System-Independent Dual-Energy Computed Tomography for Characterization of Materials

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Summary

- Context: DHS needs to detect explosives in baggage
- Objective: Develop system-independent X-ray signatures
  - Commonly used dual-energy (DECT) X-ray signatures, based on \((\mu_{\text{high}}, \mu_{\text{low}})\) or Hounsfield units, are system X-ray spectrum dependent; this makes them difficult to compare across systems

- Recent Results:
  - DHS-EXD funded development of a new method called SIRZ* using a physics-based feature space \((\rho_e, Z_e)\)
  - In test cases SIRZ was precise (<2% err.) and accurate (<3% err.) for 5 different CT spectra taken in pairwise combinations
  - SIRZ has now been automated and its accuracy confirmed to <3% error on another scanner

- Advantages:
  - SIRZ removes spectral information from the characterization feature space.


SIRZ usefulness still needs to verified for other systems, such as EDSs
Outline

- SIRZ Method
- Experiments
- Results
  - Manual & semi-automated SIRZ R&D tests
  - Automated-SIRZ tests
- Future Work
- Summary
SIRZ is a reference-calibrated dual energy decomp post-processing

\[ \rho_e = K(a_c) \] and \[ Z_e = k(a_p/a_c)^{1/n} \]

where the \( K, k \) and \( n \) constants are obtained through a calibration procedure using well-known reference materials

Photoelectric-Compton decomp* (PCD) solves a system of equations

- Attenuation generally follows the Beer-Lambert Law:
  \[ I = I_0 e^{-\mu l} \]

- Attenuation Projections (P) are obtained using the formula:
  \[ P = -\ln \frac{I}{I_0} = \mu l \]

- Photoelectric and Compton contributions \((A_c, A_p)\) of \((\mu l)\) are a function of:
  \[ P(E) = \int \mu(x, y, z, E) dl = f_{KN}(E) \int a_c dl + f_p(E) \int a_p dl = f_{KN}(E)A_c + f_p(E)A_p \]

- Integrating over the system spectral response \([S(E)]\) extends mono- to poly-energetic, then use 2 (low/high) spectra to solve a system of 2 equations with 2 unknowns \((A_c, A_p)\).
  \[ P_L = -\ln \left[ \int S_L(E) \exp\left[-f_{KN}(E)A_c - f_p(E)A_p\right] dE \right] + \ln \int S_L(E) dE \quad \text{(Low energy projection)} \]
  \[ P_H = -\ln \left[ \int S_H(E) \exp\left[-f_{KN}(E)A_c - f_p(E)A_p\right] dE \right] + \ln \int S_H(E) dE \quad \text{(High energy projection)} \]


Note: Spectral knowledge of \(S_L(E)\) and \(S_H(E)\) are needed
Ze and $\rho_e$ are system-independent decomposition features

- **Ze** is an alternative definition of effective atomic number*, instead of $Z_{\text{eff}}$
  - $Z_{\text{eff}} = \sqrt[p]{\sum_i a_i(Z_i)^p}$ is empirically derived approximation, fits poorly over broad $Z$/spectrum
  - Ze is based on X-ray cross sections, and is computed using published tables
  - ZeCalc‡ is a Java app to calculate Ze given composition and spectrum (and $\rho_e$ if density known)

- $\rho_e$ is the electron density, given as:
  $$\rho_e = \rho \frac{\sum r_iZ_i}{\sum r_jA_j},$$
  where $\rho$ is mass density, $r_i$ is molar fraction, and $A_i$ is atomic mass

- Materials with identical Ze are shown to have closer X-ray cross section than materials with identical $Z_{\text{eff}}$ (with $p=3.80$).
- SIRZ tested for $6 \leq Ze \leq 14$ and $0.5 \leq \rho_e \leq 1.2$


We chose features grounded in x-ray physics to remove system variability.
(\rho_e, Z_e) values are found by MMSE fit to known reference materials

- SIRZ uses \( \rho_e = K(a_c) \) and \( Z_e = k(a_p/a_c)^{1/n} \)
- For each dual-energy scan, constants \( K, k \) and \( n \) are found by minimum-mean-square-error (MMSE) fit from the \( a_c \) and \( a_p \) images of reference materials whose \((\rho_e, Z_e)\) values are well known
  - We used Graphite, POM (Delrin), Water, PTFE (Teflon), Magnesium, Silicon
- The \((\rho_e, Z_e)\) of the unknown specimen is directly calculated using the equations above
- Note that beam hardening compensation is not needed!
R&D experiments involved two CT systems of similar design

- Two DECT systems (HE and TB) were used for quantitative specimen characterization
  - The main differences is in their detectors and energies employed
- Reference Materials were *simultaneously* scanned with specimen

![General layout of HE and TB DECT systems](image)

<table>
<thead>
<tr>
<th>CT Scanners, Spectra and Filters Used in Experiments</th>
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<tbody>
<tr>
<td><strong>CT Scanner</strong></td>
</tr>
<tr>
<td></td>
</tr>
<tr>
<td>HE</td>
</tr>
<tr>
<td></td>
</tr>
<tr>
<td>TB</td>
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*Spectral responses used in experiments*

*The shaded boxes indicate the scans that were not acquired.*
Well-known specimens were designed to establish a baseline of performance

- Specimens covered a range of Z values (from graphite, Z=6, to Si, Z=14)
  - Homogeneous Specimens match the composition of corresponding reference materials
  - Two Heterogeneous “composite” Specimens examine system behavior for complex samples
  - High-Z Specimen of RbBr solution to observe behaviors outside of design goals
- All solid references and specimens were assayed to >99.98% purity by composition

<table>
<thead>
<tr>
<th>Name</th>
<th>Reference</th>
<th>Dia (mm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Specimen 1</td>
<td>Graphite</td>
<td>50.8</td>
</tr>
<tr>
<td>Specimen 2</td>
<td>Teflon</td>
<td>56</td>
</tr>
<tr>
<td>Specimen 3</td>
<td>Magnesium</td>
<td>25.4</td>
</tr>
<tr>
<td>Specimen 4</td>
<td>Silicon</td>
<td>25.4</td>
</tr>
<tr>
<td>Insert A</td>
<td>Teflon</td>
<td>10</td>
</tr>
<tr>
<td>Insert B</td>
<td>Delrin</td>
<td>10</td>
</tr>
<tr>
<td>Insert C</td>
<td>Magnesium</td>
<td>10</td>
</tr>
<tr>
<td>Insert D</td>
<td>Water</td>
<td>10</td>
</tr>
<tr>
<td>Substrate 1</td>
<td>Teflon Plug</td>
<td>56</td>
</tr>
<tr>
<td>Substrate 2</td>
<td>Delrin Plug</td>
<td>50.8</td>
</tr>
<tr>
<td>Specimen 7</td>
<td>Water² (60 ml)</td>
<td>36.9/38.9</td>
</tr>
<tr>
<td><strong>High-Z Specimen</strong></td>
<td><strong>19% RbBr solution</strong></td>
<td>10</td>
</tr>
</tbody>
</table>
Features based on linear attenuation coefficients discriminated poorly

- $Z_{\text{eff}}$ interpolation uses reference materials to generate $Z_{\text{eff}}$ estimates based on Low/High ratio values.
- $Z_{\text{eff}}$ interpolation significantly improves errors in the vertical dimension.
- \(YNC^*\) using PCD-estimates of $Z_{\text{eff}}$ is slightly better, but still has large horizontal errors.


The vertical (Z) uncertainty is reduced from Ratio to Interpolated-$Z_{\text{eff}}$ results.
In our R&D, SIRZ* showed better precision and accuracy over prior methods. SIRZ is system-independent and outperforms Ratio, $Z_{\text{eff}}$-interpolation.

- System-independent $\rho_e/Z_e$ (SIRZ) produces good material estimates over the interpolative range.
- Using six reference materials generates similar results to using only the four shown.
- “Actual” values on the SIRZ plot were estimated with ZeCalc.


**SIRZ**

Reference Materials used for spectral-coefficient determination are in Red Boxes.
SIRZ has been automated* and tested on a different DECT scanner. SIRZ was validated and shown to have <3% accuracy error on a new DECT scanner.

Future work

- Currently estimating spectral response of a TSA-certified explosives detection system (EDS): the Leidos(Reveal) CT80-DR
  - Using HADES, MCNP and BRL-CAD to model the spectral response of the CT80-DR and simulate material rods scanned on the CT80-DR
  - Reference rods scanned on the system match HADES-simulated attenuation values to within 5% (low energy) and 15% (high energy).
  - Iterating on the current system model to bring this closer (target of <5%).
  - HADES models of MicroCT provide estimates matching to within 6%

- Next step: Run dual energy decomposition for CT80-DR datasets, to compare with prior MicroCT results.
Open questions and future work for decomposition methods

- What is the minimum set of reference materials required? (Theoretically 2)
  - We used four to six reference materials in the ranges of \(6 \leq Z_e \leq 14\) and \(0.5 \leq \rho_e \leq 1.2\) and we kept \(\mu l \leq 2\) where \(l\) is the max chord length

- How will performance degrade for materials outside the \((\rho_e, Z_e)\) range of the reference materials? At what point will it exceed 3% error?

- What is the maximum \(Z\) supported by this feature space? (Initial investigation was performed for \(Z\) up to 20, but K-edges are an issue at higher \(Z\))

- How often does the system spectral response estimation need to be recalculated? (Due to spectrum changes or model uncertainties or noise)

- How well will these methods apply to other DECT scanners?
  - Laboratory DECT systems?
  - Other commercial explosive detection systems (EDSs), e.g., CT80-DR?
  - Other energies and applications (medical, cargo, nano-CT, etc.)?
  - Horizontally-oriented X-ray sources?

No matter the method used, these issues need to be addressed.
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The Ratio Feature Space poorly discriminated specimens in early tests.

LAC Ratio is highly-dependent on system spectral response.

Note: Water BHC was performed on 80, 100, and 125 keV sinograms using a water-filled 60-ml Nalgene bottle.
The system spectral response is estimated with standard tools

- System Spectral Response includes the X-ray source, filters and detector
- SOURCE: Monte Carlo or SpekCalc spectra used with cross-section tables to compute expected transmission vs. chord length
- DETECTOR: MCNP models the detector spectrum based on vendor specs
- Spectral estimates are modified by adding filtration until a transmission match is reached across a range of reference specimens (Carbon to Silicon).
- This modeling yields an estimated system spectral response.

Filter thickness errors <5% are sufficient for good spectral response estimates.