Bayesian Approach to Estimating Fireball Parameters from Remote Sensing Data

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Derek E. Armstrong
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Remote Sensing of High Explosive (HE) Events

• **Use of spectrometers to monitor HE events in infrared region:**
  – Information on fireball temperature
  – Information on fireball gas species concentrations (CO₂, CO, H₂O, etc.)
  – Information on presence of metals or other materials

[Image of explosion]

![Sensor fireball spectrum (･･･) Model spectrum (----) Blackbody (-----)](image)

• **Objectives of the work:**
  – Improve computational physics codes that simulate HE or similar events
  – Validation of physics codes and models
    • HE equation-of-state (EOS)
    • Metal fragmentation
Code Validation

- Improvements and validation to computational codes / models by comparing temperature, soot & fireball gas concentrations:

Image is 2D slice from 3D simulation

Models for gas species molar fractions in mixed HE/air zones

Pressure - 1.0, HE/air - 0.5
Model for Fireball Radiance

• Observed sensor radiance depends on the following:
  – Fireball temperature (blackbody function) and size
  – Fireball composition (gas and solid material emission)
  – Atmospheric transmission (depends on atmospheric conditions and distance)

At-sensor radiance $R(.)$ with gas and soot (no additional solid materials):

$$R(\nu) = I^2 \varepsilon_{FB}(\nu) B(T_{FB}, \nu) \tau_{atm}(\nu)$$

$$= I^2 (1 - e^{-\kappa_p l \sum \xi_i \sigma_i(\nu)}) B(T_{FB}, \nu) \tau_{atm}(\nu)$$

Fit parameters in red:

- $\kappa_p$ is soot absorption coefficient
- $\sigma_i$ is gas cross sections
- $\xi_i$ is gas concentrations in #/cm$^3$
Model for Fireball Radiance

At sensor radiance given by:

\[ R(\nu) = l^2 \varepsilon_{FB}(\nu) B(T_{FB}, \nu) \tau_{atm}(\nu) \]

**Red** curve is blackbody scaled to fit two wavenumber regions.

**Blue** curve is FTIR.

**Green** curve is atmospheric transmission computed with given temperature and pressure.

Line-by-line computation and convolved to sensor wavenumbers. Alternative is to use SNB.

Mismatch between green curve and data (blue) is due to fireball selective emission from fireball constituents.
Spectrometer Resolution and FTIR

• Tradeoff between different resolutions (spatial vs temporal vs spectral):
  – Sensors often sacrifice one type of resolution to improve the other two

• This presentation considers specific FTIR spectrometer:
  – FTIR (Fourier Transform Infrared): raw data is an interferogram
  – Single pixel, ~16 cm\(^{-1}\) spectral resolution, ~0.01s temporal resolution
  – Instrument uses moving mirror to change path length of part of incoming radiation and measures interference of recombined signal
Computational Challenges

Spectral Model:

\[ R(v) = l^2 \varepsilon_{FB}(v) B(T_{FB}, v) \tau_{atm}(v) \]
\[ = l^2 \left( 1 - e^{-l\kappa_p - l \sum \xi_i \sigma_i(v)} \right) B(T_{FB}, v) \tau_{atm}(v) \]
\[ R_s(v_i) = \int_0^\infty L(v - v_i) R(v) dv. \]

Optimize over model parameters in red!

Spectral model is computed at high resolution: 0.001 cm\(^{-1}\)

T = 1195K, \( l = 330\) cm, soot (cm\(^{-1}\)) = 0.001, XH2O (#/cm\(^3\)) = 7.3E17, XCO2 (#/cm\(^3\)) = 1.7E18, XCO (#/cm\(^3\)) = 9.2E16.

High Resolution Model (R)  Instrument Line Shape (L)  Sensor Response (R_s)
Computational Challenges, Continued

• Millions of \((T, P)\) dependent gas absorption lines:
  – Generally makes high resolution modeling and convolving with instrumental line shape necessary
  – Studying use of lower spectral resolution modeling for multi-fidelity approaches and improved efficiency

• SNB investigated by Zammit & Timmermans (LANL):
  – Bands averaged to 25 cm\(^{-1}\) with SNB
  – Speed-up of computation (~2000 spectra per second per core for FTIR analysis, Zammit & Timmermans)

Transmission in band is \(\tau = \exp\left(-\frac{\bar{W}}{\bar{\delta}}\right)\), where \(\bar{W}\) is mean black equivalent width of these lines and \(\bar{\delta}\) is lines per unit length in band.
Optimization Approach

• Development of Python code for full spectral modeling and utilizing hi-resolution or line-by-line cross sections:
  – Multi-process Python code used for prototyping
  – Instrumental (FTIR) line shape is modeled
  – Amoeba or downhill simplex method is used for optimization
  – Code optimizes fit by adjusting fireball temperature and width, soot absorption coefficient, plus H2O, CO2, and CO concentrations

Spectral Model:

\[ R(\nu) = l^2 \epsilon_{FB}(\nu) B(T_{FB}, \nu) \tau_{atm}(\nu) \]

Parameters found by Amoeba optimization method:

- \( T = 1195 \text{K} \)
- width = 330 cm
- soot (cm\(^{-1}\)) = 0.001
- \( X_{H2O} \) (#/cm\(^3\)) = 7.3E17
- \( X_{CO2} \) (#/cm\(^3\)) = 1.7E18
- \( X_{CO} \) (#/cm\(^3\)) = 9.2E16
Uncertainty Quantification

• Bayesian calibration for parameter estimation when metals are not included in the model:
  – Error term is assumed to be a multivariate Gaussian
  – Inverse gamma distribution used for unknown Gaussian variance

• Bayesian Model Averaging (BMA) for models including metals:
  – Quantify uncertainty in materials in fireball
  – Based on Bayesian Information Criterion (BIC)
  – Computes model probabilities with estimate of log transformation of full Bayesian posterior
Bayesian Model Averaging (BMA)

• Fireball model with additional solid materials:

\[ l^2 \varepsilon_{FB}(\nu) B(T_{FB}, \nu) \tau_{atm}(\nu) + \sum_i c_i \varepsilon_i B(T_i, \nu) \tau_{atm}(\nu) \]

• BMA to compute probabilities for materials:

\[ P(\text{material } i) = \sum_{M \text{ contains } i} P(M|d) \]

• Model probabilities computed based on an estimate using the Bayesian Information Criterion (BIC)

\[ P(M|d) = e^{-BIC/2} \]

\[ BIC = k \ln(n) - 2 \ln(L_{max}) \]

Large number of possible models \( M \): Each model defined by set of materials to include in spectrum computation.

Model probabilities computed for each of possible thousands of models.

Many possible models due to sub-setting 10s of materials.
Bayesian Information Criterion (BIC)

Based on an estimate of the log-transformation of the full Bayesian posterior probability:

\[
\ln (P(M|d)) = \ln \left( \pi(M) \int g(\theta_M|M)L(d|\theta_M)d\theta_M \right)
\]

2\textsuperscript{nd}-order Taylor’s series approximation of log transformation, expanded about the maximum likelihood estimate (MLE):

\[
BIC = k\ln(n) - 2\ln(L_{\text{max}})
\]

\[
P(M|d) \approx e^{-BIC/2}
\]

Technically, BIC is -2 times log transformation.

BIC is obtained as estimate of log-transformation after removing insignificant terms. BIC above does not use prior on models M.
NOTE: If number of potential models are large, then a method is needed to sample a collection of best models.

### Case Problem 1:

<table>
<thead>
<tr>
<th>Material</th>
<th>BMA Probability</th>
</tr>
</thead>
<tbody>
<tr>
<td>mat 12</td>
<td>0.99837</td>
</tr>
<tr>
<td>mat 03</td>
<td>0.12883</td>
</tr>
<tr>
<td>mat 05</td>
<td>0.08371</td>
</tr>
</tbody>
</table>

Material 12 is important to fit of data. High confidence for material 12.

### Case Problem 2:

<table>
<thead>
<tr>
<th>Material</th>
<th>BMA Probability</th>
</tr>
</thead>
<tbody>
<tr>
<td>mat 04</td>
<td>0.52832</td>
</tr>
<tr>
<td>mat 20</td>
<td>0.39881</td>
</tr>
<tr>
<td>mat 14</td>
<td>0.27873</td>
</tr>
</tbody>
</table>

Material 04 is not important to fit of data. Low confidence for material 04.
Bayesian Calibration

Can be used for cases with known or fixed materials. Can compute probabilities for soot and gas concentrations ($\theta$):

Likelihood: $p(d|\theta, \omega) = \left(\frac{1}{\sqrt{2\pi \omega}}\right)^{-n/2} \exp\left(-\frac{\chi^2}{2}\right)$

where $\theta$ is the set of model parameters and

$$\chi^2 = \sum_{j=1}^{n} \frac{(d_j - m(v_j, \theta))^2}{2m(v_j, \theta)^2 \omega}.$$

Inverse gamma distribution applied to unknown Gaussian variance $\omega$
Best RMS from sampling (~100000 points) for Bayesian = 1.74
Best RMS from Amoeba optimization = 1.89
Bayesian Calibration – Cont’d

Best RMS from sampling (~100000 points) for Bayesian = 1.74

$$RMS = \sqrt{\frac{\sum (m_i - d_i)^2}{n}}$$

Histogram of RMS for all sampled points

Histogram of Top 1% RMS

Histogram of Top 1% RMS

Histogram of Top 1% RMS

Histogram of Top 1% RMS

Histogram of Top 1% RMS

Histogram of Top 1% RMS

Histogram of Top 1% RMS
Summary

• Estimate fireball parameters to improve and validate computational physics codes simulating explosive events

• Uncertainty quantification is necessary due to correlation of parameters when fitting to data
  – Investigating many models allows for quantification of importance of a material to the fit of data

• Studying use of Bayesian calibration and Bayesian Model Averaging for fireball characterization:
  – Methods can be applied to general spectroscopy problem and not just fireball characterization
  – BMA for material uncertainty