A Transport-Regularized Physics-Informed Neural Network for Neutron Fluence and Boron Dose Prediction in BNCT

Ke Yang, MS[1,2] ; Fang-Fang Yin, PhD[1,2]
[1] Medical Physics Graduate Program, Duke Kunshan University, Kunshan, China
[2] Jiangsu Provincial University Key (Construction) Laboratory for Smart Diagnosis and Treatment of Lung Cancer, Kunshan, China

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ABSTRACT

Purpose:
Accurate neutron fluence and boron dose prediction is essential for boron neutron capture therapy (BNCT), but Monte Carlo (MC)-based dose calculation is computationally expensive. This study developed a transport-regularized physics-informed neural network (TR-PINN) surrogate model for beam-radius-conditioned neutron fluence and target ^{10}B dose prediction.

Methods:
PHITS simulations were performed in a simplified soft-tissue-equivalent BNCT phantom to generate time-integrated neutron fluence distributions, target ^{10}B dose, and effective absorption-coefficient data. Beam radius was used as the conditioning parameter. The proposed TR-PINN learned a continuous mapping from spatial coordinates and beam radius to MC-derived neutron fluence. A diffusion-type residual with learnable effective transport parameters was incorporated to regularize the predicted fluence field, and an MC-derived effective absorption coefficient was used to constrain parameter learning. Model performance was evaluated across training, interpolation, and extrapolation beam-radius cases and compared with a purely data-driven MLP baseline.

Results:
TR-PINN reproduced the main PHITS-derived target ^{10}B dose patterns and achieved lower target-dose errors than the Pure MLP baseline across all evaluated beam radii. The all-case target-region mean relative error decreased from 0.0409 for the baseline to 0.0288 for TR-PINN. TR-PINN also reduced the mean normalized PDE residual from 0.7477 to 0.3481, indicating improved physical consistency of the predicted fluence field.

Conclusion:
The results demonstrate the feasibility of TR-PINN as a fast, physically constrained surrogate model for BNCT neutron fluence and target ^{10}B dose prediction. Future work will extend the framework to patient-specific 3D geometries and energy-dependent transport-informed constraints.

CONTACT

Ke Yang
Duke Kunshan University
No. 8 Duke Avenue, Kunshan, Jiangsu, China 215316
ke.yang@dukekunshan.edu.cn
+86 13629604879

INTRODUCTION

Boron neutron capture therapy (BNCT) requires accurate neutron fluence and boron dose prediction because dose formation depends on neutron transport, nuclear reactions, boron concentration, and tissue composition. Monte Carlo (MC) simulation remains the standard approach for BNCT dose calculation due to its high physical accuracy, but the large number of particle histories required for statistical reliability leads to high computational cost and limits rapid beam-parameter evaluation.

Deep-learning surrogate models have been explored to accelerate BNCT dose prediction, but most existing approaches are primarily data-driven and do not explicitly incorporate transport-related physical behavior into model training. To address this limitation, this study develops a transport-regularized physics-informed neural network (TR-PINN) surrogate model for beam-radius-conditioned neutron fluence and derived ^{10}B dose prediction in a simplified BNCT phantom.

The proposed model learns a continuous mapping from spatial coordinates and beam radius to MC-derived time-integrated neutron fluence distributions. A diffusion-type residual with learnable effective transport parameters is incorporated to improve physical consistency, and an MC-derived effective absorption coefficient is used to constrain the learned absorption parameter. The objective of this study is to evaluate the feasibility of TR-PINN as a fast, physically constrained surrogate framework for BNCT neutron fluence and target boron dose estimation.

METHODS AND MATERIALS

PHITS 3.34 Monte Carlo simulations were used to generate reference neutron fluence distributions, target-region ^{10}B dose, and effective absorption-coefficient data in a simplified soft-tissue-equivalent BNCT phantom. The phantom was modeled as a $20\times20\times28$ cm³ rectangular volume with a spherical target of 2 cm radius located at (0,0,−8) cm.

A monoenergetic 20 keV cylindrical neutron beam was incident along the +z direction, and beam radius was used as the conditioning parameter. Seven beam radii were used for training, with additional interpolation and extrapolation cases for evaluation.

The proposed TR-PINN learns a continuous mapping from normalized spatial coordinates and beam radius to MC-derived time-integrated neutron fluence. The framework consists of three components: Data-Net for fluence prediction, Source-Net for effective source-term learning, and Parameter-Net for estimating beam-radius-dependent effective transport parameters $D(r0)$ and $\Sigma a(r0)$. Stage A pretrained Data-Net using supervised MC fluence data. Stage B introduced Source-Net to learn an effective source distribution under a diffusion-type residual. Stage C jointly optimized Data-Net and Parameter-Net using data-fitting loss, normalized PDE residual loss, and an MC-derived absorption-coefficient constraint.

The trained model outputs neutron fluence distributions for unseen beam-radius conditions. Target ^{10}B dose was then calculated from the predicted fluence using the effective boron absorption coefficient. Model performance was evaluated against PHITS using fluence relative error, target-region dose error, and normalized PDE residual, with comparison to a purely data-driven MLP baseline.

RESULTS

As shown in Figure 1, TR-PINN reproduced the PHITS-derived centerline target ^{10}B dose profile with good agreement for the representative beam-radius case (r0=4.00 cm). Both TR-PINN and the Pure MLP baseline captured the main depth-dependent dose trend, including the dose increase near the beam-entrance side and the gradual decrease along the target depth. However, TR-PINN showed lower local relative errors across most target-region positions, indicating improved local target-dose prediction compared with the purely data-driven baseline.

As summarized in Figure 2, TR-PINN achieved lower target ^{10}B dose mean relative errors than the Pure MLP baseline across all evaluated beam radii. This improvement was observed in training, interpolation, and extrapolation cases, suggesting that the transport-regularized formulation improved target-region prediction stability beyond simple data fitting. The lowest errors were generally observed within or near the training beam-radius range, while higher errors appeared at the smallest and largest extrapolation radii. This indicates that beam-radius extrapolation remained more challenging than interpolation, but TR-PINN still maintained consistently lower target-dose errors than the Pure MLP baseline.

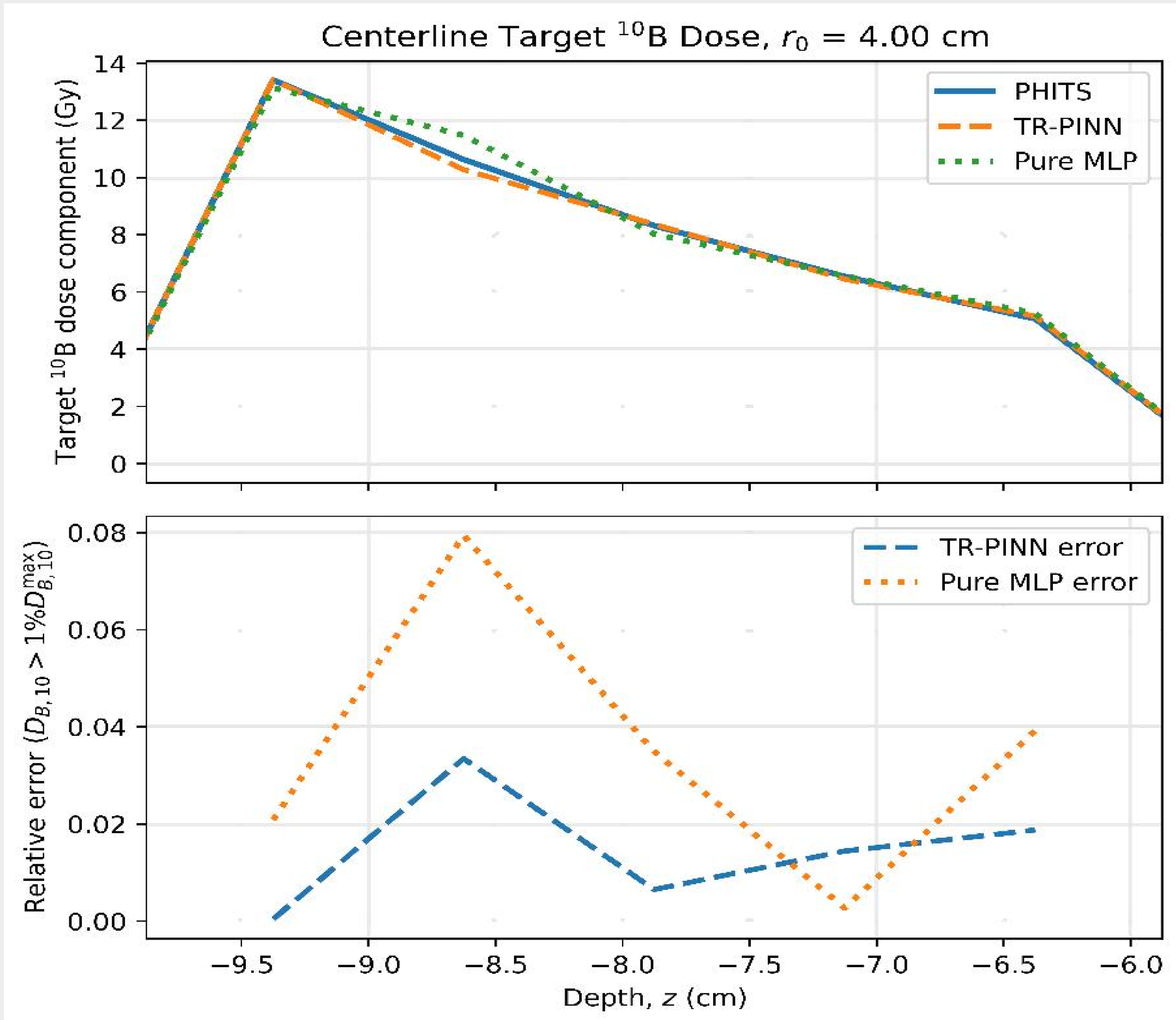

Figure 1. Centerline target ^{10}B dose comparison for r_0= 4 cm. TR-PINN and Pure MLP predictions were compared with PHITS reference results. The lower panel shows relative errors within the target-dose region.

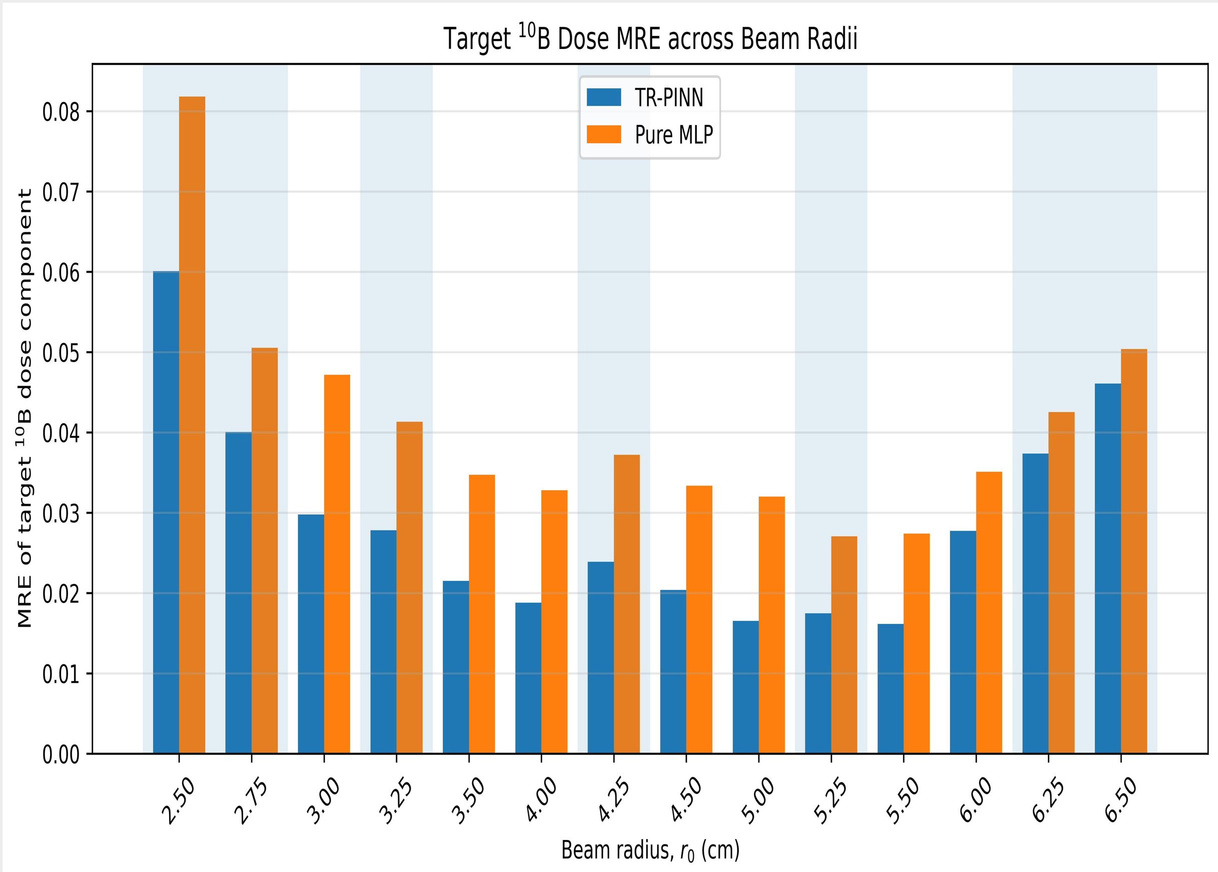

Figure 2. Target ^{10}B dose error across beam radii. Blue bars represent TR-PINN and orange bars represent the Pure MLP baseline. Shaded regions indicate interpolation and extrapolation test cases.

DISCUSSION

The present results demonstrate the feasibility of using a transport-regularized PINN surrogate model for BNCT neutron fluence and target ^{10}B dose prediction. Compared with the purely data-driven MLP baseline, TR-PINN provided more stable target-region dose prediction across training, interpolation, and extrapolation beam-radius cases. This suggests that incorporating a diffusion-type residual can improve prediction consistency beyond simple data fitting, particularly in the region most relevant to BNCT dose evaluation.

The improvement was more evident in the target region than in the global fluence field. This is reasonable because the physics-based residual was used as an effective regularization term rather than a full deterministic transport solver. It helped constrain the learned fluence field toward a smoother and more physically consistent solution, while local deviations could still occur near peak-dose regions or under beam-radius extrapolation. This study was performed in a simplified soft-tissue-equivalent phantom with beam radius as the only conditioning parameter. The effective one-group diffusion residual and case-wise absorption coefficient were used to provide a computationally efficient feasibility framework, but they do not fully describe energy- and angle-dependent neutron transport. Future work will extend the framework to three-dimensional and patient-specific geometries, incorporate additional beam and biological parameters, and investigate multigroup or energy-dependent transport-informed constraints. Despite these limitations, TR-PINN shows promising potential as a fast, physically constrained surrogate model for BNCT dose-related prediction tasks.

CONCLUSIONS

This study demonstrates the feasibility of a transport-regularized PINN surrogate model for BNCT neutron fluence and target ^{10}B dose prediction. By incorporating a diffusion-type residual and learnable effective transport parameters, TR-PINN improved target-region prediction stability compared with a purely data-driven MLP baseline. The model achieved consistently lower target-dose errors across training, interpolation, and extrapolation beam-radius cases, suggesting that physics-based regularization can enhance surrogate dose prediction under limited training data. Future work will extend the framework to patient-specific 3D geometries and more detailed energy-dependent transport constraints.

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