A Case Study in Improvement of a Multiphysics Model Through the Application of Verification & Validation Methods

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Ian Tregillis*, Aaron Koskelo‡, Brandon Wilson‡

Los Alamos National Laboratory

*XCP-6: Plasma Theory and Applications
‡XCP-8: Verification and Analysis

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This talk is a direct sequel to VVS2019-5137; both talks cover work documented in Tregillis & Koskelo, JVVUQ 4(4):041004 (2019)

• Brief Recap of Earlier Work
  – The RMI+SSVD Ejecta Source Model in Theory & Simulation
  – Model Performance in Validation & Verification Spaces
• Expanding Scope to Encompass Other Physics Data
• Boundary Conditions for an Entire Class of Source Models
• A Modified (“BC Aware”) Version of the RMI+SSVD Model
• Validation Meta-Analysis
• Refinements to the “Compatibility Score” Metric
• Summary
A physics hypothesis for ejecta production at shocked free surfaces: the RMI+SSVD source model

The RMI source model posits that imperfections on the free surface seed the growth of a Richtmyer-Meshkov fluid instability, and that ejecta originate from the disintegration of RMI spike features.

Proton radiography data suggest the spikes evolve self-similarly, thereby yielding a velocity distribution (SSVD) for the ejecta mass.

Our goal is to evaluate the source model & the quality of its numerical implementation in FLAG.

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Buttler et al. J. Fluid Mech. 703:60 (2012);
Dimonte et al. J. Appl. Phys. 113:024905 (2013);

The RMI+SSVD ejecta source model has been implemented as a sub-grid model in FLAG†.

This simulation capability has been applied to HE-driven, singly shocked tin coupons fielded in vacuum:


Getting the right amount of material at the right place at the right time requires:

- HE modeling
- strength modeling
- equations of state
- numerical methods
- ejecta modeling (subgrid)

†Fung et al., Computers & Fluids 83:177 (2013); Harrison, LA-UR-15-26632
The assumptions built into the piezo analysis describe a system with a closed-form solution. We have derived that solution* for LANL’s RMI+SSVD model.

Source Function for RMI+SSVD

\[ m_c(w, t_c) = \frac{2}{3} m_0 \cdot \frac{1}{t_c + \beta \tau} \cdot \frac{\xi e^{-\frac{\xi w}{\eta^2}} + 1}{(2 - e^{-\xi}) \eta^s} \cdot \Pi(t_c) \]

True Mass Accumulation on Sensor

\[ m_t(t) = \left\{ \begin{array}{ll}
\frac{2m_0 \xi}{3 \eta^s (2 - e^{-\xi})} \int_{t / \eta^s}^{h - u_{fs}} e^{-\frac{\xi w}{\eta^2}} \ln \left[ p(t) + \frac{q(t)}{w} \right] dw & (t > t^*) \\
+ \frac{2m_0}{3 \eta^s (2 - e^{-\xi})} \ln \left( 1 + \frac{t_{cf}}{\beta \tau} \right) & (t \leq t^*)
\end{array} \right. \]

Error Imposed by Instant-Production Assumption

\[ \Delta m(t) = m_t(t) - m_t(t_{cf}) \]

These expressions aren’t coded into FLAG.

This is a framework for mathematical verification†.

\[ \beta \tau: \text{ RMI timescale} \]
\[ \tilde{w} = \hat{\eta}^s: \text{ max. relative velocity} \]
\[ \hat{u}: \text{ max. lab-frame velocity} \]
\[ \xi: \text{ self-similarity parameter} \]
\[ m_0: \text{ mass normalization} \]
\[ t^*: \text{ time of } \hat{u} \text{ depletion} \]
\[ t_{cf}: \text{ ejecta shut-off time} \]
\[ t_{oa}: \text{ time of first arrival} \]
\[ h: \text{ sensor distance} \]

\[ p(t) = 1 + \frac{t}{\beta \tau} \quad q(t) = \frac{u_{fs} - h}{\beta \tau} \quad t^* = \frac{h + \hat{\eta}^s t_{cf}}{\tilde{w}} \]


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Verification: FLAG calculations adhere to the model.
Validation: The model deviates from the data.

Vogan 06: Predicted, Simulated, & Piezoelectrically Inferred Mass Data
(3.8.Alpha.14: nisites = 0, floor_npackets = 1, Npp = 10^5)

100% data ± 1σ at t₀ (linear: 100% → 10%)
FLAG ejfoil (corrected for u_r ≠ 0 & u_f,t): Original SSVD
Analytic m_r ± 1σ (pinned to data endpoints): Original SSVD

Theory

"Verification"

"Validation"

Data

Simulations

Compatibility Score*

FLAG / data
13.9

Theory / data
39.7

FLAG / Theory
64.9
Piezoelectric voltage datasets from these and related experiments exhibit two apparently global properties.

The time-dependent piezoelectric voltages:

- rise smoothly from the baseline, and
- are continuous.

These properties encode requirements for the model prediction, including:

\[
V(t_{a0}) = 0 \\
V'(t_{a0}) = 0 \\
\lim_{t \to t^-} V(t) = \lim_{t \to t^+} V(t) \forall t
\]

The voltage properties can be expressed mathematically for a class of ejecta source models encompassing RMI+SSVD.

Any ejecta source model with a stationary velocity distribution, or which is well-approximated as such, has a source areal mass function of the generic form

$$m_c(w, t_c) = m_0 g(t_c) f(w) \prod_{t_0}^{t_{cf}}(t_c)$$

One can show analytically* that such a source function will predict

$$V(t_{a0}) = \kappa_p \frac{m_0}{h} \frac{\hat{u}^4}{\hat{w}} g(0) f(\hat{w})$$

$$V'(t_{a0}) = \kappa_p \left\{ \frac{m_0}{h^2} \left[ \frac{\hat{u}^6}{\hat{w}^2} - 4 \frac{\hat{u}^5}{\hat{w}} \right] g(0) f(\hat{w}) + \frac{m_0}{h} \frac{\hat{u}^5}{\hat{w}^2} g'(0) f(\hat{w}) - \frac{m_0}{h^2} \frac{\hat{u}^6}{\hat{w}} g(0) f'(\hat{w}) \right\}$$

$$\Delta V(t^*) = \kappa_p \frac{m_0}{h - u_{fs} t_{cf}} \frac{\hat{u}^4}{\hat{w}} g(t_{cf}) f(\hat{w})$$

where the fastest particles are depleted at $t^*$ and $\kappa_p$ is a constant defined by the pin.

*Full derivation in Tregillis, LA-UR-18-27420 (2018); see also Tregillis & Koskelo, JVVUQ 4:041004 (2019)
The RMI+SSVD source model violates the required boundary conditions. A simple modification can fix that.

\[ V(t_{a0}) = 0 \implies g(0) = 0 \text{ or } f(\hat{w}) = 0 \]
\[ V'(t_{a0}) = 0 \implies g(0) = g'(0) = 0, \text{ or } g(0) = f(\hat{w}) = 0, \text{ or } f(\hat{w}) = f'(\hat{w}) = 0 \]
\[ \Delta V(t^*) = 0 \implies g(t_{cf}) = 0 \text{ or } f(\hat{w}) = 0 \]

RMI+SSVD (stationary approx.)

\[ g(t_c) = \frac{2}{3} \frac{1}{t_c + \beta' \tau} \]
\[ f(w) = \frac{\xi e^{-\xi \frac{w}{\hat{w}}} + 1}{(2 - e^{-\xi})\hat{w}} \]

<table>
<thead>
<tr>
<th>Condition</th>
<th>Equation</th>
</tr>
</thead>
<tbody>
<tr>
<td>( V(t_{a0}) \neq 0 )</td>
<td>( g(0) = ) 0 \text{ or } ( f(\hat{w}) = 0 )</td>
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<td>( \Delta V(t^*) \neq 0 )</td>
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All requirements can be satisfied with a simple modification to the SSVD:

\[ \tilde{f}(w) = \kappa[f(w) - f(\hat{w})] \]  
(\( \kappa \) is required to conserve mass)

will have \( \tilde{f}(\hat{w}) = 0, \tilde{f}'(\hat{w}) \approx 0 \) for sufficiently large \( \xi \) (FLAG uses 7.2).

Let’s consider a model that combines RMI with this “modified” SSVD.
One change to the SSVD corrects three discrepancies in the model’s voltage predictions.

- **ANY** source model will exhibit these problems if it violates the required BCs.
- These problems **ARE NOT CAUSED** by attempting to fit nuances of the data.
- Thresholding the data **DOES NOT CHANGE** this result.

*Vogan et al. J. Appl. Phys. 98:113508 (2005); piezoelectric data courtesy of William Buttler.*
Synthetic (analytic) radiographs illustrate the beneficial effect of modifying the SSVD in accordance with the boundary condition requirements.

The ejecta leading edge is typically invisible in X-ray transmission data.
Recomputing the analytic mass prediction using the modified SSVD.

Vogan 06: Predicted, Simulated, & Piezoelectrically Inferred Mass Data
(3.8.Alpha.14: nsites = 0, floor_npackets = 1, Npp = 10)

- 100% data ±1σ at tf (linear: 100% → 10%)
- FLAG efoil (corrected for uv ≠ 0 & uf,): Original SSVD
- Analytic m1 ± 1σ (pinned to data endpoints): Original SSVD

Original SSVD

<table>
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<tr>
<th>Score</th>
<th>FLAG / 100% data</th>
<th>~14%</th>
</tr>
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<tbody>
<tr>
<td>Theory / 100% data</td>
<td>~40%</td>
<td></td>
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**Graph:**
- Cumulative Ejecta Mass/Area on Sensor [mg/cm²]
- Time since Shock Breakout [µs]

**Key Points:**
- **Original SSVD** score for 100% data is ~14%.
- **Theory** score for 100% data is ~40%.

...yields a significantly improved comparison to the unthresholded mass data.

The original SSVD has at $t_{a0}$

$$\dot{m}_{t,i} = 0; \bar{m}_{t,i}, \ddot{m}_{t,i} \neq 0$$

The modified SSVD has at $t_{a0}$

$$\dot{m}_{t,i} = \bar{m}_{t,i} = \ddot{m}_{t,i} = 0$$

Vogan 06: Predicted, Simulated, & Piezoelectrically Inferred Mass Data

(3.8.Alpha.14: nsites = 0, floor_npackets = 1, N_{tp} = 10^3)
But there are many ways to conduct the comparisons...

- **SSVD**: Free parameter. FLAG uses 7.2, based on empirical comparison to data
- **Ejecta**: Predicted: Derived strictly from the RMI model prediction
  Pinned: Pinned to the value implicit in the data (1st arrival time)
- **Data**: Unthresholded: 100% of recorded mass domain
 Thresholded: 99% of recorded mass domain
- **Production interval**: Tuned: tuned to match the total observed mass for each shot
  Prescribed: set by ansatz*: $t_{cf} = a \lambda / u_{fs}$; $a = 40 \pm 10$
- **Time-dependent data uncertainty**: Constant: $1\sigma$ uncertainty is 10% at all times
  Linear: $1\sigma$ uncertainty declines linearly 100% → 10%

…so we computed the model / data compatibility score for 115,200 scenarios.

**Ensemble Parameters**

- $\xi$: 400 values: $2 \leq x \leq 22$
- data: 100% & 99%
- $t_{cf}$: tuned (1) & prescribed (3)
- $t_{a0}$: predicted & pinned to data
- SSVD: original & modified
- shots: Vogan 3-8 & 10-12

**Score Calculations**

- data $\pm 1\sigma$ ("constant"); model $\pm 0.2\sigma$

Narrow band on the model elucidates trends at the cost of lowered scores.

- Modifying SSVD is more effective than thresholding the data.
- Model compatibility is very sensitive to the unknown ejecta production interval, even within the range allowed by the mass measurement uncertainty.

![Compatibility Scores: Vogan Piezo Data & RMI+SSVD Model Predictions](image)
The model compatibility score can be sensitive to undetectable changes in the measurement. We’re assessing alternate approaches and metrics.

- The compatibility score is sensitive to changes in the model inputs that shift the diagnostic prediction within the $1\sigma$ error bars.

- The score is computed from the global integral over a binary-valued function (true when the uncertainty bands overlap, false otherwise).

- A better approach might use a smoother argument, such as confidence intervals, and might think in terms of model acceptability* rather than model compatibility†.

• We started out with **good verification results** (high compatibility scores for FLAG/theory comparison), but **undesirable validation results** (low compatibility scores for theory/data comparison).

• Global properties of piezoelectric voltage data can be translated into boundary conditions for a very wide range of ejecta source models.

• The original RMI+SSVD exhibits **model-form error** because it violates these boundary conditions.

• A small modification brings the model into alignment with these conditions.

• The modification was implemented in FLAG.

• We now find **good verification results** and **excellent validation results** (very high compatibility scores for theory/data comparison).

• Further advances might come from a more nuanced consideration of metrics.