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Title: Uncertainty in High Explosive Equations of State

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Uncertainty in High Explosive Equations of State

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Background

MOTIVATION

Equations of state (EOS) are essential in characterizing high explosives. Computing the EOS of an explosive given experimental data requires inverting the experimental output to produce optimal parameters for that data. Here, we compare parameters calibrated to different shots of a cylinder test from Pemberton et al. 2011. Estimates of EOS parameters exist, but are calibrated under the assumption that different shots have the same resulting optimal parameters. **It is still unknown if these results agree between individual shots.** This work aims to determine if shots of the Pemberton experiment can be used as one collective result, or if each run should be treated separately.

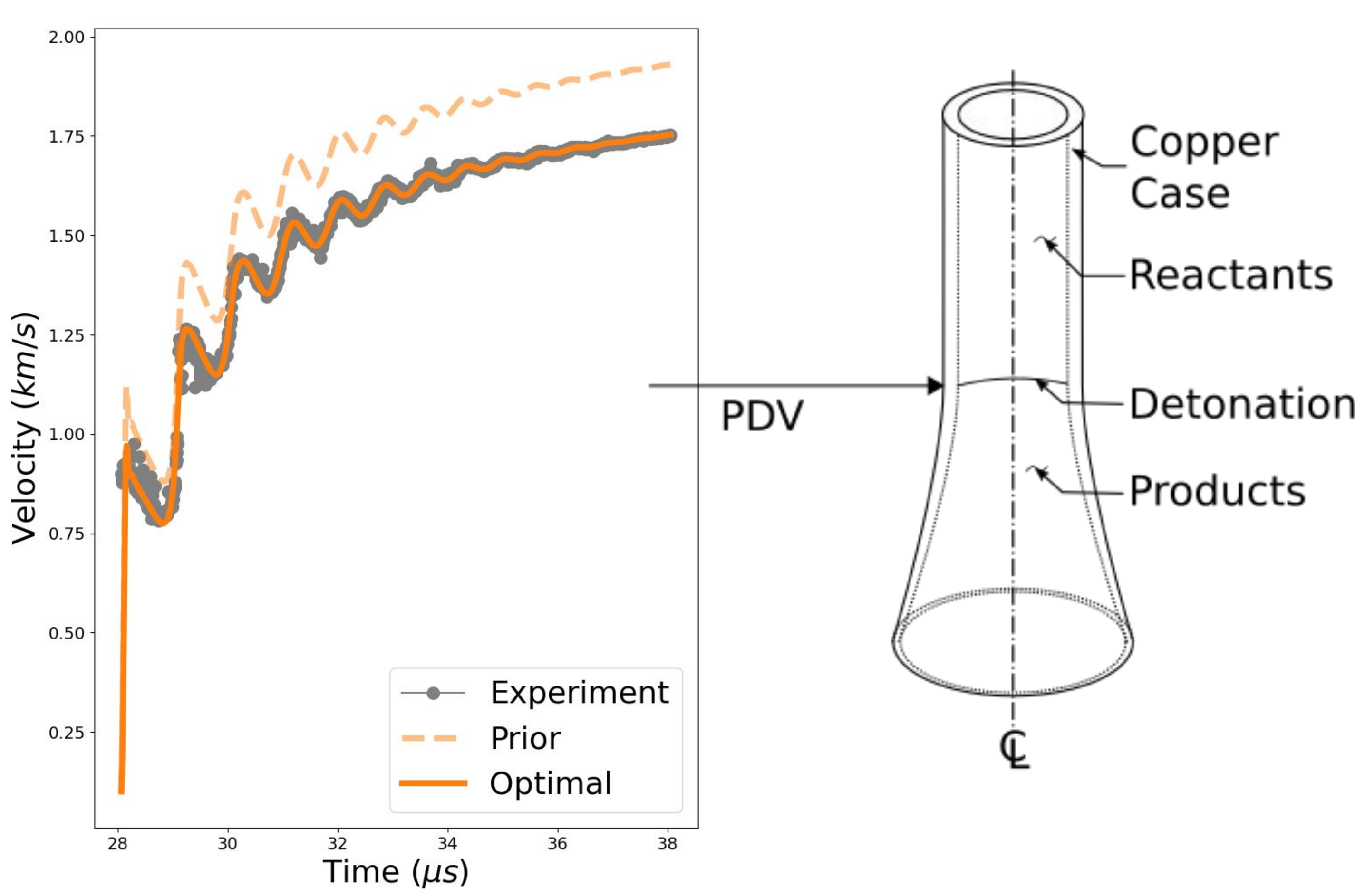

Fig. 1: Left: Velocity of the cylinder wall from the experiment, the simulation using the prior EOS, and the simulation using the optimized EOS. **Right:** Setup of a cylinder test. Compacted explosive is encased in a cylindrical case, and the detonation products form a conical outflow from the bottom of the cylinder. A Photon Doppler Velocimeter (PDV) probe is used to measure the wall velocity in the radial direction.

THE DAVIS PRODUCTS EQUATION OF STATE (EOS)

The Davis Products EOS is a functional form describing the relationship between state variables for explosive detonation products. It has seven degrees of freedom (DOF) that are adjusted during calibration: *a, k,* v_c, p_c, *n, b,* and C_{vp}. For this work, we want to investigate the assertion that separate shots in Pemberton et al.'s experiment series are consistent with each other; i.e. that they can be fitted with the same functional form of the Davis products EOS within reported experimental uncertainty. To do this, we optimize parameters to each shot separately, and compare the parameter values, uncertainties, and the physical implications of these optimal parameters in pressure-volume space.

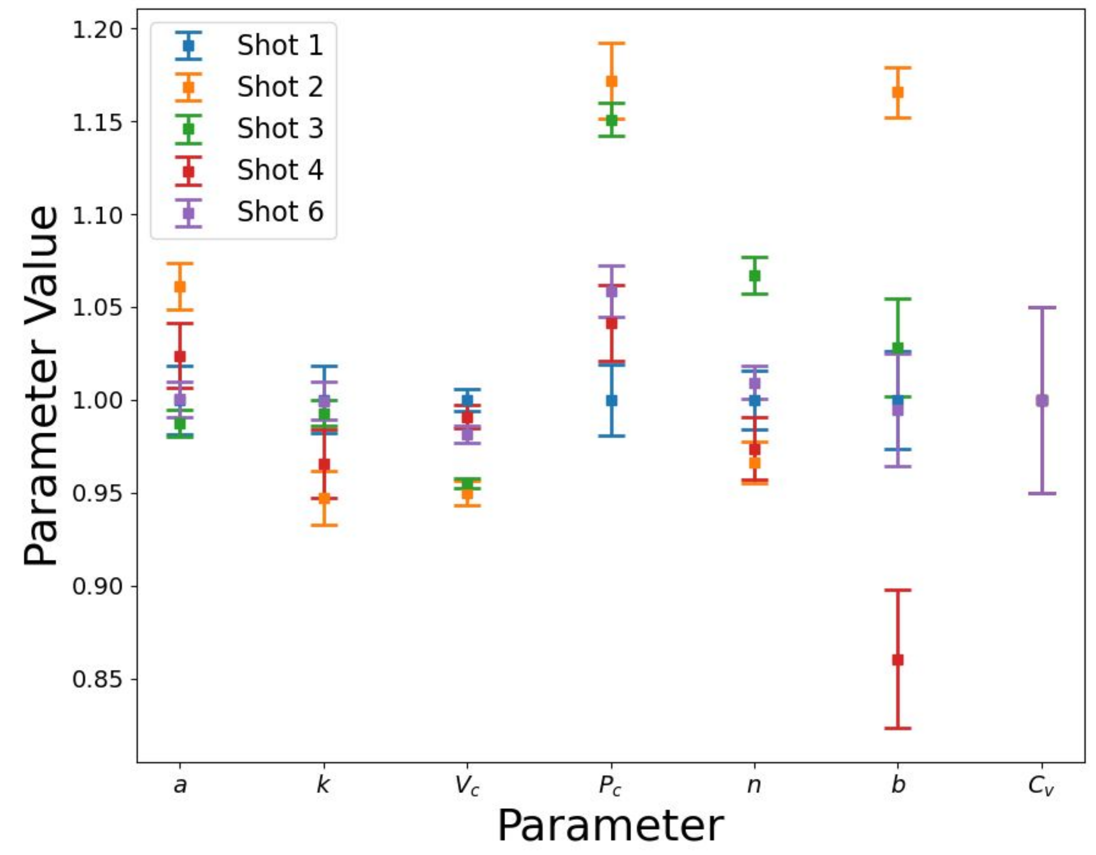

Fig 2. Davis EOS parameters calibrated according to each shot in the experiments of Pemberton et al. 2011. The parameter values are normalized to the optimal value calibrated to shot one, chosen arbitrarily. While some parameters agree, the spread in other parameters show that different solutions yield similar results.

Methods

VARIATIONAL BAYESIAN INFERENCE

Our inversion method uses gradient descent to optimize the posterior probability of the Davis EOS DOF given the data. If θ is the DOF vector and *y* represents the experimental data, then by Bayes' theorem, the posterior is given by $P(\theta|y) \propto P(y|\theta)P(\theta)$. The likelihood probability of the data given the parameters is computed by considering the difference of the simulation and the experiment. The prior probability is assumed to be a multivariate normal distribution whose mean and variance are chosen reasonably. Practically, the probabilities are computed in log space. The optimal DOF values are given by:

$$\arg\max_{\theta}\left(\underbrace{\log P(\theta|\mathcal{Y})}_{\text{Posterior}}\right) = \arg\max_{\theta}\left(\underbrace{\log P(\mathcal{Y}|\theta)}_{\text{Likelihood}} + \underbrace{\log P(\theta)}_{\text{Prior}}\right)$$

SOFTWARE

This work makes use of the Functional UNcertainty Constrained by Law and Experiment (F_UNCLE) package created by Stephen Andrews (XCP-8) and Andrew Fraser. We specifically implement the above methods using variational Bayesian inference in the VBayes class. The free Lagrangian (FLAG) hydrocode is used to simulate the PDV probe output data of a cylinder experiment given the parameters to the Davis EOS model.

REFERENCES

F_UNCLE: Tools for understanding functional uncertainty. Copyright (C) 2016 Andrew M. Fraser and Stephen A. Andrews.
William C. Davis. Equation of State for Detonation Products.
Pemberton, Steven & Herrera, Dennis & Herrera, Tommy & Arellano, Jesus & Sandoval, Thomas. (2022). Steady Deflagration of PBX9501 Within a Copper Cylinder. 0.2172/1044857.

ALGORITHMIC IMPROVEMENTS

VBayes includes a naïve line search as the last step in its optimization, which evaluates the log posterior probability at each DOF vector for *n* steps along the direction of the optimal step. While this method will return an *approximate* minimum, its boundary constraint — stopping at the input DOF — may exclude the true optimal DOF from even being evaluated by the line search. To fix this possible omission, we revise VBayes to include a cubic interpolation over the *n* steps to find the optimal functional form of log posterior probability versus DOF vector, then calculate the absolute maximum on this function.

Results

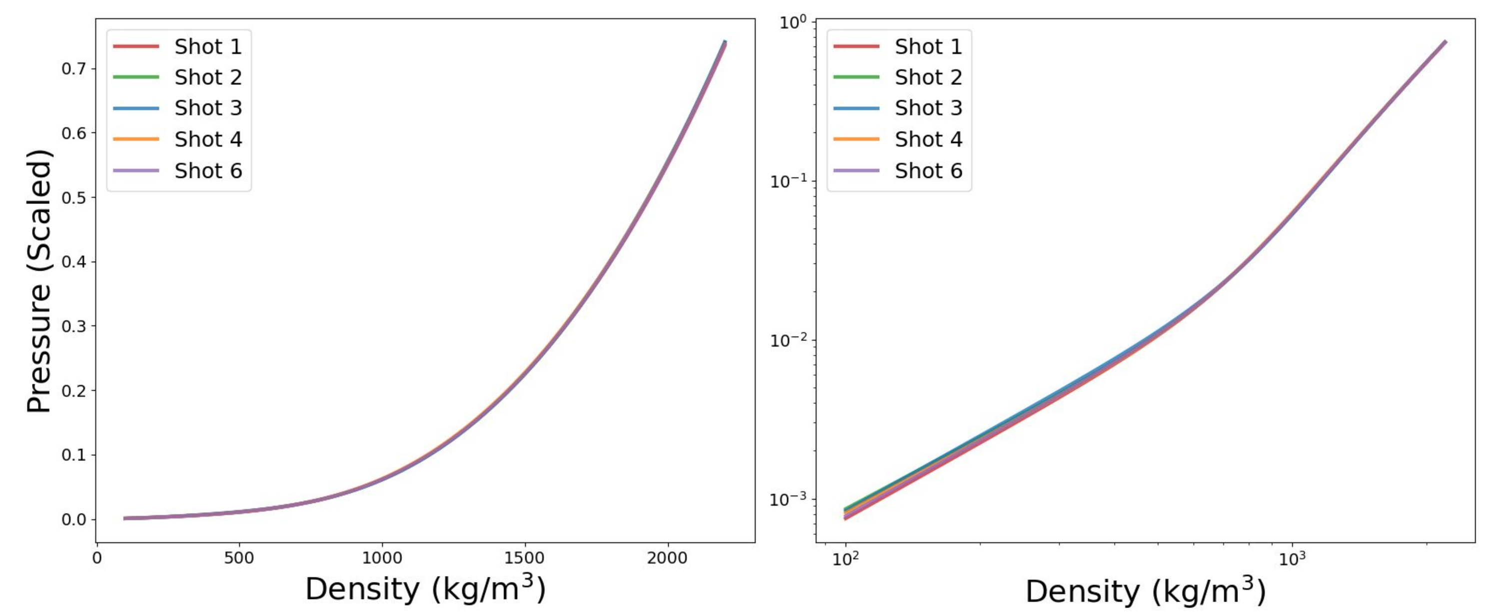

Fig 3. Isentropes of the Davis Products EOS optimized to different shots. Despite having different resulting parameters, each shot yields overlapping isentropes. **Left:** Linear scale. **Right:** Log scale.

PARAMETERS IN PHYSICAL SPACE

In Fig. 2, some of the optimal parameters for each shot are consistent; for example, the specific heat C_v is stable since the simulation and experiments do not incorporate temperature. Besides these exceptions, the optimal parameters for each shot's inversion vary; however, different shots still give consistent results in pressure-volume space. In Fig. 3, we see that the optimal isentrope of each shot overlaps for the majority of the volume range of the experimental data. Thus, multiple DOF solutions can lead to accurate simulation data. We conclude that the Pemberton et al. cylinder experiments alone are insufficient to differentiate between sets of optimal Davis Products EOS parameters. Including additional experiments into the inversion is necessary to determine accurate EOS models.

FUTURE WORK

Future work will optimize and compare the presented EOS according to other experiments, including those of different geometries. We are also working to improve the likelihood probability distribution by using Gaussian process regression to return a better estimate for the experimental uncertainty.

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