Gaussian Process Regression with Component Splitting for MCNP-Based Neutron Flux Reconstruction in OPR-1000 Baffle

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1. Introduction

Activation evaluation of reactor internal structures provides essential information for decommissioning planning, radioactive waste classification, disposal strategy development, and worker dose management [1,2]. Because the activation level of reactor structures is governed by the local neutron flux, energy spectrum, and irradiation history, reliable evaluation of the spatial neutron flux distribution over the entire structure is important for estimating activation inventories, source terms, and dose-related quantities. However, collecting a sufficient number of samples and performing activation analysis over the whole structure are limited by cost, time, manpower, and accessibility. Therefore, a calculation-based irradiation flux evaluation method is required to complement limited measurement data and in-core or ex-core monitoring data, and to estimate activation levels at locations where direct sampling is difficult.

For this purpose, MCNP, a Monte Carlo neutron transport code, can be used to estimate the irradiation neutron flux at baffle locations in an OPR-1000 reactor [2]. MCNP can provide particle flux tallies for user-defined cells, surfaces, detector points, or mesh bins, while accounting for complex material effects around reactor structures. However, MCNP tallies provide discrete or mesh-cell-averaged flux estimates for user-defined tally regions, rather than a continuous three-dimensional flux field over the structure [3]. In particular, an FMESH tally provides mesh-cell-averaged flux values, and its output includes the bin center coordinates, tally results, and associated relative errors.

Therefore, the continuous three-dimensional flux field reconstructed in this study is not intended to replace MCNP tally results, but to provide a post-processing representation of the discrete MCNP estimates for activation evaluation. This representation can support flux estimation at arbitrary structural locations, on meshes different from the original MCNP tally mesh, and over irregular geometries of reactor internal structures [3,4]. In this study, MCNP neutron flux tally results for an OPR-1000 baffle were used to evaluate whether a component-splitting Gaussian Process Regression (GPR) method can reconstruct a continuous 3D neutron flux trend from discrete tally results. In particular, this study examined whether the baffle flux field can be represented as a combination of transverse and axial components, and evaluated how accurately this splitting representation reconstructs the MCNP flux trend.

2. Methods

2.1 MCNP Baffle Flux Dataset

The target structure in this study is the OPR-1000 baffle, and neutron flux tally results obtained from MCNP calculations were used. The baffle dataset consists of spatial coordinates and the corresponding neutron flux values. Each data point represents a spatial location inside or near the surface of the baffle, and the corresponding MCNP flux estimate was used for GPR training or validation depending on the dataset. MCNP provides the CTME option to specify the maximum computer time, in minutes, allocated to a Monte Carlo calculation [5]. In this study, CTME was used as a representative measure of computational cost when generating MCNP tally datasets. The MCNP calculations were performed on an Intel(R) Core(TM) Ultra 7 270K Plus processor using 20 cores. Therefore, the comparison between CTME=2,400 and CTME=130,000 should be interpreted under this computing configuration. The GPR model was trained using tally data generated with CTME = 2,400, whereas the validation dataset was generated with CTME = 130,000 and was used as the higher-cost MCNP reference.

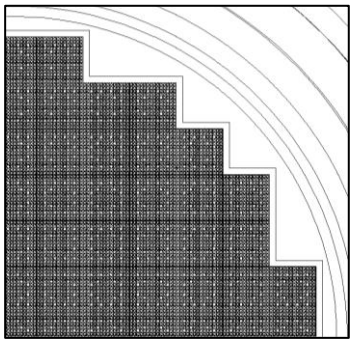


Fig. 1. OPR-1000 baffle geometry modeled in MCNP

2.2 Component-Splitting Flux Representation

The baffle flux field can be expressed as a function of three-dimensional spatial coordinates. In this study, the 3D neutron flux field in the baffle was assumed to be

approximated by a combination of transverse and axial flux components, based on the expectation that the dominant spatial variation can be separated into the cross-sectional flux distribution and the axial flux shape of the reactor internal structure. The transverse component represents flux variation in the radial and azimuthal directions, whereas the axial component represents flux variation along the height direction. This splitting representation separates the major flux variations according to the geometric directions of the structure, rather than directly learning the entire 3D flux field over all spatial locations.

$$\Phi(r,\theta,z) \approx AF(r,\theta)G(z) \quad (1)$$

where F(r,θ) and G(z) represent the transverse and axial flux components, respectively, and A is a scale factor. If the separability is sufficiently high, the major flux trend can be efficiently reconstructed without calculating or measuring the full 3D flux field at every location. In this study, separability was evaluated by comparing the original MCNP flux field with the component-splitting approximation represented by AF(r,θ)G(z). The agreement was quantified using R^2 for both the entire baffle and the individual geometric regions defined by the baffle shape.

2.3 Gaussian Process Regression Model

GPR was used as a surrogate model to learn a spatially continuous flux trend from MCNP tally results [6,7,8]. Because MCNP tally data provide flux estimates only at discrete locations, GPR uses these data points to predict the flux at unobserved locations and to provide the corresponding prediction uncertainty.

GPR training was performed separately for the transverse and axial components. The transverse and axial GPR models used a Matérn 5/2 kernel with a constant scaling factor. The hyperparameters were selected separately for each component model by maximizing the log marginal likelihood over predefined candidate grids. The transverse model used (r,θ), or the corresponding normalized spatial coordinates, as input variables, whereas the axial model used the z-coordinate as its input variable. Considering the large spatial variation of the flux, the output variable can be defined as a log-transformed or normalized flux shape. The 3D flux prediction is then obtained by combining the GPR predictions for each component [4].

2.4 Reconstruction Procedure

The reconstruction procedure used in this study is as follows.

I. Organize the MCNP tally results for the OPR-1000 baffle.
II. Construct separate datasets for the transverse and axial flux components from the tally results.
III. Select valid data points for each component and preprocess the corresponding coordinates and flux values.
IV. Train separate GPR models for the transverse and axial components.
V. Predict the transverse and axial flux components using the trained GPR models.
VI. Combine the predicted components to reconstruct the 3D neutron flux field.
VII. Evaluate the reconstruction performance by comparing the reconstructed flux with both the comparison dataset generated under the same CTME=2,400 condition and the validation dataset generated as the higher-cost MCNP reference with CTME=130,000.

2.5 Evaluation Metrics

The model performance was evaluated by comparing the MCNP flux and the GPR predictions. The main evaluation metrics were the coefficient of determination on the flux scale, the coefficient of determination on the log scale, the median prediction-to-MCNP ratio, and the relative residual distribution.

$$R^2 = 1 - \frac{\Sigma_i\left(\Phi_i^{\mathrm{MCNP}} - \hat{\Phi}_i\right)^2}{\Sigma_i\left(\Phi_i^{\mathrm{MCNP}} - \bar{\Phi}^{\mathrm{MCNP}}\right)^2} \quad (2)$$

In addition, R^2 based on log Φ was evaluated to assess the reconstruction performance on the log flux scale. This metric is useful for evaluating relative spatial trends when the flux values have a large dynamic range.

The central tendency between the predicted values and the MCNP reference values was evaluated using the following ratio.

$$\text{median ratio} = \text{median}_i\left(\frac{\hat{\Phi}_i}{\Phi_i^{\mathrm{MCNP}}}\right) \quad (3)$$

The relative residual was defined as follows.

$$\text{relative residual}_i = \left|\frac{\hat{\Phi}_i - \Phi_i^{\mathrm{MCNP}}}{\Phi_i^{\mathrm{MCNP}}}\right| \quad (4)$$

Using these metrics, this study evaluated whether the component-splitting GPR method can appropriately reconstruct both the absolute magnitude and the log-scale spatial trend of the baffle MCNP flux field. The resulting R^2 values on the flux and log-flux scales, median prediction-to-MCNP ratio, and relative residuals were summarized separately for the comparison and validation datasets.

3. Results and Discussion

Table I summarizes the separability evaluation of the baffle MCNP flux field using the component-splitting approximation. The normalized MCNP tally field was compared with the rank-1 approximation constructed from the transverse and axial flux components. The

overall min-max normalized comparison yielded R^2=0.890, indicating that the main spatial trend of the baffle flux field can be represented by the separable component product. For the individual baffle region, R^2 increased to 0.940 - 0.968, suggesting that the separable structure becomes more distinct within regions that have more consistent local geometry. was approximately 0.890 in the overall min-max normalized. These results indicate that the baffle flux field can be largely explained by a combination of transverse and axial components, and that the separability can become more distinct when geometric shape is considered.

Table I. Separability evaluation of the baffle MCNP flux using the component-splitting approximation.

Case	R^2	RMSE to identity	MAE to identity
Entire baffle	0.890	0.158	0.149
Region 1	0.946	0.197	0.193
Region 2	0.968	0.092	0.085
Region 3	0.962	0.158	0.155
Region 4	0.965	0.103	0.096
Region 5	0.963	0.184	0.179

Based on this separability, the component-splitting GPR method was applied to reconstruct the major spatial trends of the baffle flux field. Figures 2-5 compare the reconstructed flux distributions with the MCNP results at representative axial locations, and Figure 6 summarizes the prediction agreement for the comparison and validation datasets. In particular, the comparison with the validation dataset yielded R^2=0.983 on the flux scale and R^2=0.984 on the log-flux scale, while the median prediction-to-MCNP ratio was approximately 1.004. These results show that the central tendency of the GPR predictions is very close to the higher-cost MCNP reference values. Also, these results demonstrate that component-splitting GPR can be effective as an MCNP post-processing approach for reconstructing a continuous 3D flux trend from discrete tally estimates used in activation evaluation.

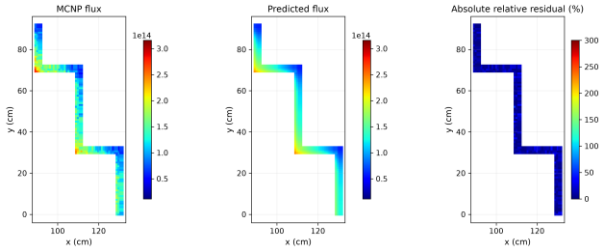


Fig. 2. Comparison of MCNP and reconstructed neutron flux distribution for the comparison dataset at z = -0.36 cm

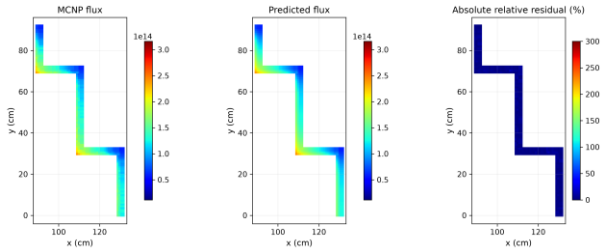


Fig. 3. Validation of the reconstructed neutron flux distribution against the higher-cost MCNP reference at z = -0.36 cm

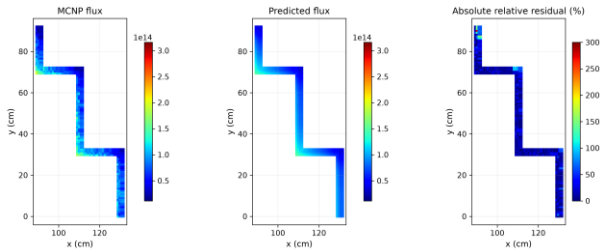


Fig. 4. Comparison of MCNP and reconstructed neutron flux distributions for the comparison dataset at z = -186.55 cm

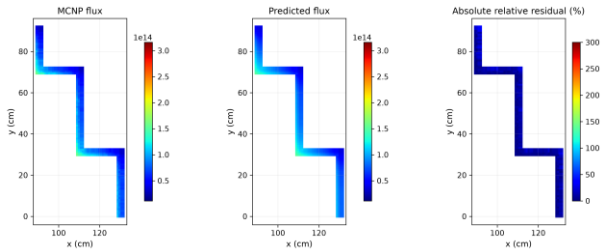


Fig. 5. Validation of the reconstructed neutron flux distribution against the higher-cost MCNP reference at z = -186.55 cm

The comparison dataset was generated with the same CTME setting as the MCNP tally data used for GPR training, CTME = 2,400, whereas the validation dataset was generated with a higher CTME setting, CTME = 130,000. When the GPR predictions were compared with these two datasets, the prediction scatter was larger for the lower-cost comparison dataset but narrower against the higher-cost MCNP reference. This behavior can be interpreted as the effect of GPR smoothing on the statistical noise included in the low-cost MCNP tally results. Therefore, the closer agreement with the higher-cost reference does not imply that the low-cost tally values themselves are more accurate, but indicates that the GPR reconstruction captured the dominant spatial flux trend while reducing local Monte Carlo noise.

Consequently, the baffle case can be interpreted as an initial application demonstrating that component-splitting GPR can be used as a surrogate post-processing method for reconstructing neutron flux fields in reactor internal structures.

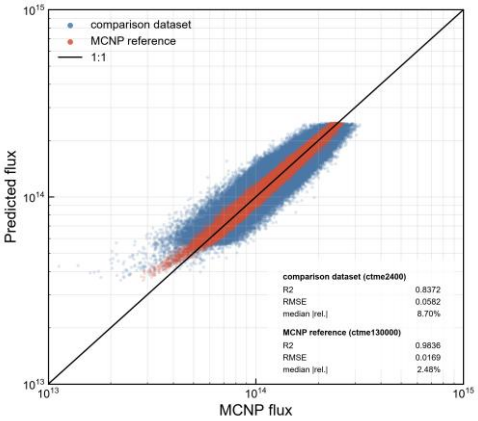


Figure 6. Scatter plot of GPR predictions against comparison dataset and higher-cost MCNP reference

4. Conclusions

In this study, the applicability of a component-splitting GPR-based neutron flux reconstruction method was evaluated using MCNP results for an OPR-1000 baffle. Although MCNP is useful for estimating the neutron flux at baffle locations, its tally results are provided as discrete or mesh-cell-averaged flux estimates for user-defined cells or mesh bins. The proposed GPR-based reconstruction therefore serves as a post-processing method for constructing a continuous spatial flux trend needed in activation evaluations that require flux information beyond the original tally support.

The analysis results showed that the baffle flux field can be largely explained by a combination of transverse and axial components, and that the GPR model effectively reconstructed the major spatial trends of the MCNP reference flux. In the best case, the R^2 on the log flux scale was approximately 0.984, and the median prediction-to-MCNP ratio was approximately 1.004. These results confirm that component-splitting GPR can be used to reconstruct a continuous 3D neutron flux trend from discrete MCNP tally results. These findings also suggest that, under the specified computing configuration, component-splitting GPR can reproduce flux trends comparable to the higher-cost MCNP results generated with CTME = 130,000, while using training data generated with CTME = 2,400. This indicates the potential to reduce the MCNP computational cost required for flux-field reconstruction.

Therefore, this study can be interpreted as an initial application showing that component-splitting GPR can be used as a surrogate modeling technique for reconstructing neutron flux fields in reactor internal structures to support activation evaluation. Future work should extend the application to structures located farther from the neutron source, such as the core barrel, thermal shield, and reactor vessel, where MCNP relative error and tally support issues become more important. In addition, incorporating MCNP tally relative errors as weights or noise information in the GPR model should be investigated to improve the treatment of spatially varying Monte Carlo uncertainty.

Acknowledgement

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REFERENCES

[1] OECD Nuclear Energy Agency, *Radiological Characterisation from a Waste and Materials End-State Perspective: Practices and Experience*, OECD/NEA, Paris, France, 2017.
[2] H. D. Sohn, K. S. Park, H. W. Kim, C. W. Kim, Y. H. Hwang, and J. Y. Yoon, "The study for activation evaluation on activated structures in nuclear power plant with 40 years operation history," *Annals of Nuclear Energy*, Vol. 141, 107305, 2020.
[3] A. Osborne, J. Dorville, and P. Romano, "Upsampling Monte Carlo neutron transport simulation tallies using a convolutional neural network," *Energy and AI*, Vol. 13, 100247, 2023.
[4] W. Chen, D. Yang, J. Zhang, C. Zhang, H. Gong, B. Xia, Y. Quan, and L. Wang, "Study of non-intrusive model order reduction of neutron transport problems," *Annals of Nuclear Energy*, Vol. 162, 108495, 2021.
[5] C. J. Werner, J. S. Bull, C. J. Solomon, et al., *MCNP6.3 Theory & User Manual*, LA-UR-22-30006, Rev. 1, Los Alamos National Laboratory, 2022.
[6] C. E. Rasmussen and C. K. I. Williams, *Gaussian Processes for Machine Learning*, MIT Press, Cambridge, MA, 2006.
[7] B. A. Khuwaileh and W. A. Metwally, "Gaussian process approach for dose mapping in radiation fields," *Nuclear Engineering and Technology*, Vol. 52, pp. 1807-1816, 2020.
[8] W. Cho, S.-G. Shin, M.-J. Lee, S. Jang, J. Lee, S. Han, H. Jo, and S.-H. Kim, "3D radiation map reconstruction strategy using Gaussian process regression with attenuation effects and radiation characteristics," *Nuclear Engineering and Technology*, Vol. 57, 103612, 2025.