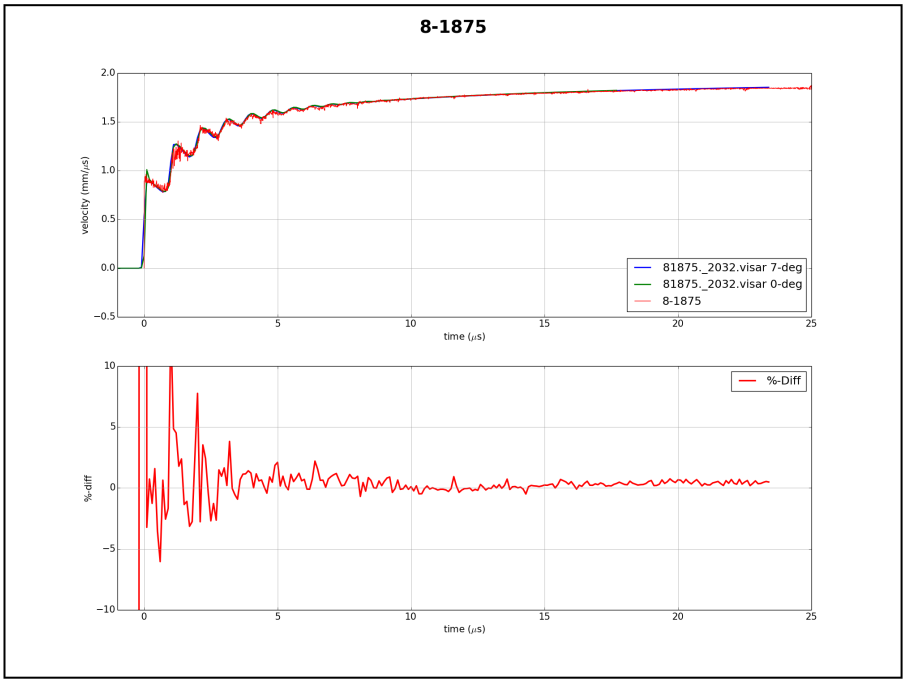

Figure A.10. Radial wall velocity, FLAG vs. measured, for shot 8-1875
Appendix B.

Appendix B.
FLAG pressure-volume distributions

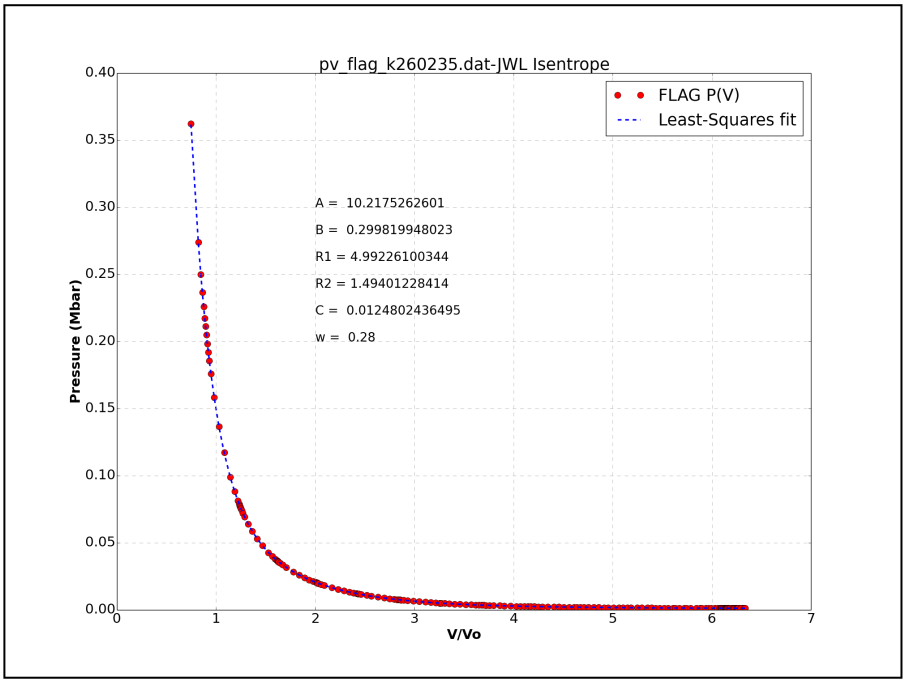

Figure B.1. FLAG pressure vs. volume (data and JWL fit) for shot K-260235.

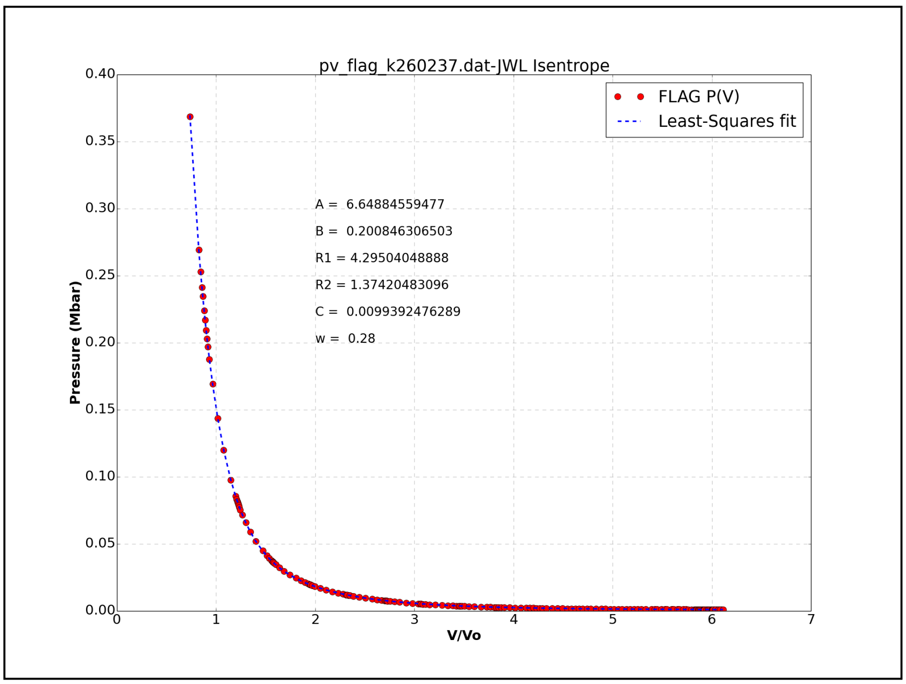

Figure B.2. FLAG pressure vs. volume (data and JWL fit) for shot K-260237.

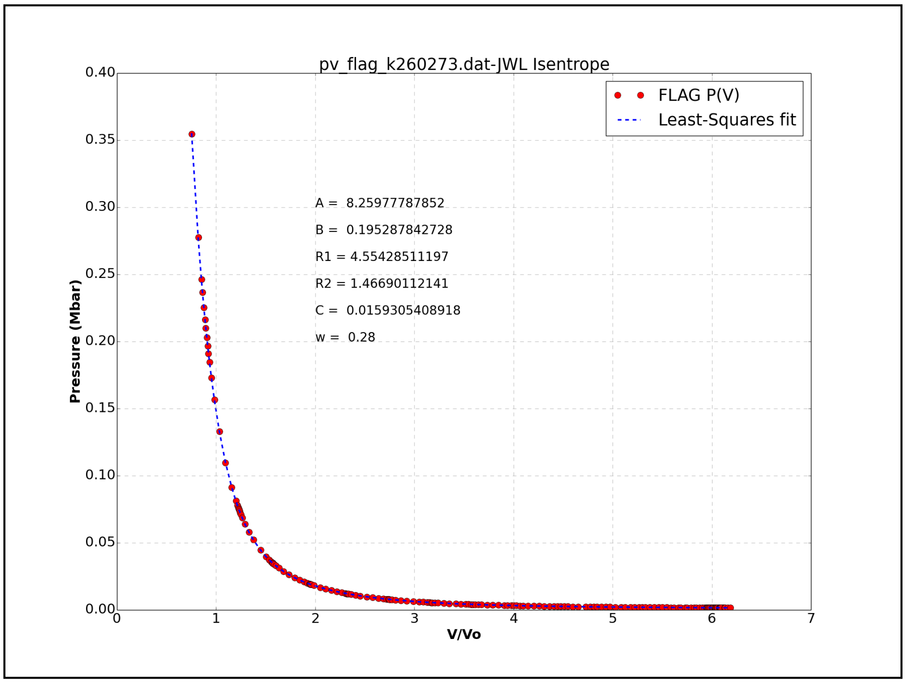

Figure B.3. FLAG pressure vs. volume (data and JWL fit) for shot K-260273.

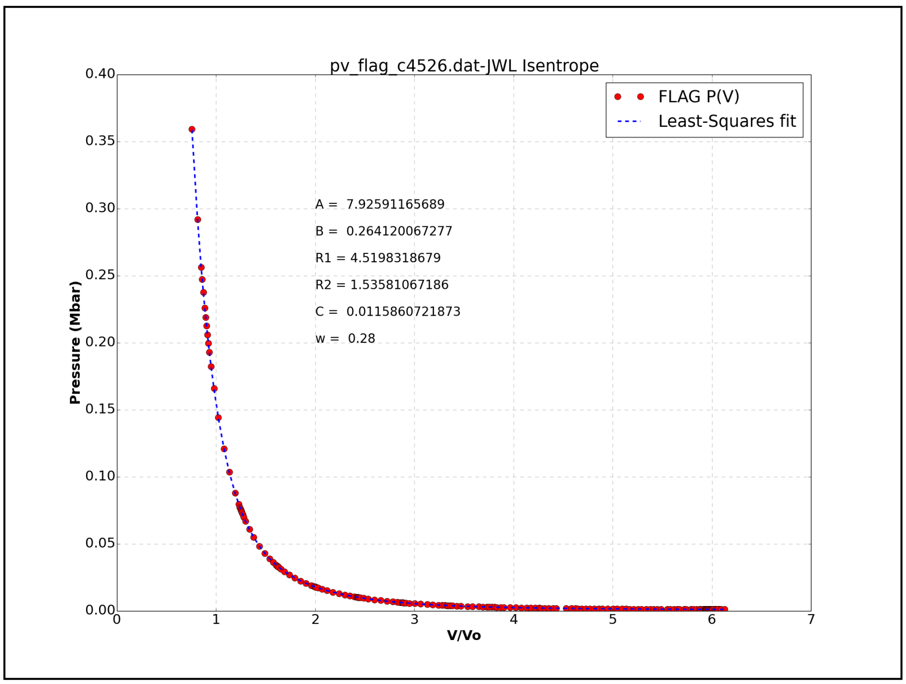

Figure B.4. FLAG pressure vs. volume (data and JWL fit) for shot C4526.

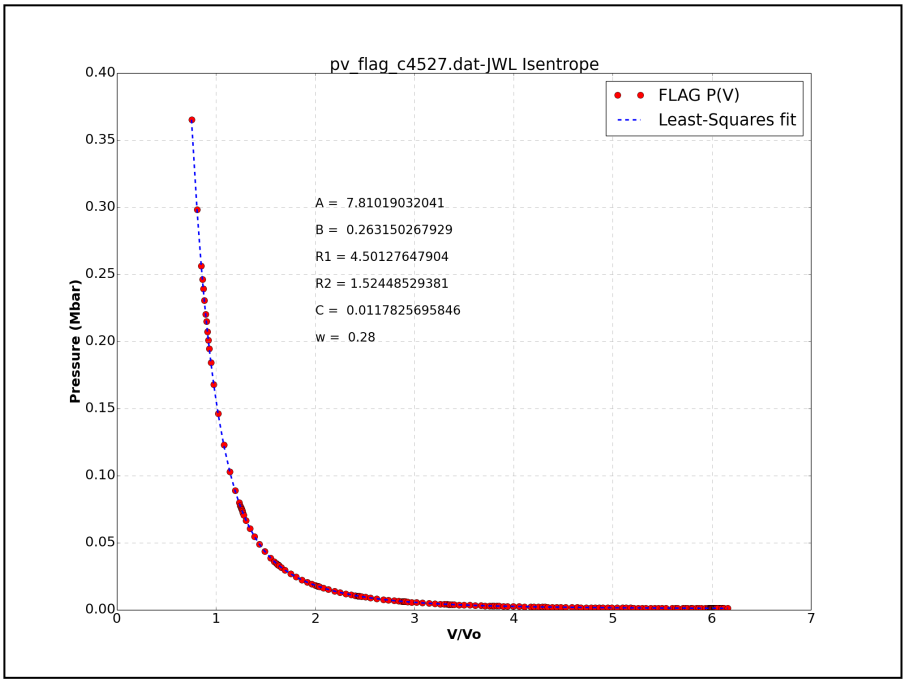

Figure B.5. FLAG pressure vs. volume (data and JWL fit) for shot C4527.

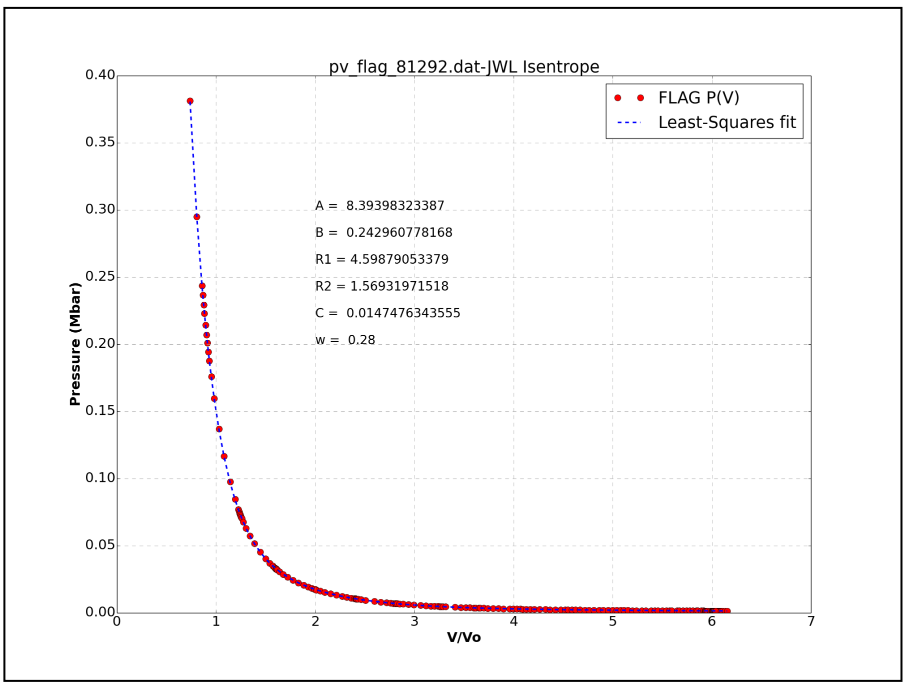

Figure B.6. FLAG pressure vs. volume (data and JWL fit) for shot 8-1892.

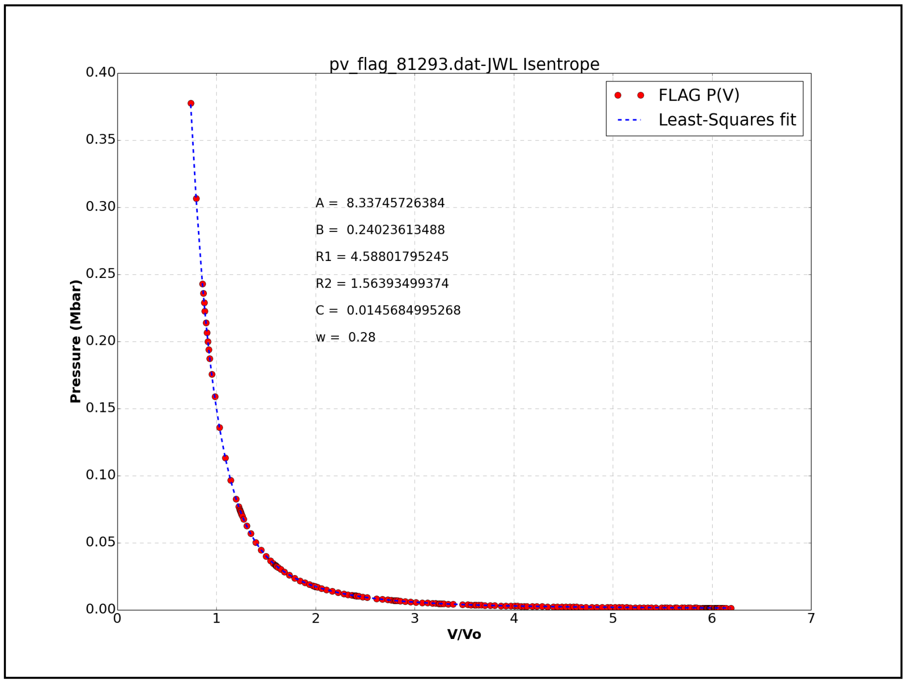

Figure B.7. FLAG pressure vs. volume (data and JWL fit) for shot 8-1893.

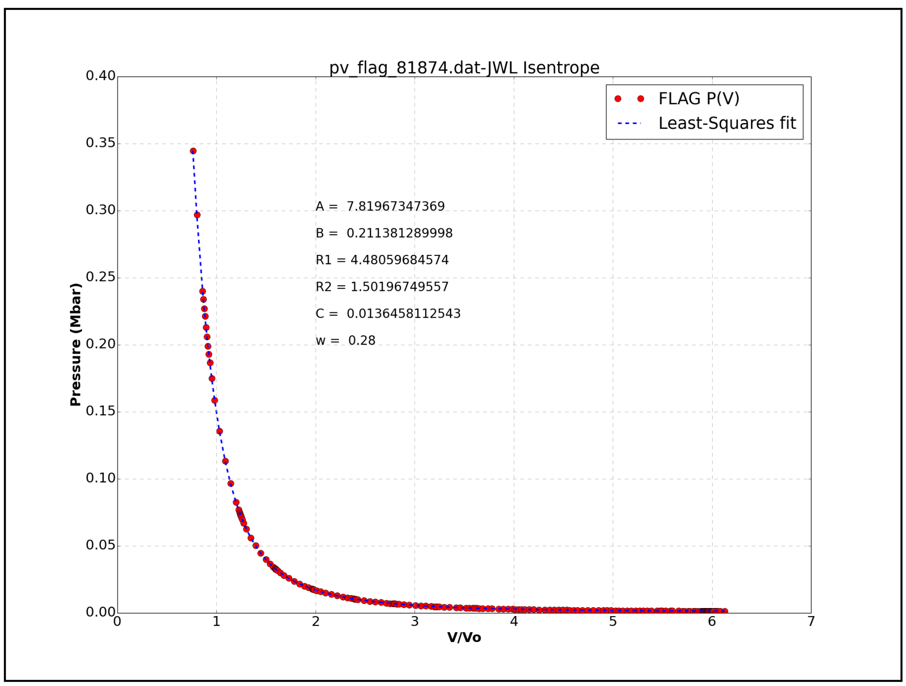

Figure B.8. FLAG pressure vs. volume (data and JWL fit) for shots 8-1874/75.

Appendix C.
Example Ingen input script for shot 8-1874

```
import ingen
from ingen import gwiz, altair, materials, csv
ingen.startModel(name='mesh/cylinder', convenience = globals())

HErad=1.2705
Cuthick=0.2535
Length=30.48

cntr.center1=gwiz.rLine(r=0.0,z1=0.0,z2=Length)
cntr.HE_Cu1=gwiz.rLine(r=HErad,z1=0.0,z2=Length)
cntr.Cu_Outer=gwiz.rLine(r=HErad+Cuthick,z1=0.0,z2=Length)
altair.contours2Segments(contours=cntr,segments=seg)

res = 0.01
seg.center1.equalArcDistrib(dx=res)
seg.HE_Cu1.equalArcDistrib(dx=res)
seg.Cu_Outer.equalArcDistrib(dx=res)

squareRule=altair.squareDistrib()

blk.HE = altair.block2(jMin=seg.center1, jMax=seg.HE_Cu1,rule=squareRule, material =
materials.material(1))
blk.Cu = altair.block2(jMin=seg.HE_Cu1, jMax=seg.Cu_Outer, rule=squareRule, material =
materials.material(2))

blk.HE.iMin().tag("fixedZ_Bottom")
blk.Cu.iMin().tag("fixedZ_Bottom")
#blk.Air3.iMin().tag("fixedZ_Bottom")

#blk.Air1.iMax().tag("fixedZ_Top")
#blk.Air2.iMax().tag("fixedZ_Top")
#blk.Air3.iMax().tag("fixedZ_Top")

#blk.Air3.jMax().tag("fixedR")

#blk.HE.jMin().tag("fixedCenterR")
#blk.Cu_Plug.iMax().tag("fixedCenterR")
#blk.Air1.jMin().tag("fixedCenterR")

seg.HE_Cu1.slide("slideHE_Cu")

seg.Cu_Outer.tag("visar")
ingen.endModel(metadata=True,x3d=True,npes=128)

#csv.mkDeck("Triptest.flg",db,"deck")
```

Appendix D.
Example FLAG input deck for shot 8-1874

```
!-------------------------------------------------
!
! UNIT SET
!
!-------------------------------------------------
setunits "cgmu"
!-------------------------------------------------
!
! GLOBAL CONSTANTS
!
!-------------------------------------------------
real LENGTH, INTERFACE               ! length of tube, HE/Cu interface
LENGTH = 30.48
INTERFACE = 2.54
real RADIUSCUO, DENSITYCU,DENSITYHE  ! Cu outer radius, Cu & HE density
RADIUSCUO = 3.05
DENSITYCU = 8.94
DENSITYHE = 1.845
!-------------------------------------------------
!
! GLOBAL
!
!-------------------------------------------------
mk /global
    title     = "81874" ! The problem title
    tstop     = 40.0    ! The problem stop time
    dtinitial = 0.001   ! The first timestep.
    dtmax     = 0.01   ! The maximum timestep.
    dump_local_path = "./restarts"
mk /global/signal
    eventlist = "Zdump" "ENSIGHT"
!-------------------------------------------------
!
! MESH
!
!-------------------------------------------------
!--------------------
!  Ingen Mesh
!--------------------
! donor mesh - will be repartitioned
mk /global/mesh(Donor)/geometry/axis2
mk /global/mesh(Donor)/zoner/importx3d
    filepath = "./mesh"
```

```
    file = "cylinder.x3d"
! the actual mesh, with repartitioner
mk /global/mesh/geometry/axis2
mk /global/mesh/zoner/repartition
    meshname = "Donor"
mk /global/mesh/zoner/repartition/partitioner/oned
    isysdir = 2
    isystem = 1
    origin(:) = 0.0 0.0
! makes dendrites behave like dendrites, rather than just 5 sided zones
mk /global/mesh/splitend
!
!mk /global/mesh/zoner/pszoner
!    kkprocll = 16 32       ! (512) Set the parallel decomposition. For
!                           ! (512) this problem each processor will contain
!                           ! (512) a tenth-slice along the length of the domain
!    kk3z = 304 3040        ! (512) Zone count in each direction.
!!
!!   kkprocll = 4 64        ! (256) Set the parallel decomposition. For
!!                          ! (256) this problem each processor will contain
!!                          ! (256) a tenth-slice along the length of the domain
!!   kk3z = 64 640          ! (256) Zone count in each direction.
!    pmin = 0.0 0.0         ! Low (x, y) coordinates
!    pmax = RADIUSCUO LENGTH! High (x,y)
!-------------------------------------------------
!
! FUNCTIONS
!
!-------------------------------------------------
mk /global/mesh/func(Axis)/planex
    c = 0.0
mk /global/mesh/func(Interface)/planex
    c = INTERFACE
mk /global/mesh/func(Outer)/planex
    c = RADIUSCUO
mk /global/mesh/func(Bottom)/planey
    c = 0.0
mk /global/mesh/func(Top)/planey
    c = LENGTH
mk /global/mesh/func(Universe)/universe
!-------------------------------------------------
!
! BOUNDARIES
!
!-------------------------------------------------
mk /global/mesh/kbdy(Axis)/onefunc
```

```
    fname = "Axis"
!mk /global/mesh/kbdy(Interface)/onefunc
!    fname = "Interface"
!mk /global/mesh/kbdy(Outer)/onefunc
!    fname = "Outer"
mk /global/mesh/kbdy(Bottom)/onefunc
    fname = "Bottom"
mk /global/mesh/kbdy(Top)/onefunc
    fname = "Top"

!
!-------------------------------------------------
!
! REGIONS
!
!-------------------------------------------------
!mk /global/mesh/kregion(Universe)/onefunc
!    fname = "Universe"
!mk /global/mesh/kregion(HE)/boolfunc
!    kbool = Expr(int(int(int(Axis comp(Interface)) Bottom) comp(Top)))
!mk /global/mesh/kregion(Cu)/boolfunc
!    kbool = Expr(int(int(int(Interface comp(Outer)) Bottom) comp(Top)))
!
mk /global/mesh/kregion(Universe)/universe
mk /global/mesh/kregion(HE)/linked
   fname = "link.1"
mk /global/mesh/kregion(Cu)/linked
   fname = "link.2"
!
!--------------------------------------
! DETONATION TIMES
!--------------------------------------

!--------------------------------------
!  MATERIALS
!    JWL PBX-9404 from LLNL Explosives Ref Guide (ERG)
!--------------------------------------
mk /global/mesh/mat(he1)/gas
    region = "HE"
mk /global/mesh/mat(he1)/gas/model/twoeoss/eos1/gruneisen ! from Von W.
    r0 = DENSITYHE    ! g/cc
    g0 = 0.7989
    a  = 0.0
    s1 = 1.737
    s2 = 0.0
    s3 = 0.0
```

```
    c  = 0.2339    ! cm/u-sec
    cv = 2.99e-6   ! Mb-cc/g-degK
    tzero = 300.0  ! degK
mk /global/mesh/mat(he1)/gas/model/twoeoss/eos2/jwl ! from ExpRefGuide #1
    ieosburn = 0
    r0 = 1.845
    a  = 7.696566552
    b  = 0.204099805
    r1 = 4.455
    r2 = 1.485
    w  = 0.28
    tzero = 300.0  ! degK
    iusecalc = 1

mk /global/mesh/mat(he1)/gas/model/twoeoss/eoscriteria/eosburn

mk /global/mesh/mat(he1)/gas/element/hepoly
    detvelhe = 0.882937339228328
    heenergy = *(/(0.122 1.843) 0.935)

mk /global/mesh/mat(he1)/gas/initialize/ptre
    density = DENSITYHE
    energy  = 0.0
!--------------------------------------
!  Q MATERIAL
!--------------------------------------
mk /global/mesh/mat(MyQ)/modq
    region="HE"
    q2  = 2.0
    q1  = 0.1
    q1n = 0.1
mk /global/mesh/mat(MyQ)/modq/mqbarton
    iqproj = 3
    qbart  = 1
mk /global/mesh/mat(MyQ)/modq/mqtts
     alfa = 0.5
     beta = 0.0
     q1   = 0.3
     q2   = 2.0
     q1n  = 0.3
     itqs = 1
!-------------------------------------
!  Copper
!--------------------------------------
mk /global/mesh/mat(Cu)/solid
    region = "Cu"
```

```
cd /global/mesh/mat(Cu)
    mk +solid
       ss=0.0001
    mk +solid/element/fvpoly
    mk +solid/model/decoupled/pvol/eos/gruneisen  ! from ShapedCharge example
       r0          = DENSITYCU     ! g/cc
       c           = 0.394         ! cm/us
       g0          = 2.02
       a           = 0.47
       s1          = 1.489
       s2          = 0.
       s3          = 0.
       cv          = 0.3835e-5     ! Mbar-cc/g-degK
       tzero       = 294.0         ! degK
       ixten = 1
    mk +solid/model/decoupled/strength/ptwmod1  ! from ShapedCharge example
       r = 0.
       theta0=0.025
       p=3.0
       kappa=0.17
       gamma=8.0e-6
       alpha=0.447
       g0=0.525                ! Mbar
       tm=1356                 ! deg-K
       am=1.0552e-22           ! g/atom
       s0=0.0092
       sinf=0.0022
       y0=0.0001
       y1=0.094
       y2=0.575
       yinf=0.0001
       beta=0.25
    mk +solid/initialize/stre
       density= DENSITYCU              ! g/cc
       energy=0.0                  ! Mbar-cc/g
    mk +solid/model/q/barton
       q1  = 0.3
       q1n = 0.0
       q2  = 1.3

mk /global/mesh/mat(Cu)/solid/tracers
    vars = "velocity"
    filepath = "./diagnostics"
mk /global/mesh/mat(Cu)/solid/tracers/initialize/prescribe
    max_ptcl = 305
    start_coords(:,1:25)=    1.524   0.000 &
```

```
                      1.524   0.100 &
                      1.524   0.201 &
                      1.524   0.301 &
                      1.524   0.401 &
                      1.524   0.501 &
                      1.524   0.602 &
                      1.524   0.702 &
                      1.524   0.802 &
                      1.524   0.902 &
                      1.524   1.003 &
                      1.524   1.103 &
                      1.524   1.203 &
                      1.524   1.303 &
                      1.524   1.404 &
                      1.524   1.504 &
                      1.524   1.604 &
                      1.524   1.704 &
                      1.524   1.805 &
                      1.524   1.905 &
                      1.524   2.005 &
                      1.524   2.106 &
                      1.524   2.206 &
                      1.524   2.306 &
                      1.524   2.406
start_coords(:,26:50)= 1.524   2.507 &
                      1.524   2.607 &
                      1.524   2.707 &
                      1.524   2.807 &
                      1.524   2.908 &
                      1.524   3.008 &
                      1.524   3.108 &
                      1.524   3.208 &
                      1.524   3.309 &
                      1.524   3.409 &
                      1.524   3.509 &
                      1.524   3.609 &
                      1.524   3.710 &
                      1.524   3.810 &
                      1.524   3.910 &
                      1.524   4.011 &
                      1.524   4.111 &
                      1.524   4.211 &
                      1.524   4.311 &
                      1.524   4.412 &
                      1.524   4.512 &
                      1.524   4.612 &
```

```
                        1.524   4.712 &
                        1.524   4.813 &
                        1.524   4.913
start_coords(:,51:75)=  1.524   5.013 &
                        1.524   5.113 &
                        1.524   5.214 &
                        1.524   5.314 &
                        1.524   5.414 &
                        1.524   5.514 &
                        1.524   5.615 &
                        1.524   5.715 &
                        1.524   5.815 &
                        1.524   5.916 &
                        1.524   6.016 &
                        1.524   6.116 &
                        1.524   6.216 &
                        1.524   6.317 &
                        1.524   6.417 &
                        1.524   6.517 &
                        1.524   6.617 &
                        1.524   6.718 &
                        1.524   6.818 &
                        1.524   6.918 &
                        1.524   7.018 &
                        1.524   7.119 &
                        1.524   7.219 &
                        1.524   7.319 &
                        1.524   7.419
start_coords(:,76:100)= 1.524   7.520 &
                        1.524   7.620 &
                        1.524   7.720 &
                        1.524   7.821 &
                        1.524   7.921 &
                        1.524   8.021 &
                        1.524   8.121 &
                        1.524   8.222 &
                        1.524   8.322 &
                        1.524   8.422 &
                        1.524   8.522 &
                        1.524   8.623 &
                        1.524   8.723 &
                        1.524   8.823 &
                        1.524   8.923 &
                        1.524   9.024 &
                        1.524   9.124 &
                        1.524   9.224 &
```

```
                        1.524   9.324 &
                        1.524   9.425 &
                        1.524   9.525 &
                        1.524   9.625 &
                        1.524   9.726 &
                        1.524   9.826 &
                        1.524   9.926
start_coords(:,101:125)= 1.524  10.026 &
                        1.524  10.127 &
                        1.524  10.227 &
                        1.524  10.327 &
                        1.524  10.427 &
                        1.524  10.528 &
                        1.524  10.628 &
                        1.524  10.728 &
                        1.524  10.828 &
                        1.524  10.929 &
                        1.524  11.029 &
                        1.524  11.129 &
                        1.524  11.229 &
                        1.524  11.330 &
                        1.524  11.430 &
                        1.524  11.530 &
                        1.524  11.631 &
                        1.524  11.731 &
                        1.524  11.831 &
                        1.524  11.931 &
                        1.524  12.032 &
                        1.524  12.132 &
                        1.524  12.232 &
                        1.524  12.332 &
                        1.524  12.433
start_coords(:,126:150)= 1.524  12.533 &
                        1.524  12.633 &
                        1.524  12.733 &
                        1.524  12.834 &
                        1.524  12.934 &
                        1.524  13.034 &
                        1.524  13.134 &
                        1.524  13.235 &
                        1.524  13.335 &
                        1.524  13.435 &
                        1.524  13.536 &
                        1.524  13.636 &
                        1.524  13.736 &
                        1.524  13.836 &
```

```
                         1.524  13.937 &
                         1.524  14.037 &
                         1.524  14.137 &
                         1.524  14.237 &
                         1.524  14.338 &
                         1.524  14.438 &
                         1.524  14.538 &
                         1.524  14.638 &
                         1.524  14.739 &
                         1.524  14.839 &
                         1.524  14.939
start_coords(:,151:175)= 1.524  15.039 &
                         1.524  15.140 &
                         1.524  15.240 &
                         1.524  15.340 &
                         1.524  15.441 &
                         1.524  15.541 &
                         1.524  15.641 &
                         1.524  15.741 &
                         1.524  15.842 &
                         1.524  15.942 &
                         1.524  16.042 &
                         1.524  16.142 &
                         1.524  16.243 &
                         1.524  16.343 &
                         1.524  16.443 &
                         1.524  16.543 &
                         1.524  16.644 &
                         1.524  16.744 &
                         1.524  16.844 &
                         1.524  16.944 &
                         1.524  17.045 &
                         1.524  17.145 &
                         1.524  17.245 &
                         1.524  17.346 &
                         1.524  17.446
start_coords(:,176:200)= 1.524  17.546 &
                         1.524  17.646 &
                         1.524  17.747 &
                         1.524  17.847 &
                         1.524  17.947 &
                         1.524  18.047 &
                         1.524  18.148 &
                         1.524  18.248 &
                         1.524  18.348 &
                         1.524  18.448 &
```

```
                        1.524  18.549 &
                        1.524  18.649 &
                        1.524  18.749 &
                        1.524  18.849 &
                        1.524  18.950 &
                        1.524  19.050 &
                        1.524  19.150 &
                        1.524  19.251 &
                        1.524  19.351 &
                        1.524  19.451 &
                        1.524  19.551 &
                        1.524  19.652 &
                        1.524  19.752 &
                        1.524  19.852 &
                        1.524  19.952
start_coords(:,201:225)= 1.524  20.053 &
                        1.524  20.153 &
                        1.524  20.253 &
                        1.524  20.353 &
                        1.524  20.454 &
                        1.524  20.554 &
                        1.524  20.654 &
                        1.524  20.754 &
                        1.524  20.855 &
                        1.524  20.955 &
                        1.524  21.055 &
                        1.524  21.156 &
                        1.524  21.256 &
                        1.524  21.356 &
                        1.524  21.456 &
                        1.524  21.557 &
                        1.524  21.657 &
                        1.524  21.757 &
                        1.524  21.857 &
                        1.524  21.958 &
                        1.524  22.058 &
                        1.524  22.158 &
                        1.524  22.258 &
                        1.524  22.359 &
                        1.524  22.459
start_coords(:,226:250)= 1.524  22.559 &
                        1.524  22.659 &
                        1.524  22.760 &
                        1.524  22.860 &
                        1.524  22.960 &
                        1.524  23.061 &
```

```
                              1.524  23.161 &
                              1.524  23.261 &
                              1.524  23.361 &
                              1.524  23.462 &
                              1.524  23.562 &
                              1.524  23.662 &
                              1.524  23.762 &
                              1.524  23.863 &
                              1.524  23.963 &
                              1.524  24.063 &
                              1.524  24.163 &
                              1.524  24.264 &
                              1.524  24.364 &
                              1.524  24.464 &
                              1.524  24.564 &
                              1.524  24.665 &
                              1.524  24.765 &
                              1.524  24.865 &
                              1.524  24.966
start_coords(:,251:275)= 1.524  25.066 &
                              1.524  25.166 &
                              1.524  25.266 &
                              1.524  25.367 &
                              1.524  25.467 &
                              1.524  25.567 &
                              1.524  25.667 &
                              1.524  25.768 &
                              1.524  25.868 &
                              1.524  25.968 &
                              1.524  26.068 &
                              1.524  26.169 &
                              1.524  26.269 &
                              1.524  26.369 &
                              1.524  26.469 &
                              1.524  26.570 &
                              1.524  26.670 &
                              1.524  26.770 &
                              1.524  26.871 &
                              1.524  26.971 &
                              1.524  27.071 &
                              1.524  27.171 &
                              1.524  27.272 &
                              1.524  27.372 &
                              1.524  27.472
start_coords(:,276:300)= 1.524  27.572 &
                              1.524  27.673 &
```

```
                              1.524  27.773 &
                              1.524  27.873 &
                              1.524  27.973 &
                              1.524  28.074 &
                              1.524  28.174 &
                              1.524  28.274 &
                              1.524  28.374 &
                              1.524  28.475 &
                              1.524  28.575 &
                              1.524  28.675 &
                              1.524  28.776 &
                              1.524  28.876 &
                              1.524  28.976 &
                              1.524  29.076 &
                              1.524  29.177 &
                              1.524  29.277 &
                              1.524  29.377 &
                              1.524  29.477 &
                              1.524  29.578 &
                              1.524  29.678 &
                              1.524  29.778 &
                              1.524  29.878 &
                              1.524  29.979
    start_coords(:,301:305)= 1.524  30.079 &
                              1.524  30.179 &
                              1.524  30.279 &
                              1.524  30.380 &
                              1.524  30.480 &

!--------------------------------------
! HIGH EXPLOSIVE LUND LIGHTING
!--------------------------------------
mk /global/mesh/heburn/helund
    alias phet phet
    alias zhet zhet
    alias zhetmin zhetmin
    alias zhetmax zhetmax
mk /global/mesh/heburn/hedet
    kkdll  = 20
!            x     y    t
    dxt    = 0.0  0.0   0.0

!--------------------------------------
! HIGH EXPLOSIVE DSD LIGHTING
!--------------------------------------
!mk /global/mesh/kregion(HE_All)/boolregion
```

```
!    kbool = Expr(un(HE HE))
!
!mk /global/mesh/kbdy(HE_All_Bdy)/regbdy
!    region = "HE"
!
!mk /global/mesh/heburn
!    alias zhet zhet
!
!mk /global/mesh/heburn/hedsd
!    dxgrid = 0.01
!    ibdyptsfac = 20
!    region = "HE_All"
!    bdy    = "HE_All_Bdy"
!!    writefile = "./dsddump"
!
!mk /global/mesh/kbdy(HE_DSDBdy)/matbdy
!    matb = "he1"
!
!mk /global/mesh/heburn/hedsd/he(HE)
!    region = "HE_All"
!    bdy = "HE_DSDBdy"
!    dcj = 0.88254459
!    dmax = 1.00
!    rkmax = 19.35464
!    omega_s = 0.940796
!    a = 1.18764
!    b = 0.004180
!    c = 21.2891   0.00653  0.000  0.49497  0.000
!    e = 0.0778    1.00000  2.000  1.00000  2.0000
!
!mk /global/mesh/kbdy(Cu_DSDBdy)/matbdy
!    matb = "Cu"
!
!mk /global/mesh/heburn/hedsd/he(HE)/inert(HE_Cu)
!    region = "Cu"
!    bdy = "Cu_DSDBdy"
!    omega_c = 0.9
!
!mk /global/mesh/heburn/hedsd/dsddet/hecircledet
!    kkdetll = 1
!det_def(:,1) = 0.00000 -2.54000 2.7000 0.00000 0.88254459

!-------------------------------------
!  HYDRO PARAMETERS
!-------------------------------------
mk /global/mesh/hydro/lhydro
```

```
!    dtmax = 1000.0
    alias velocity pu
    alias pressure zp
    alias density zr
    alias temperature zt
    alias energy ze
    alias qeff zqeff
!---------------------------------------
!  HYDRO BOUNDARY CONDITIONS
!---------------------------------------
mk /global/mesh/hydro/lhydro/kbc(Axis)/kfix
    bdy = "Axis"
    nfix = 1 0
mk /global/mesh/hydro/lhydro/kbc(Top)/kfix
    bdy = "Top"
    nfix = 0 1
!mk /global/mesh/hydro/lhydro/kbc(Interface)/kfix
!    bdy = "Interface"
!    nfix = 0 0
mk /global/mesh/hydro/lhydro/kbc(Bottom)/kfix
    bdy = "Bottom"
    nfix = 0 1
! import each slide boundary
mk /global/mesh/kbdy(slideHE_Cu)/importdefn
    filepath = "./mesh"
    file = "cylinder.slideHE_Cu.Bdy"

! create the slideline boundary conditions
! slideline #1
mk /global/mesh/hydro/lhydro/kbc(slideHE_Cu)/slide   $ note the name of the kbc
   bdy = "slideHE_Cu"
   cut_angle  = 175.0
mk /global/mesh/hydro/lhydro/kbc(slideHE_Cu)/slide/enforcement/newton
  vel_enf_frac = 0.95
mk /global/mesh/hydro/lhydro/kbc(slideHE_Cu)/slide/parallel/ghost/bbox/proj_cycles
!---------------------------------------
!  ALIASES
!---------------------------------------
cd /global/mesh/hydro/lhydro
  alias velocity pu
  alias pressure zp
  alias density zr
  alias temp zt
  alias energy ze
!---------------------------------------
! ENSIGHT OUTPUT
```

```
!---------------------------------------
mk /global/mesh/output/ensight
    filepath = "./ens"
    vars = "pressure" "energy" "density" "temp" "velocity"
    iensmatint = 1
    iensvisar = 1
!---------------------------------------
! VISAR PDV OUTPUT
!---------------------------------------
mk /global/mesh/kbdy(pdvbdy)/importdefn
 filepath = "./mesh"
 file="cylinder.visar.Bdy."

mk /global/mesh/output/visar_pdv(1524_2032)
    filepath = "./diagnostics"
    bdy = "pdvbdy"
    matlist = "Cu"
    icoord_dump = 2
    nlayers = 1
    vars = "velocity"
    vorigin = 10.0     0.0   15.24 &       ! (x,z,y) NOT (x,y,z)
              10.0     0.0   20.32 &
              10.0     0.0   15.24 &       ! (x,z,y) NOT (x,y,z)
              10.0     0.0   20.32
    vdir =    -0.99254 0.0 -0.12187 &  ! 7 degrees from normal
              -0.99254 0.0 -0.12187 &
              -1.000 0.0 0.0        &  ! 0 degrees from normal
              -1.000 0.0 0.0
    iens_2d_switch = 1
    sense = 0
!---------------------------------------
!  EXECUTION
!---------------------------------------
!---------------------------------------
!  EVENTS
!---------------------------------------
dot ENSIGHT every 2.0 from 0.0
dot ENSIGHT at 25.98
dostop ENSIGHT
ENSIGHT
doc DTC every 20
dot BuffVisarPDV every 0.1
dot VisarPDVDump every 0.1
dot TracerSample every 0.1
doc Zdump every 5000 from 5000
!---------------------------------------
```

```
!  EXECUTION
!-------------------------------------
run
end
```