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Hybrid Density-Constrained Dynamic Framework for Five-Material Decomposition and Quantitative Physical Properties Via Multi-Energy Spectral Analysis in Photon-Counting CT

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ABSTRACT

Purpose:
To develop a density-constrained dynamic framework for five-material decomposition (water, fat, bone, iodine, lung) using three-energy Photon-Counting CT (PCCT). This approach solves the mathematical underdetermination from three energy measurements, enabling accurate mass density (MD), effective atomic number (EAN), and stopping power ratio (SPR) estimation.

Methods:
PCCT images (40, 70, 190 keV; NAEOTOM Alpha) were analyzed using an adaptive algorithm with three stages: (1) Lung separation for voxels < −400 HU; (2) Dynamic fat basis inclusion via NNLS for voxels matching fat spectral gradients and densities (0.85–1.02 g/cm³); and (3) Iodine exclusion in high-density voxels (> 1.30 g/cm³) to prevent cortical bone misclassification. Validation utilized electron density (062M) and multi-energy phantoms with iodine inserts.

Results:
The framework successfully decomposed five materials. In the 062M phantom, soft tissue MD and SPR errors were ≤ 2.11% and ≤ 2.75%, respectively. Density constraints effectively suppressed false iodine in cortical bone (Bone 800 MD/SPR errors < 0.5%). Lung (Inhale) MD was underestimated by 5.38%. Iodine quantification demonstrated excellent linearity ($R^2 \approx 1.0$) down to 0.2 mg/mL.

Conclusion:
This density-constrained dynamic framework enables robust five-material decomposition from PCCT data, yielding accurate physical parameters for proton/heavy-ion therapy planning and quantitative imaging.

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INTRODUCTION

Photon-Counting CT (PCCT) holds great potential for advanced quantitative imaging and radiotherapy planning. However, decomposing five distinct materials from only three energy measurements poses a mathematically underdetermined inverse problem. Separating spectrally similar materials such as cortical bone and iodine remains a critical challenge, often leading to severe crosstalk and limiting the accuracy of physical parametric maps.

This study aims to develop and validate a novel physics-constrained adaptive optimization framework for solving the mathematically underdetermined five-material decomposition problem (water, fat, bone, iodine, and lung) using three-energy PCCT.

METHODS AND MATERIALS

Three-energy PCCT images (40, 70, and 190 keV) were acquired using the NAEOTOM Alpha (Siemens Healthineers). The proposed framework addresses the underdetermined five-material decomposition problem by combining density-constrained material selection, adaptive basis selection, and physics-constrained material decomposition (**Fig. 1**). Low-density voxels were first classified as lung, while soft-tissue voxels underwent voxel-wise adaptive selection between three- and four-material basis models according to spectral characteristics and estimated density.

The decomposed material fractions were subsequently used to derive mass density (MD), relative electron density (RED), effective atomic number (EAN), and stopping power ratio (SPR). Validation was performed using the CIRS 062M Electron Density Phantom and the Sun Nuclear Multi-Energy Phantom containing iodine inserts (0.2–20 mg/mL).

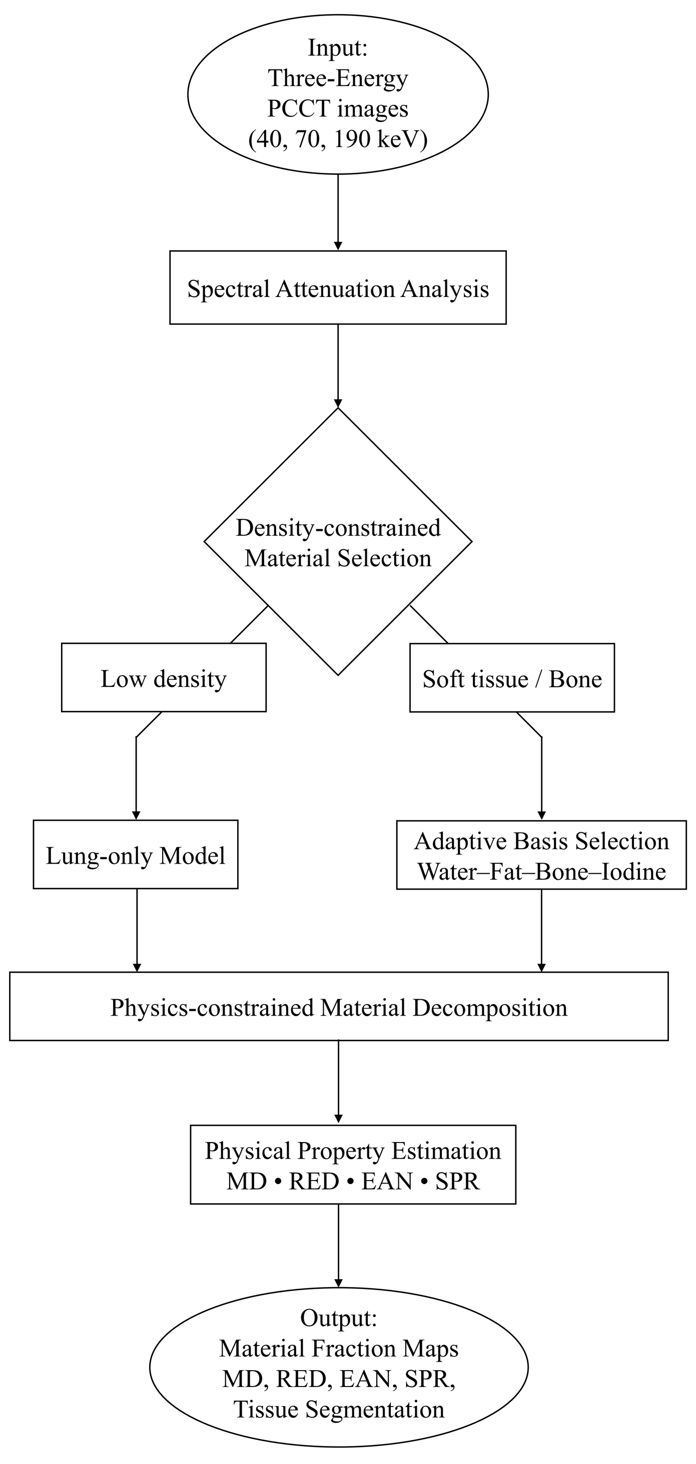

Figure 1. Conceptual workflow of the proposed density-constrained adaptive material decomposition framework for three-energy PCCT.

RESULTS

The proposed physics-constrained optimization framework successfully resolved the underdetermined five-material decomposition problem while generating physically consistent material fractions and quantitative parametric maps.

Soft Tissue Accuracy: In the 062M phantom, soft tissues (Adipose, Muscle, Liver, Breast 50/50) showed MD errors ranging from -0.69% to -2.11% and SPR errors from -0.55% to -2.75% relative to theoretical values (**Figs. 2, 3, and 4**).

Bone/Iodine Separation: The bone-preserving regularization effectively suppressed false iodine decomposition in high-density cortical bone (Bone 800; MD: +0.24%, SPR: +0.47%) (**Figs. 2, 3, and 4**).

Low-Density Regions: The dedicated lung classification stabilized decomposition in low-density regions, although Lung (Inhale) still exhibited an MD underestimation of -5.38% (**Figs. 2 and 4**).

Iodine Linearity: Iodine quantification demonstrated excellent linearity ($R^2 \approx 1.0$) down to 0.2 mg/mL, preserving mass conservation and spectral consistency (**Figs. 3 and 4**).

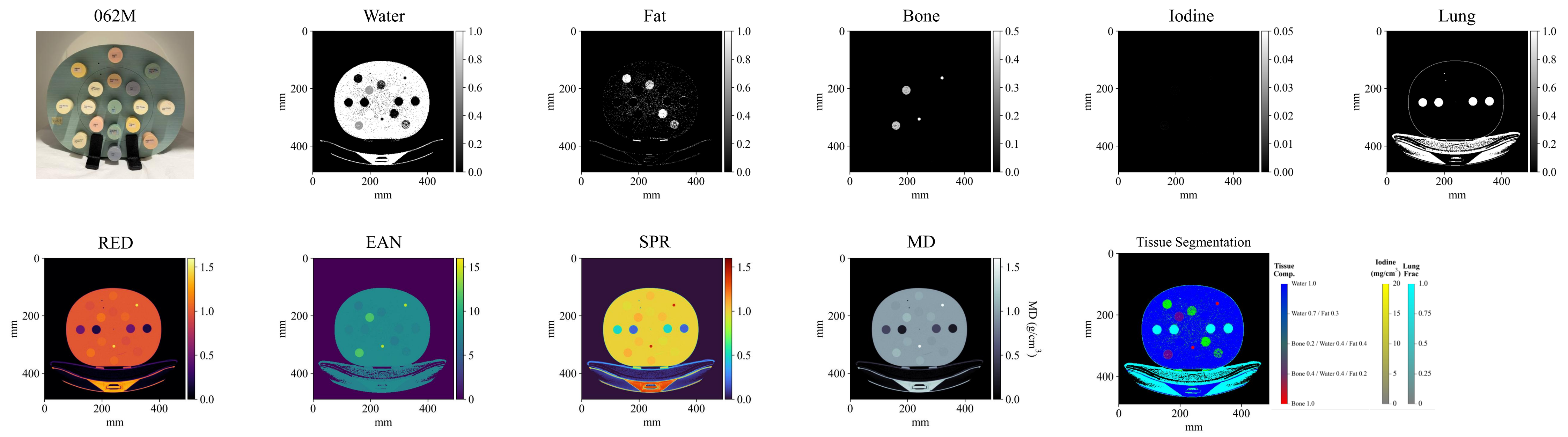

Figure 2. Generated Parametric Maps: four materials, physical properties and tissue segmentation for a multi-energy phantom (062M).

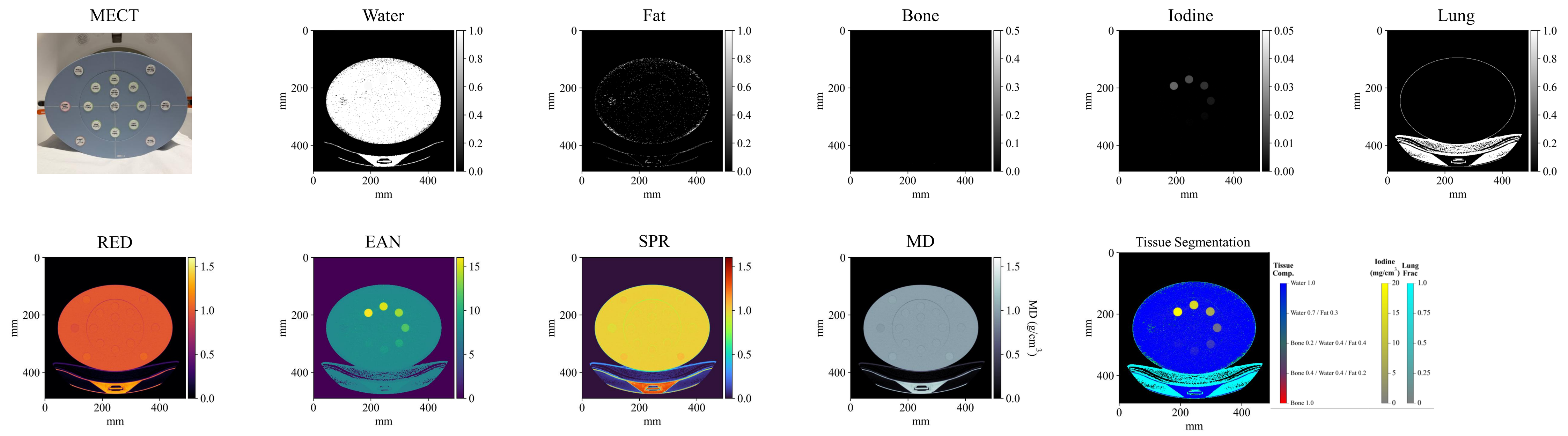

Figure 3. Generated Parametric Maps: four materials, physical properties and tissue segmentation for an electron density phantom (MECT).

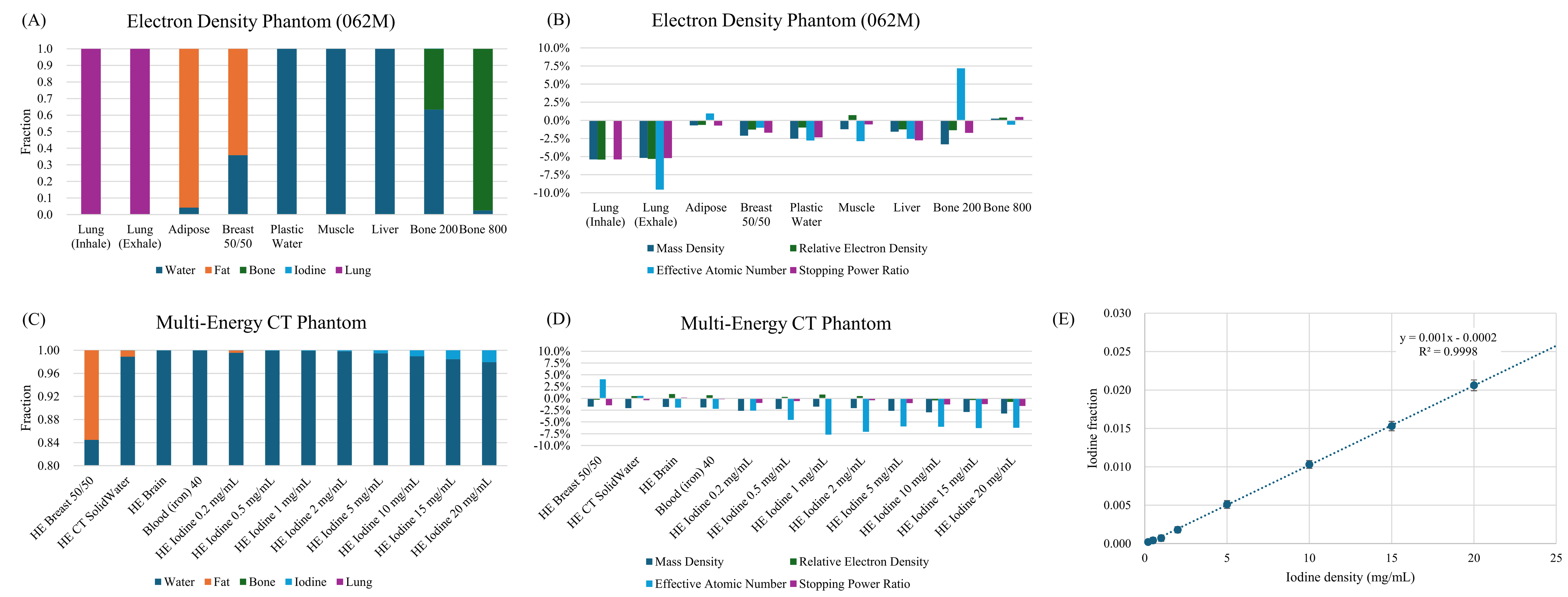

Figure 4. Quantitative Accuracy Analysis: decomposed material fractions and physical properties for 062M (A and B) and MECT (C and D); Iodine linearity (E).

CONCLUSIONS

The proposed framework demonstrates that hierarchical physical constraints and adaptive optimization can transform a mathematically underdetermined five-material decomposition problem into a stable inverse problem, enabling accurate estimation of MD, RED, EAN, and SPR from only three spectral measurements. This framework provides a practical quantitative imaging platform for proton and heavy-ion therapy planning as well as advanced spectral CT applications.