

Empirical Correlations Between the Function of Entropy (Z_s) and Net Artificial Viscous Work in a Shock Physics Hydrocode

Session EE02: Equation of State
11:15 AM-12:45 PM, Friday, June 23, 2023

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Group on Shock Compression of Condensed Matter (SCCM 2023)
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Section 1. Background and Motivation



- 1) Increasingly, analysts need/want new material models (e.g., strength, constitutive, phase change, kinetics, reactive burn) that depend on **entropy of the shock state**.
 - Examples include the UK CREST burn model [1] and multi-material shocks [2] (e.g., cavitation).
- 2) The Any Mie-Grüneisen equation of state (AMGL) was implemented into Sandia's Eulerian shock physics hydrocode CTH. This model can compute the shock entropy.
 - AMGL is distributed with version 13.0 and is under active development for the 13.1 release.
- 3) Verification activities uncovered **inherent numerical errors** and **empirical correlations** that have never before been documented.
 - These inherent errors in entropy mean that entropy-dependent material model parameters must be re-calibrated for use in CTH.
 - Large dataset for 2023 APS GSCCM consisting of 1D shock wave simulations (**= 56,304 total**)
 - 46 calibrated AMGL library materials
 - 24 mesh resolutions between 2 and 25 zones per millimeter
 - 51 Hugoniot points each, for impact velocities between 200 and 3500 m/s

^[1] Kittell, D., Schmitt, R., Tuttle, L., and Harstad, E., "Implementation of a CREST multistate reactive burn model in CTH for two solid high explosives," *Proceedings of the 16th International Detonation Symposium*, pp. 1021-1031, Cambridge, MD, July 2018.

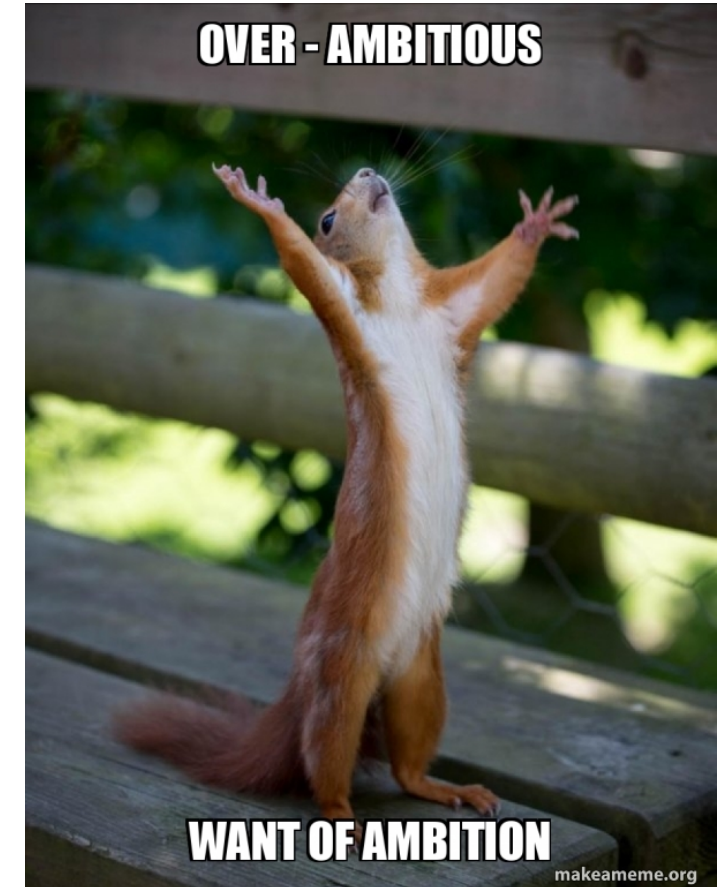
^[2] Schumacher, S. C., and Baer, M. R., "Generalized continuum mixture theory for multi-material shock physics." *International Journal of Engineering Science* **183**:103807, 2023.

Section 1. Objectives



- 1) Convince you that the new AMGL thermodynamic state variables in CTH are mesh resolved for sufficiently large number of zones [**Easy**]
- 2) Propose a numerical method to correct the shock state entropy in CTH using artificial viscosity, based upon two empirical correlations supported by results for 46 calibrated library materials [**Harder, and a little controversial**]
- 3) Speculate about possible ties between the empirical correlations to a physical law [**Too ambitions, but it is addressed on the last slide**]

Overall this APS talk is...



Section 2. Root-Mean-Squared Error for 46 Materials



PROBLEM → Reduce the Hugoniot curve into a single data point, in order to show mesh convergence and to quantify the numerical errors.

SOLUTION → Plot the shifted RMSE, with equation given below,

Root-mean-squared
error at arbitrary
mesh resolution

Root-mean-squared error
at max resolution $k=25$
zones per millimeter

$$Y = \text{RMSE}_{P,k} - \text{RMSE}_{P,k=25} + \langle \text{RMSE}_{P,k=25} \rangle_{\text{mats}}$$

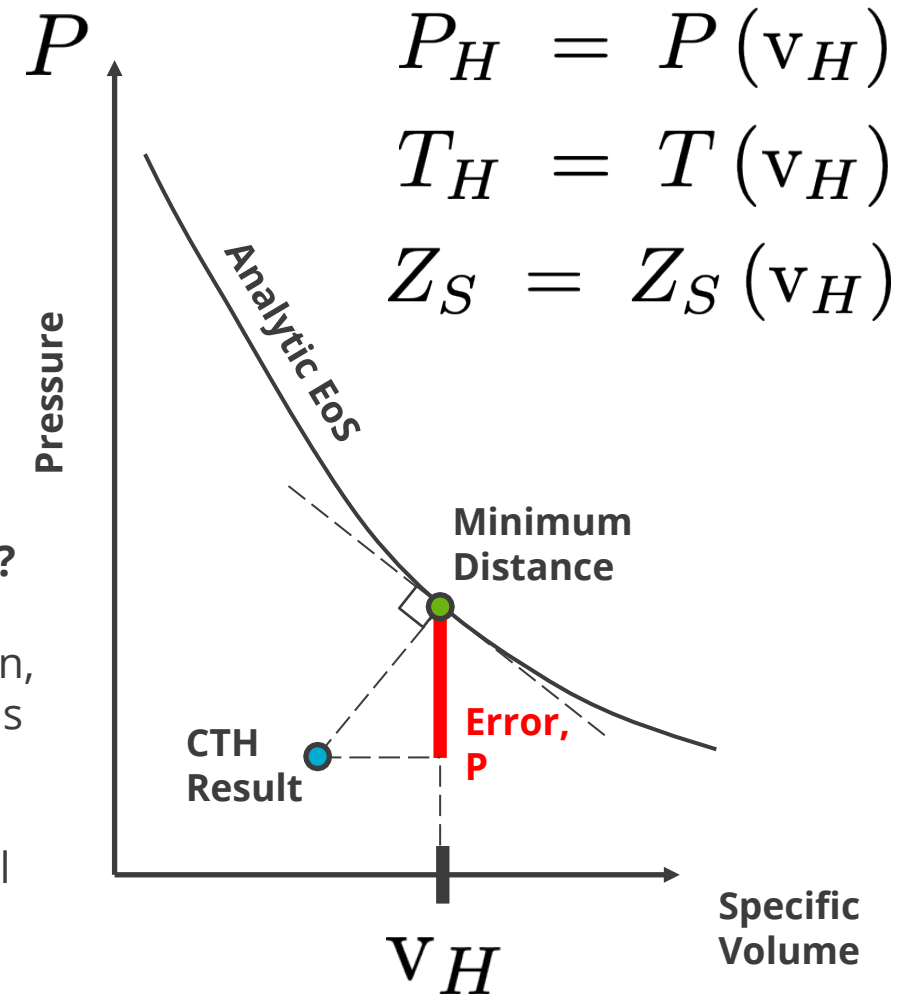
RMSE as a function of
material and $k=2$ to 25
zones per millimeter

Mean RMSE over
all materials at
max resolution

$$\text{RMSE}_{P,k} = \sqrt{\frac{1}{N} \sum_{i=1}^N (P_{CTH} - P_H)^2}$$

How calculated?

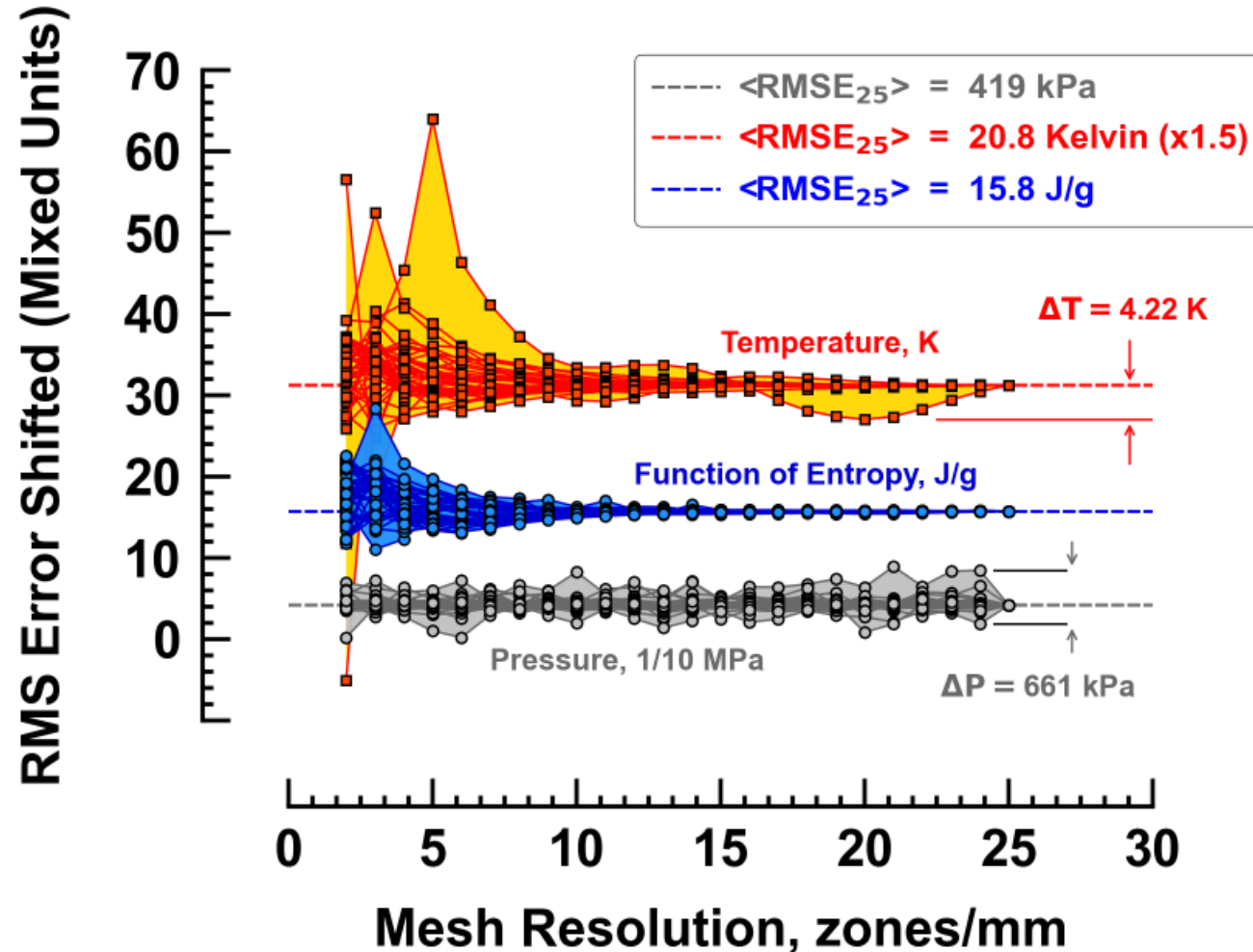
In the minimum distance equation, the analytic EoS is approximated (locally) by a 5th-order polynomial



Section 2. Root-Mean-Squared Error for 46 Materials



1D Mesh Convergence for 46 Materials



Discussion Points

- Mesh convergence after **10 to 15 zones per millimeter**.
- RMSE for pressure is **hundreds of kPa**, which is rather small when dealing with GPa.
- Mean RMSE values of **20.8 Kelvin and 15.8 J/g are not insignificant errors**, especially for reactive burn models AWSD [3] and CREST [4].
- The shock width is coupled to the accuracy of **advection and remap algorithms**, as well as to **artificial viscosity**, which affects T and ZS.
- Material with the oscillatory temperature RMSE is Tantalum, which also has the highest shock temperatures.

[3] Aslam, T. D., "Shock temperature dependent rate law for plastic bonded explosives," *J. Appl. Phys.*, **123**:145901, 2018.

[4] Handley, C. A., Lambourn, B. D., Whitworth, N. J., James, H. R., and Belfield, W. J., "Understanding the shock and detonation response of high explosives at the continuum and meso scales," *Appl. Phys. Rev.*, **5**:011303, 2018.

Section 2. Artificial Viscosity Definitions



DEFINITION #1 Artificial viscosity is a diffusive process that spreads the discontinuous shock front over a finite number of cells. It is a tensor quantity in most modern hydrocodes.

$$\mathbf{Q} = \begin{pmatrix} q_x & s_x & 0 \\ s_y & q_y & 0 \\ 0 & 0 & q_z \end{pmatrix} \xrightarrow{\text{1DR}} q_x = B_L \Delta x c \left| \frac{d\rho}{dt} \right| + B_Q \rho (\Delta x)^2 \left| \frac{d\rho}{dt} \cdot \frac{1}{\rho} \right|^2$$

Linear Term
Quadratic Term

1D, 2D, and 3D CTH simulations use Wilkins' Q, Ref. [5]

DEFINITION #2 Net artificial viscous work is analogous to pressure-volume work, and it is added to internal energy, incrementally, as the shock wave passes through a material.

$$\mathbf{Q} : \Delta \mathbf{V} \xrightarrow{\text{Net}} \sum_{\text{cycles}} \mathbf{Q} : \Delta \mathbf{V} \xrightarrow{\text{1DR}} \sum_{\text{cycles}} |q_x \Delta V_x|$$

Single Time Step

Extra variable called "QWORK" in CTH 13.0

Converges in:
18 to 25
zones/mm – see
backup slides

[5] Wilkins, M.L., "Use of artificial viscosity in multidimensional fluid dynamic calculations," *J. Comp. Phys.*, **36**(3):281-303, 1980.

Section 3. Empirical Correlation for 46 AMGL Materials



During the code development activities, we began to realize that Z_S is related to the net $Q:DV$, i.e.,

$$Z_S \sim fcn \left(\sum_{cycles} Q : \Delta V \right)$$

This is the formula that was programmed into AMGL EoS in CTH version 13.0

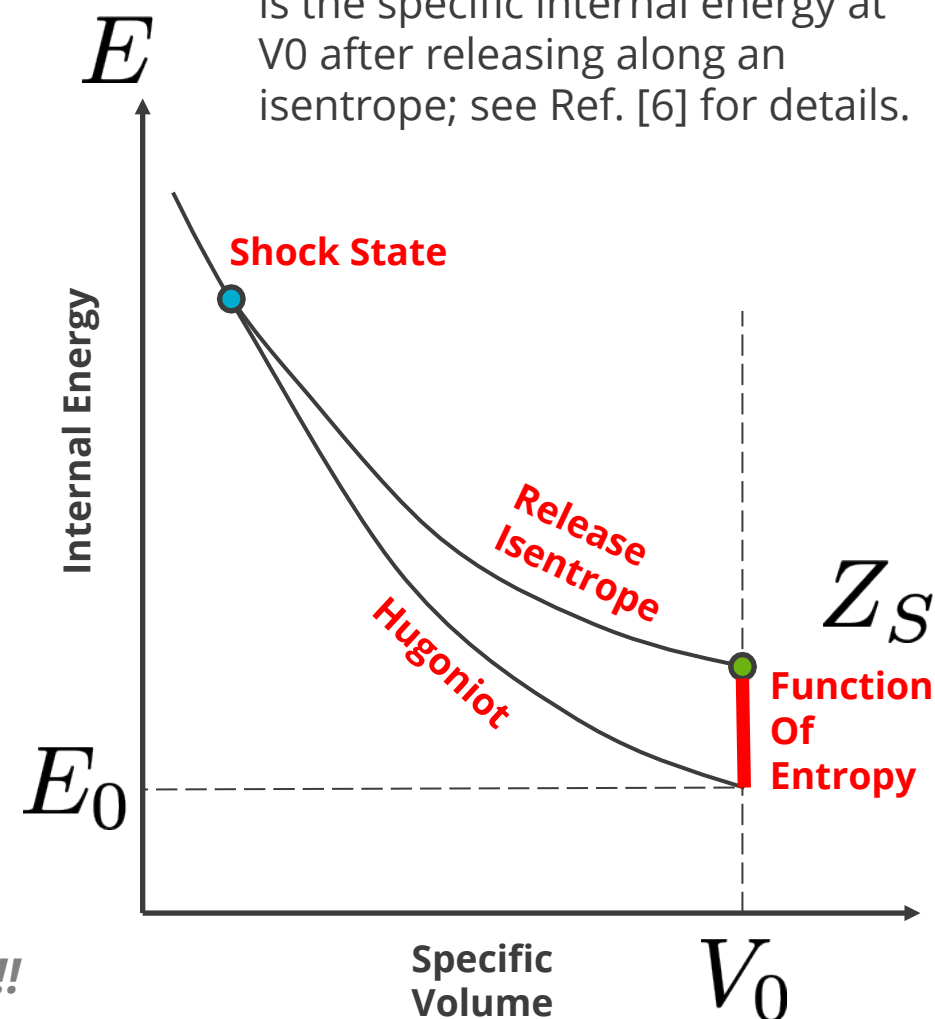
$$Z_S = s_f \left(\sum_{cycles} Q : \Delta V \right) + q_t \left(\sum_{cycles} Q : \Delta V \right)^2$$

Linear scale factor, or parameter "SF" in CTH

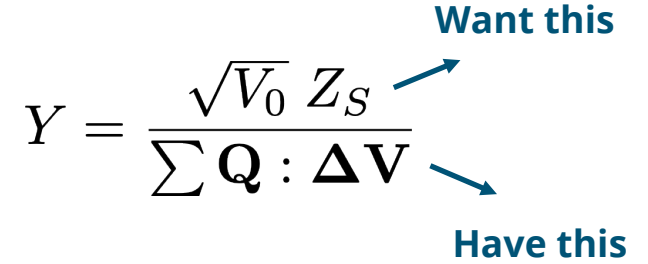
Quadratic term coefficient, or parameter "QT" in CTH

Each of the 46 library materials has unique SF and QT values !!!

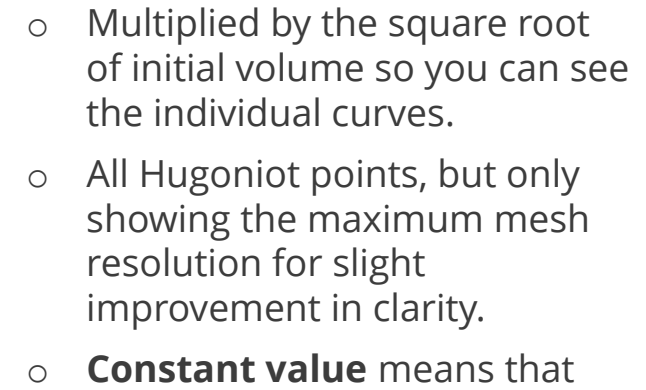
By the way, **Function of entropy** is the specific internal energy at V_0 after releasing along an isentrope; see Ref. [6] for details.



[6] Lambourn, B. D., "An improved EOS for non-reacted explosives," in 14th American Physical Society Topical Conference on Shock Compression of Condensed Matter, AIP Publishing, Baltimore, MD, July 31-August 5, pp.165-168, 2005.



Discussion Points



$$Z_S \propto \sum \mathbf{Q} : \Delta \mathbf{V}$$

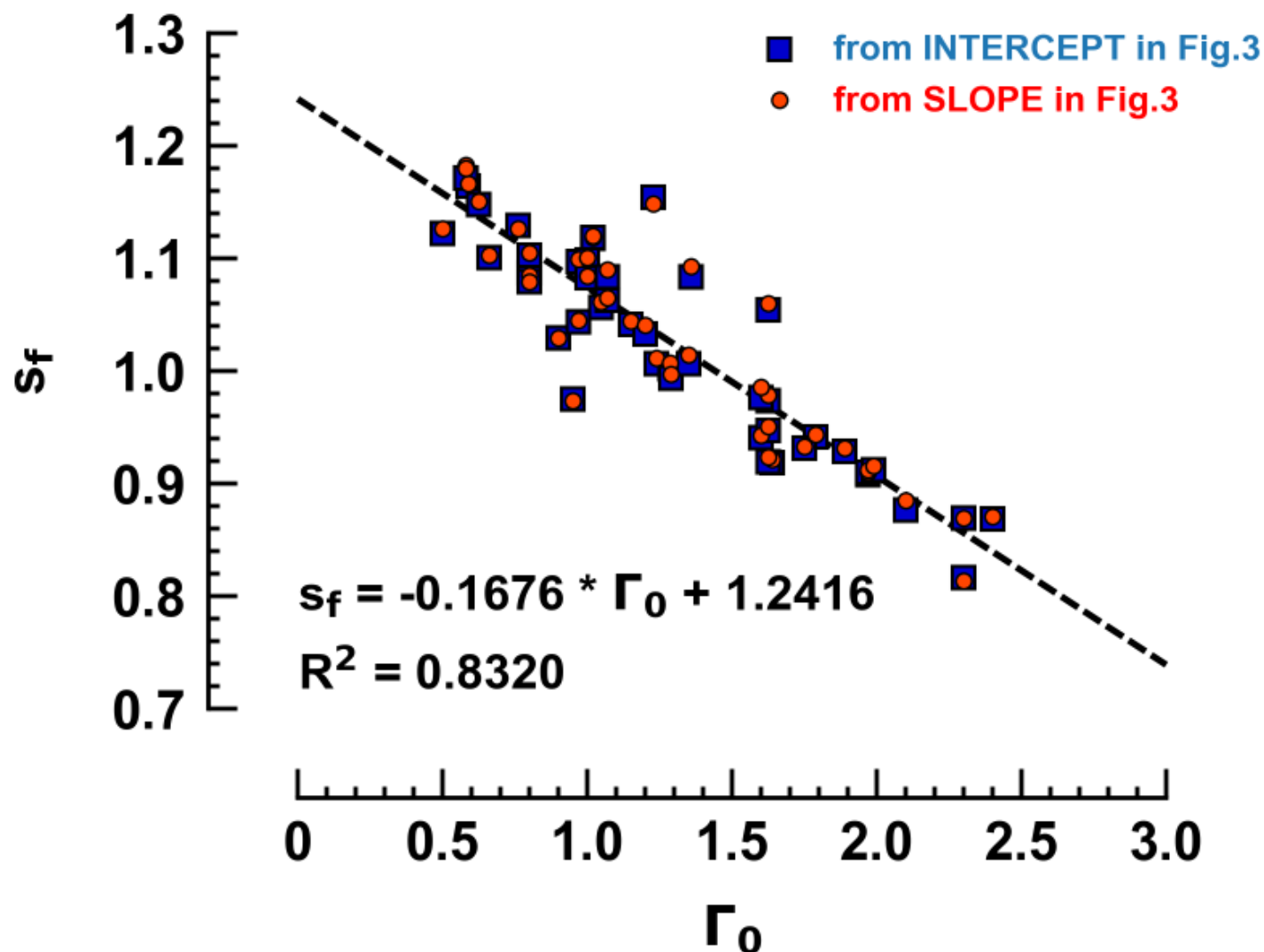
- **Linear slope** means that

$$Z_S \sim \left(\sum \mathbf{Q} : \Delta \mathbf{V} \right)^2$$

Section 3. Empirical Correlation for 46 AMGL Materials



Second Empirical Correlation



Linear fit from the previous slide

$$\frac{\sqrt{V_0} Z_S}{\sum Q : \Delta V} \approx$$

$$A \left(\sum Q : \Delta V \right) + B$$

Parameter s_f can be calculated from the INTERCEPT

$$s_f = \frac{B}{\sqrt{V_0}}$$

Parameter s_f can be calculated from the SLOPE by performing a second curve fit to the function

$$Z_S - q_t \left(\sum Q : \Delta V \right)^2$$

and $q_t = \frac{A}{\sqrt{V_0}}$

Section 4. Summary and Conclusions



- 1) AMGL thermodynamic state variables in CTH 13.0 begin to converge as early as **10 zones per millimeter**, but may require up to **18 zones per millimeter** for the net artificial viscous work to converge. After that, the shock state is mesh independent.
- 2) The shock state function of entropy can be **accurately determined** knowing the **net artificial viscous work** across a shock wave.
- 3) We talked about artificial viscosity, but real **shock viscosity** may change the equation.

Function of Entropy in CTH
(ignore quadratic term)

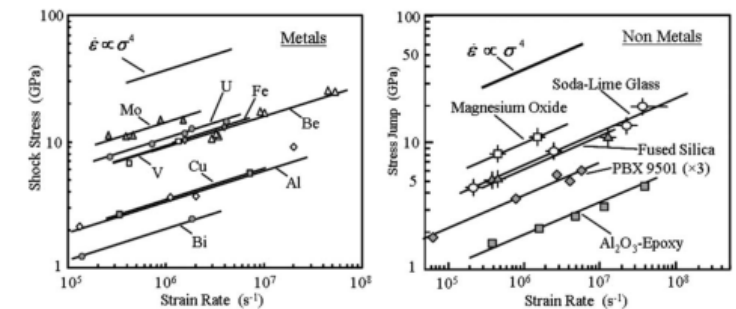
$$Z_S \approx (-0.1676 \Gamma_0 + 1.2416) \sum_{cycles} \mathbf{Q} : \Delta \mathbf{V}$$

$$\mathbf{Q} = \begin{pmatrix} q_x & s_x & 0 \\ s_y & q_y & 0 \\ 0 & 0 & q_z \end{pmatrix}$$

$$Z_S = \int \mathbf{Q}_{real} : \Delta \mathbf{V}$$

Function of
Entropy in
Nature?

+



Fourth power law of Dennis Grady [7]

[7] Grady, D. E., "Structured shock waves and the fourth-power law," *J. Appl. Phys.*, **107**(1):013506, 2010.

Acknowledgements



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- [1] Kittell, D., Schmitt, R., Tuttle, L., and Harstad, E., "Implementation of a CREST multistate reactive burn model in CTH for two solid high explosives," *Proceedings of the 16th International Detonation Symposium*, pp. 1021-1031, Cambridge, MD, July 2018.
- [2] Schumacher, S. C., and Baer, M. R., "Generalized continuum mixture theory for multi-material shock physics." *International Journal of Engineering Science* **183**:103807, 2023.
- [3] Aslam, T. D., "Shock temperature dependent rate law for plastic bonded explosives," *J. Appl. Phys.*, **123**:145901, 2018.
- [4] Handley, C. A., Lambourn, B. D., Whitworth, N. J., James, H. R., and Belfield, W. J., "Understanding the shock and detonation response of high explosives at the continuum and meso scales," *Appl. Phys. Rev.*, **5**:011303, 2018.
- [5] Wilkins, M.L., "Use of artificial viscosity in multidimensional fluid dynamic calculations," *J. Comp. Phys.*, **36**(3):281-303, 1980.
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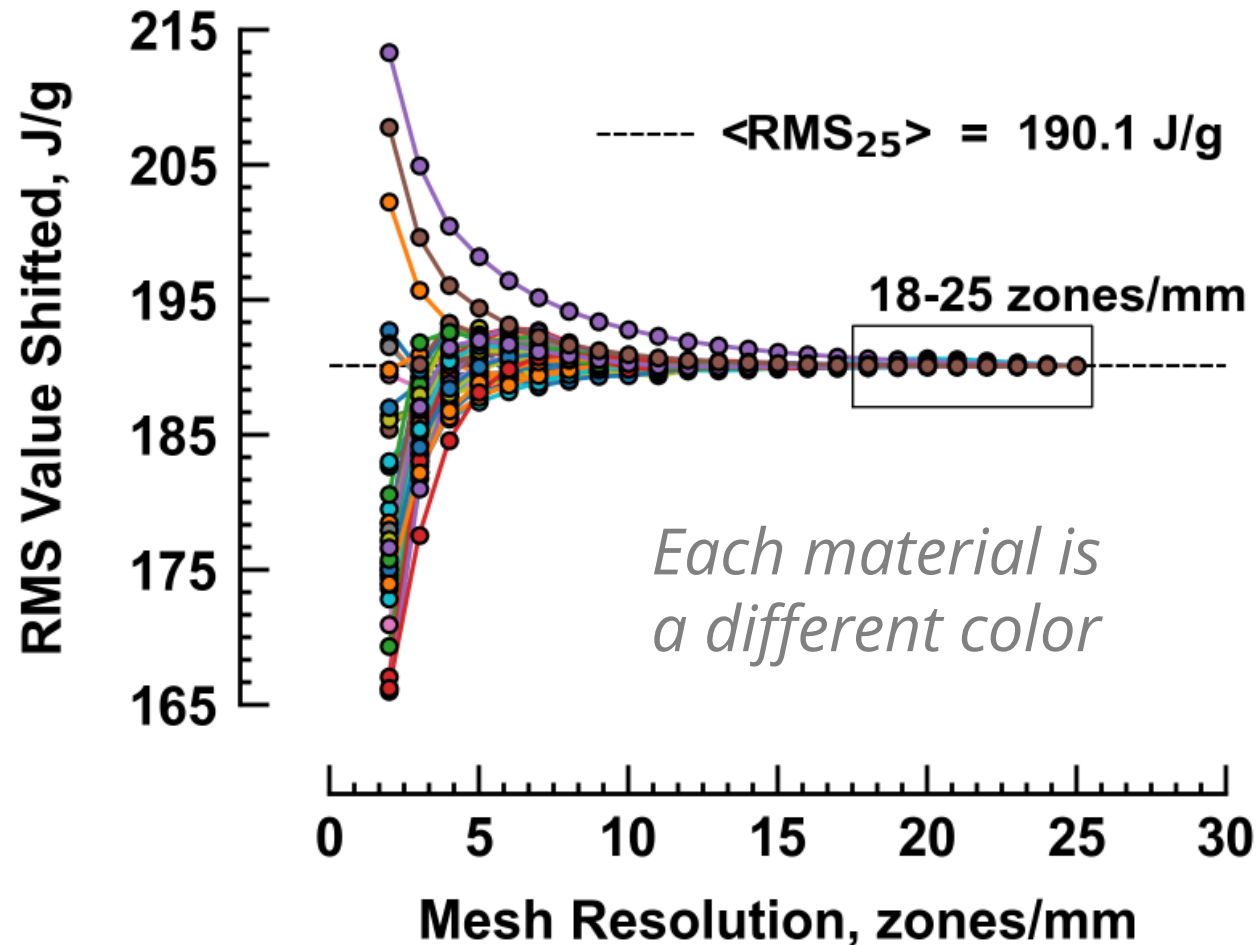


Thank You!
Questions?

Section 2. Artificial Viscosity Results (Omitted)



Net Artificial Viscous Work for 46 Materials



Discussion Points

- Most materials converge after 10 to 15 zones per millimeter like the EoS, but **18 to 25 zones per millimeter** is needed to guarantee convergence.
- Convergence isn't strictly monotonic, but it is a **more well-defined envelope** than for EoS thermodynamic state variables.

$$Y = \text{RMS}_k - \text{RMS}_{k=25} + \langle \text{RMS}_{k=25} \rangle_{\text{mats}}$$

Same as done previously for pressure, except we use the **RMS value** not error.

$$\text{RMS}_k = \sqrt{\frac{1}{N} \sum_{i=1}^N \text{QWORK}^2}$$

Abstract Title (305 characters):

Empirical Correlations Between the Function of Entropy (Z_s) and Net Artificial Viscous Work in a Shock Physics Hydrocode

Abstract Body (1,300 characters):

Concerning the reactive burn models that are used to model shock-induced reactions, the CREST model is unique in that it uses entropy as a reaction potential. Entropy is a thermodynamic state variable, and it is solved from the equation of state (EOS). However, it is susceptible to numerical errors [1], especially for Eulerian hydrocodes during the mass advection and remap steps. During a renewed effort to implement the CREST model into Sandia National Laboratories' shock physics hydrocode CTH, several methods were explored to reduce the numerical errors in the function of entropy, i.e., Z_s . Empirical correlations were found between the function of entropy and the net artificial viscous work during the passage of a shock wave. Here, these empirical correlations are discussed with respect to mesh convergence and the EOS parameters. Additionally, results are shown for 46 different EOS, consisting of metals and metal alloys, polymers, and unreacted energetic materials. Future work is planned to study higher-dimensional shock waves, shock wave interactions, and possible ties to a physical law (e.g., the fourth-power law of Grady [2]).

^[1]Kittell, D., Schmitt, R., Tuttle, L., and Harstad, E. "Implementation of a CREST multistate reactive burn model in CTH for two solid high explosives," *Proceedings of the 16th International Detonation Symposium*, pp. 1021-1031, Cambridge, MD, July 2018.

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