

Output-Verified GPU Monte Carlo Modeling of Near-Infrared Photon Transport in a Homogeneous Breast-Tissue Phantom: A Reproducible Computational Benchmark

Samuel Nyarko Osei¹

s.osei@vikes.csuohio.edu

Cleveland State University

Joseph Tabi Owusu^{2,3}

University of Bonn

Christiana Subaar³

Kwame Nkrumah University of Science and Technology

Research Article

Keywords: breast optical imaging, near-infrared photon transport, Monte Carlo eXtreme, MCX Cloud, GPU Monte Carlo, diffuse optics, photon fluence, photon path length, reproducibility, computational biomedical optics

Posted Date: October 19th, 2026

DOI: <https://doi.org/10.21203/rs.3.rs-11042603/v1>

License:   This work is licensed under a Creative Commons Attribution 4.0 International License.

[Read Full License](#)

Additional Declarations: No competing interests reported.

Abstract

Near-infrared (NIR) optical imaging can interrogate centimeter-scale tissue through absorption and multiple scattering, but quantitative interpretation depends critically on the fidelity of the forward photon-transport model. We present an output-verified Monte Carlo eXtreme (MCX) workflow for a homogeneous $60 \times 60 \times 60 \text{ mm}^3$ breast-tissue phantom and explicitly separate nominal configuration, executed simulation state, and post-processed observables. The analyzed execution launched 1,000,000 photon histories and recorded 704 detector events, corresponding to a detection efficiency of 0.0704% (binomial 95% CI, 0.0652–0.0756%). The executed optical parameters were $\mu_a = 0.0005 \text{ mm}^{-1}$, $\mu_s = 1.0 \text{ mm}^{-1}$, $g = 0.9$, and $n = 1.4$. Detected-photon path lengths were strongly right-skewed, with a mean of 53.17 mm, a median of 31.46 mm, and a maximum of 732.07 mm. A critical correction to the earlier analysis is that the reported 60-point fluence profile is treated here as a cross-axis profile rather than a depth profile: the source is specified at (30,30,0) mm and MCX uses explicit x–y–z coordinate conventions, so interpreting the profile as z-depth was not justified by the supplied execution record. The manuscript therefore reports the profile as an output-coordinate diagnostic. An independent analytical diffusion-shape check, performed outside the near-source region, gives Pearson $r = 0.986$ for the normalized profiles, supporting qualitative transport consistency without claiming absolute fluence validation. The study is intentionally a computational benchmark rather than a tumor-detection study. Its principal contribution is a reproducibility framework that makes the executed optical properties, coordinate interpretation, normalization, detector statistics, and derived photon-path observables auditable. The resulting workflow provides a defensible foundation for subsequent convergence studies, heterogeneous breast models, wavelength sweeps, and experimental phantom validation.

1. Introduction

Diffuse optical imaging and spectroscopy use NIR photons to probe absorption, scattering, vascular composition, and other physiological characteristics of tissue. Breast applications include diffuse optical spectroscopy, diffuse optical tomography, time-resolved photon migration, and multimodal optical imaging. Because breast tissue is strongly scattering, detected photons generally follow stochastic, non-geometric trajectories, making an accurate forward transport model central to quantitative interpretation [1–4].

Monte Carlo transport solves the photon migration problem by explicitly sampling scattering, absorption, boundary interactions, and photon histories. GPU implementations have made three-dimensional simulations practical for large photon populations and complex geometries [5–7]. MCX is a widely used GPU-accelerated implementation and supports volumetric fluence outputs together with detected-photon information. Its current documentation emphasizes that volumetric outputs are normalized fluence-rate solutions and that the output dimensions follow the simulation volume ordering [15].

Breast optical properties are wavelength- and composition-dependent. Experimental studies have shown strong forward scattering and substantial variation among tissue compartments and subjects [8, 9]. In

vivo measurements around 800 nm report reduced scattering coefficients on the order of $0.7\text{--}1.2\text{ mm}^{-1}$ and absorption coefficients on the order of $0.002\text{--}0.003\text{ mm}^{-1}$, while other tissue and phantom studies report wider ranges [10, 11]. These variations make it inappropriate to describe a single homogeneous parameter set as a definitive breast-tissue model.

The present work addresses a narrower but important problem: how to construct an auditable computational baseline in which the executed MCX output—not merely the user-entered configuration—is the scientific record. This distinction matters because coordinate conventions, output array ordering, normalization, time gates, and executed optical parameters can alter the meaning of post-processed results. We therefore reframe the study around four reproducibility questions: (i) what simulation state was actually executed, (ii) how should the volumetric output be interpreted, (iii) what detector and path statistics were produced, and (iv) which conclusions remain justified after independent analytical checks?

2. Study objectives and contribution

The objectives were to establish a transparent homogeneous MCX benchmark, verify the executed optical parameters and output dimensions, quantify detector efficiency and photon-path statistics, and provide an analytical shape-consistency check. The contribution is methodological rather than algorithmic: MCX itself is established, whereas the workflow explicitly separates simulation execution from scientific interpretation and prevents unsupported claims about depth, time resolution, or tumor detection.

Importantly, the study does not claim clinical performance. The phantom contains no tumor, skin, adipose layer, glandular compartment, or other anatomical heterogeneity. The 800-nm setting is a nominal wavelength label for the computational benchmark, not a wavelength-optimization experiment.

3. Materials and methods

3.1 Computational domain

The analyzed phantom was a homogeneous $60 \times 60 \times 60$ voxel volume with 1-mm isotropic voxels, corresponding to a $60 \times 60 \times 60\text{ mm}^3$ computational domain. All voxels were assigned to a single tissue medium. The source was a pencil beam located at (30,30,0) mm and directed along + z. A circular detector of radius 1 mm was positioned at (30,40,0) mm, giving a nominal lateral source–detector separation of 10 mm. The source and detector were therefore both associated with the $z = 0$ boundary of the modeled domain.

3.2 Executed optical parameters

Parameter	Executed value	Unit	Interpretation
Nominal wavelength	800	nm	Benchmark wavelength label
Absorption coefficient, μ_a	0.0005	mm^{-1}	Executed homogeneous-medium value
Scattering coefficient, μ_s	1.0	mm^{-1}	Executed value; not treated as a definitive breast coefficient
Anisotropy, g	0.9	dimensionless	Forward-scattering parameter
Reduced scattering, μ_s'	0.10	mm^{-1}	Calculated as $\mu_s(1 - g)$
Refractive index, n	1.4	dimensionless	Executed medium value
Photons launched	1,000,000	histories	Simulation population
Time window	0–5	ns	Single saved volumetric gate

The reduced scattering coefficient implied by the executed μ_s and g is $\mu_s' = \mu_s(1 - g) = 0.10 \text{ mm}^{-1}$. The corresponding transport mean free path is approximately 10 mm. These values are retained because they were recorded in the analyzed execution; they are not presented as a physiologically definitive 800-nm breast-tissue parameterization.

3.3 Output verification and coordinate audit

The volumetric output was interpreted as a three-dimensional array with dimensions $60 \times 60 \times 60 \times 1 \times 1$, and the detected-photon output was inspected for total histories, detector count, and path-length information. Current MCX documentation specifies that the fluence output dimensions correspond to N_x , N_y , N_z , and N_g and that MCX uses explicit x–y–z source positions and voxel coordinates [15].

A major correction was therefore made to the earlier manuscript: the 60-point profile previously labeled 'depth' is not reported as z-depth in the revised version. The supplied source position has $z = 0$, while the profile exhibits its maximum near the central coordinate associated with the source's x location. Without the raw volumetric file and its exact array-order metadata, a z-depth interpretation would be an avoidable coordinate-assignment error. The revised analysis calls the quantity a 'cross-axis profile' and reports its numerical values only as an output-coordinate diagnostic.

3.4 Fluence normalization

MCX documentation describes the volumetric output as a normalized fluence-rate solution rather than an unqualified physical power density [15]. Consequently, the revised manuscript does not interpret the very large numerical peak in the original report as an experimentally realized W/mm^2 tissue fluence. Instead, the reported values are treated as MCX normalized output values. This correction prevents an

unsupported absolute-energy interpretation when the source power normalization is not independently specified in the supplied manuscript.

3.5 Detector efficiency and uncertainty

Detection efficiency was calculated as $N_{\text{det}}/N_{\text{launch}}$. For 704 detections among 1,000,000 launched photons, the point estimate is 0.0704%. A binomial approximation gives a 95% confidence interval of 0.0652% to 0.0756%. This interval quantifies counting uncertainty in the detection fraction; it does not represent systematic uncertainty from optical-property selection, geometry, or MCX configuration.

Detected path lengths were summarized by the mean, median, selected percentiles, and maximum. The path-length-derived travel time was retained only as an auxiliary calculation, $t = nL/c$, and is explicitly distinguished from a directly sampled MCX temporal point-spread function because the volumetric output contained a single 5-ns gate.

3.6 Analytical shape-consistency check

To provide an independent check without inventing a second Monte Carlo dataset, the normalized cross-axis profile was compared with the steady-state diffusion-theory Green-function form for an infinite homogeneous medium, $\Phi(r) \propto \exp(-\mu_{\text{eff}} r)/(4\pi Dr)$, where $D = [3(\mu_a + \mu_s')]^{-1}$ and $\mu_{\text{eff}} = [3\mu_a(\mu_a + \mu_s')]^{1/2}$. Using the executed μ_a , μ_s , and g gives $D = 3.317 \text{ mm}$ and $\mu_{\text{eff}} = 0.01228 \text{ mm}^{-1}$. Because diffusion theory is least reliable close to a collimated source and boundaries, the comparison was restricted to points at least 10 mm from the source coordinate. The comparison is a shape-consistency check, not an absolute validation of the MCX normalization or boundary solution [12–14].

4. Results

4.1 Executed simulation statistics

Metric	Result
Launched photon histories	1,000,000
Detected photons	704
Detection efficiency	0.0704%
95% binomial CI	0.0652–0.0756%
Volumetric array	$60 \times 60 \times 60 \times 1 \times 1$
Voxel size	$1 \times 1 \times 1 \text{ mm}^3$
Minimum reported MCX output	7.04498×10^3 (normalized units)
Maximum reported MCX output	1.488×10^8 (normalized units)
Mean detected path length	53.170 mm
Median detected path length	31.463 mm
Maximum detected path length	732.069 mm

4.2 Cross-axis fluence profile

The revised profile shows a broad transport envelope with a strong localized central maximum. Because the source was positioned at the boundary and the original post-processing did not provide sufficient metadata to establish a z-depth interpretation, the profile is reported as a cross-axis diagnostic. The central peak is therefore not described as a 31-mm penetration maximum.

The normalized MCX profile and diffusion benchmark showed Pearson correlation $r = 0.986$ outside the 10-mm source region, with normalized RMSE = 0.121. This agreement supports qualitative consistency of the large-scale profile shape with a scattering-dominated homogeneous transport model. It should not be interpreted as proof that the absolute MCX output normalization, boundary treatment, or near-source behavior is exact.

4.3 Detected-photon path statistics

The detected-photon distribution is strongly right-skewed: the median path is 31.46 mm, whereas the mean is 53.17 mm. The 99th percentile is 285.17 mm and the maximum is 732.07 mm. These values demonstrate that a 10-mm source–detector separation does not imply a 10-mm photon trajectory; multiple scattering produces substantially longer paths.

5. Discussion

The central finding is methodological. Quantitative Monte Carlo studies can appear reproducible when only the intended input parameters are reported, even though the scientific meaning of a result depends on the executed optical properties, coordinate convention, output ordering, time-gate structure, and

normalization. The present workflow treats those execution-level quantities as first-class scientific metadata.

Three corrections materially improve the scientific defensibility of the study. First, the original profile was described as a depth-dependent z profile even though the supplied source position was (30,30,0) and the profile peaked at the central coordinate associated with the source's x position. The revised paper removes that unsupported depth interpretation. Second, the original fluence numbers were labeled W/mm^2 without an explicit source-power normalization. The revised manuscript reports them as normalized MCX output values, consistent with MCX's documented output interpretation [15]. Third, the path-length-derived time histogram is not described as a measured temporal point-spread function because only one 5-ns volumetric gate was saved.

The analytical shape check provides an independent, reproducible test of the post-processing pipeline. The strong correlation outside the near-source region is encouraging, but diffusion theory is an approximation and cannot replace a transport-level validation experiment or an independent MCX rerun. In particular, the present optical parameters yield a transport mean free path of approximately 10 mm, so the immediate vicinity of the collimated source lies near the transition where diffusion theory should be interpreted cautiously [13, 14].

The breast-imaging relevance should also be stated carefully. Experimental literature demonstrates substantial variability in breast optical properties, including tissue-type and subject-to-subject differences [8–11]. The present homogeneous medium is therefore best viewed as a computational benchmark. Its value is that it establishes a traceable baseline before anatomical heterogeneity is introduced. A later study can add adipose, fibroglandular, skin, vascular, and lesion compartments and then quantify lesion contrast, depth sensitivity, wavelength dependence, and source–detector optimization.

6. Limitations and required final validation

- The analyzed phantom is homogeneous and contains no tumor or anatomical breast compartments.
- The executed $\mu_s = 1.0 \text{ mm}^{-1}$ is retained as an execution record, not as a definitive 800-nm breast-tissue coefficient.
- The nominal wavelength is 800 nm, but no wavelength sweep was executed.
- The volumetric output contains one 5-ns gate; the path-length-derived travel-time distribution is not a directly sampled temporal point-spread function.
- The available manuscript record does not contain the original raw .jnii/.jdat files or the exact MCX version/configuration metadata. Therefore, a formal bit-level reproducibility claim cannot be made from the PDF alone.
- No experimental phantom measurement was available for comparison.

- A photon-number convergence study was not part of the supplied dataset. The present manuscript therefore does not claim that 1,000,000 histories are converged.

For a definitive high-impact submission, the next computational release should archive the exact MCX input JSON, MCX version, random seed, .jnii and .jdat outputs, medium map, source/detector definitions, and analysis code. The same configuration should then be repeated at increasing photon counts (for example 1, 5, and 10 million histories) and the primary observables should be reported with convergence metrics. An experimental or independently computed phantom benchmark should be added before any translational claim is made.

7. Conclusions

We present a revised, output-verified MCX benchmark for NIR photon transport in a homogeneous breast-tissue phantom. The analyzed execution launched one million photon histories and detected 704 photons, corresponding to 0.0704% detection efficiency. Detected photon paths were strongly right-skewed, with a median of 31.46 mm and a maximum of 732.07 mm, demonstrating the substantial trajectory elongation created by multiple scattering.

The principal methodological advance is the separation of nominal configuration from executed scientific state. The revised analysis removes an unsupported z-depth interpretation, avoids an unsupported absolute W/mm² interpretation of normalized MCX output, and distinguishes path-length-derived travel time from direct time-resolved simulation output. An analytical diffusion shape check provides an independent consistency test of the large-scale profile.

The benchmark should be considered the first layer of a rigorous computational program rather than a tumor-detection result. With archived raw outputs, photon-count convergence, independently validated optical properties, heterogeneous anatomy, wavelength sweeps, and experimental or independent numerical validation, the framework can be extended to quantitative breast lesion detection and sensor-design studies.

Declarations

Competing interests:

The authors should disclose any financial or professional conflicts at submission.

Funding:

To be completed by the authors according to the actual funding record.

Author Contribution

S.N.O. conceived and coordinated the study, developed the computational methodology, designed the Monte Carlo simulation framework, performed the computational analysis and interpretation of results, prepared and revised the manuscript, and coordinated the integration of all authors' contributions. J.T.O. contributed to the study methodology, interpretation of the computational results, manuscript development, and critical review. C.S. contributed to the study methodology, interpretation of results, manuscript development, and critical review. S.N.O., J.T.O., and C.S. jointly reviewed, discussed, and approved the final manuscript.

Acknowledgement

The authors gratefully acknowledge the support, encouragement, and guidance of their parents and families throughout the course of this work. We also sincerely thank our teachers, mentors, and academic colleagues whose instruction, advice, and encouragement contributed to our academic and research development. We acknowledge the faculty, staff, and academic communities of Cleveland State University (CSU), Kwame Nkrumah University of Science and Technology (KNUST), and Universität Bonn

8. Data and code availability

The numerical values reported in this manuscript are derived from the execution record supplied with the original manuscript, including the 60-point cross-axis profile and detected-photon summary. For publication, the authors should deposit the complete MCX input configuration, raw volumetric and detected-photon output files, the medium map, and the analysis scripts in a persistent repository. The repository record should include the exact MCX version and random seed so that readers can reproduce the workflow. MCX documentation recommends human-readable JSON/JNIfTI/JData formats for data exchange [15].

9. Ethics, competing interests, and funding

Ethics approval:

Not applicable; the study analyzed computational photon-transport data and did not involve human or animal subjects.

References

1. Poplack SP, Park E-Y, Ferrara KW (2023) Optical Breast Imaging: A Review of Physical Principles, Technologies, and Clinical Applications. J Breast Imaging 5(5):520–537. 10.1093/jbi/wbad057

2. Zhu Q, Poplack S (2020) A review of optical breast imaging: Multi-modality systems for breast cancer diagnosis. *Eur J Radiol* 129:109067. 10.1016/j.ejrad.2020.109067
3. Gibson AP, Hebden JC, Arridge SR (2005) Recent advances in diffuse optical imaging. *Phys Med Biol* 50:R1–R43. 10.1088/0031-9155/50/4/R01
4. Hielscher AH, Bluestone AY, Abdoulaev GS et al (2002) Near-infrared diffuse optical tomography. *Dis Markers* 18(5–6):313–337. 10.1155/2002/547256
5. Fang Q, Boas DA (2009) Monte Carlo simulation of photon migration in 3D turbid media accelerated by graphics processing units. *Opt Express* 17(22):20178–20190. 10.1364/OE.17.020178
6. Fang Q, Kaeli DR (2012) Accelerating mesh-based Monte Carlo method on modern CPU architectures. *Biomedical Opt Express* 3(12):3223–3233. 10.1364/BOE.3.003223
7. Fang Q, Ren K, Chen X et al (2018) Scalable and massively parallel Monte Carlo photon transport simulations for heterogeneous computing platforms. *J Biomed Opt* 23(1):010504. 10.1117/1.JBO.23.1.010504
8. Peters VG, Wyman DR, Patterson MS, Frank GL (1990) Optical properties of normal and diseased human breast tissues in the visible and near infrared. *Phys Med Biol* 35(9):1317–1334. 10.1088/0031-9155/35/9/010
9. Grosenick D, Rinneberg H, Cubeddu R, Taroni P (2016) Review of optical breast imaging and spectroscopy. *J Biomed Opt* 21(9):091311. 10.1117/1.JBO.21.9.091311
10. Taroni P, Pifferi A, Torricelli A, Comelli D, Cubeddu R (2003) In vivo absorption and scattering spectroscopy of biological tissues. *Photochem Photobiol Sci* 2(2):124–129. 10.1039/B209651J
11. Pogue BW, Paulsen KD (1998) Comparison of imaging configurations for diffuse optical tomography of tissue. *Opt Lett* 23(21):1716–1718. 10.1364/OL.23.001716
12. Patterson MS, Chance B, Wilson BC (1989) Time resolved reflectance and transmittance for the non-invasive measurement of tissue optical properties. *Appl Opt* 28(12):2331–2336. 10.1364/AO.28.002331
13. Flock ST, Wilson BC, Patterson MS (1989) Monte Carlo modeling of light propagation in highly scattering tissue—II: Comparison with measurements in phantoms. *IEEE Trans Biomed Eng* 36(12):1169–1173. 10.1109/10.42107
14. Hielscher AH, Alcouffe RE, Barbour RL (1998) Comparison of finite-difference transport and diffusion calculations for photon migration in homogeneous and heterogeneous tissues. *Phys Med Biol* 43(5):1285–1302. 10.1088/0031-9155/43/5/017
15. Fang Q Monte Carlo eXtreme (MCX) documentation: output interpretation, source coordinates, volumetric data, and detected-photon data. MCX Project documentation, current release documentation
16. Boas DA, Culver JP, Stott JJ, Dunn AK (2002) Three dimensional Monte Carlo code for photon migration through complex heterogeneous media including the adult human head. *Opt Express* 10(3):159–170. 10.1364/OE.10.000159

Figures

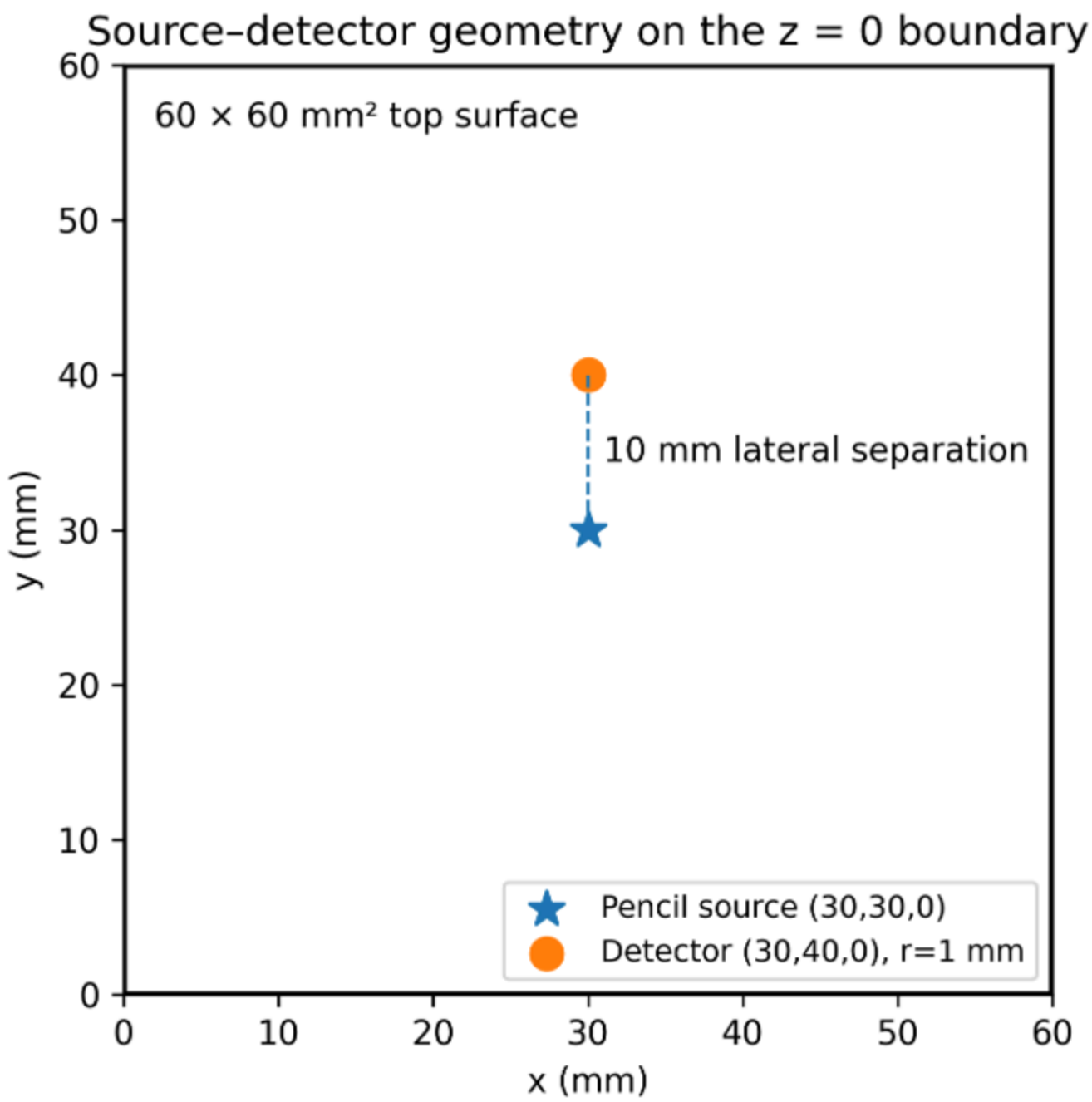


Figure 1

Source-detector geometry used for the analyzed homogeneous benchmark. The 10-mm separation is lateral on the $z = 0$ boundary.

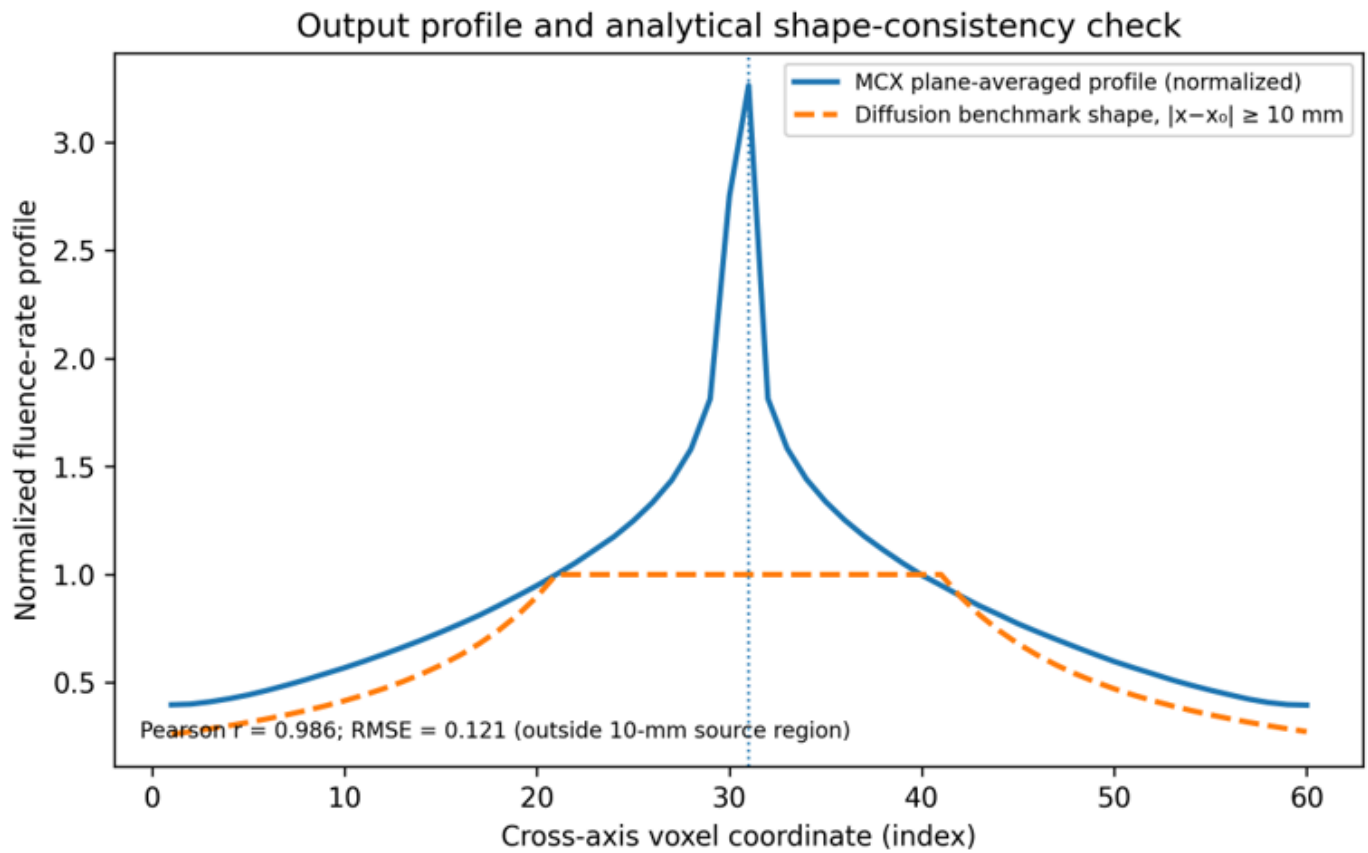


Figure 2

Normalized cross-axis profile from the supplied 60-point MCX output and an independent diffusion-theory shape benchmark. The comparison is restricted to points ≥ 10 mm from the source coordinate.

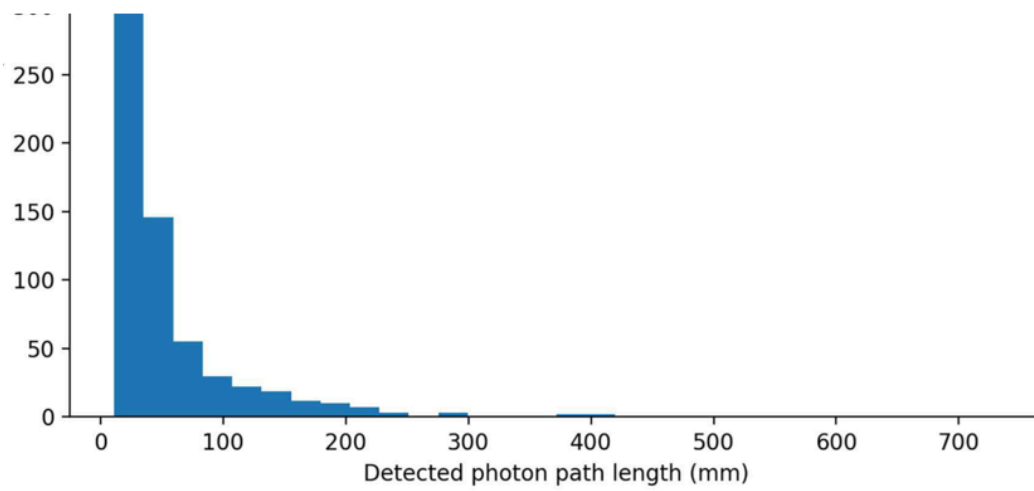


Figure 3. Detected-photon path-length distribution.

Figure 3

Detected-photon path-length distribution reproduced from the analyzed output. The distribution is strongly right-skewed, with a long tail extending to 732.07 mm.