# A Comparative Performance Study of Deep Learning-Based Surrogate Models for APR1400 Core Design: Prediction of Boron Concentration and Power Peaking Factor ($F_q$)

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## 1 Introduction

- Loading-pattern (LP) search in PWR core design is a combinatorial optimization problem that needs repeated depletion calculations — a major bottleneck [1]. It is tackled with GA/PSO meta-heuristics [2], increasingly combined with machine learning [3].
- Critical boron concentration (CBC) and $F_q$ are key safety- and margin indicators, but detailed core codes are too costly to evaluate for every LP candidate.
- Deep-learning surrogates can predict them from core state variables [4]; a prior study predicted them from k-inf and burnup for an Angra-1-like core [5].
- **Objective:** build MLP-, CNN- [6] and Transformer- [7] based surrogates for the APR1400 core, compare their boron and $F_q$ accuracy, and analyze the training instability seen for $F_q$.

### Surrogate modeling workflow

**ASTRA depletion**
999 random LPs × 23 burnup steps

↓

**Input 9×9×2**
k-inf & burnup per assembly (¼ core)

↓

**MLP · CNN · Transformer**
one dedicated model per output

↓

**Outputs**
critical boron (ppm) · Fq

## 2 Methods

### 2.1 Dataset construction

- LPs randomly configured to reflect core designers' experience; depletion with the core analysis code ASTRA.
- APR1400 modeled as a ¼ core on a 9×9 assembly grid; k-inf and burnup of every assembly extracted at each burnup step.
- 23 burnup steps per LP → 22,977 samples (999 LPs × 23).
- Split at the LP (case) level, 7 : 1.5 : 1.5, so correlated steps of one LP never leak across sets.
- Z-score normalization of inputs and outputs with training-set statistics only; non-fuel grid positions excluded.

**Table I. Dataset composition**

| Dataset | Loading patterns | Steps | Data count |
|---|---|---|---|
| Train | 699 | 23 | 16,077 |
| Validation | 150 | 23 | 3,450 |
| Test | 150 | 23 | 3,450 |
| **Total** | **999** | **23** | **22,977** |

### 2.2 Model architectures

#### MLP

162 (flattened 9×9×2) → 256 → 128 → 64 → 1, ReLU · **82,945 params**

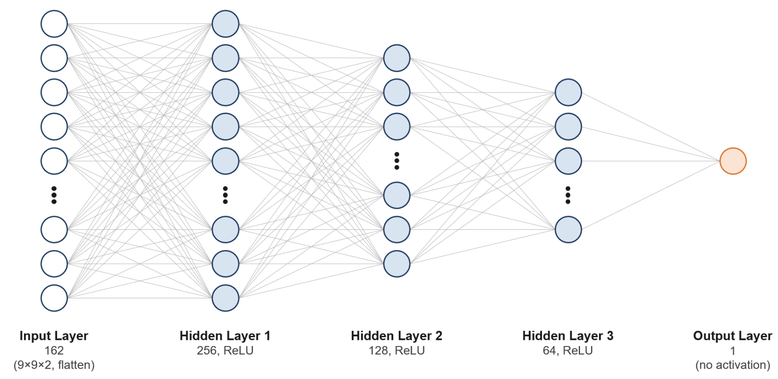



*Fig. 1(a). MLP*

#### CNN

2-channel 9×9 map → 2 × Conv 3×3 (32 ch, pad 1, no pooling) → FC 64 → 1, ReLU · **175,873 params**

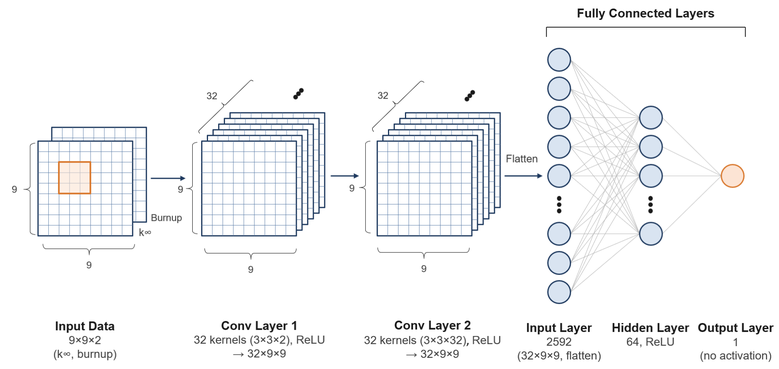



*Fig. 1(b). CNN*

#### Transformer

81 tokens (patch 1) + learned positional embedding → 2 encoder layers (d_model 32, 4 heads, FFN 128, dropout 0.1) → mean pooling · **28,129 params**

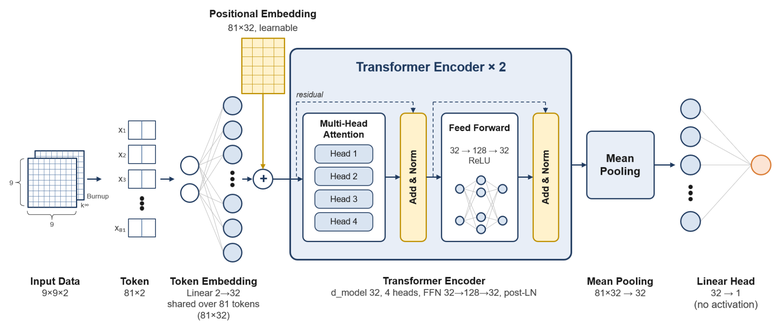



*Fig. 1(c). Transformer*

### Training configuration

- Loss: MSE = (1/N) Σ $(y_i - \hat{y}_i)^2$
- Adam (no weight decay), learning rate 1e-3, batch 64, 500 epochs
- Weights at minimum validation loss kept (no early stopping)
- Seeds 0, 1, 2 with a fixed split; deterministic GPU ops; capacities not matched

### 2.3 Evaluation metrics

- Boron — absolute error (values can be near zero): $AE_i = |\hat{y}_i - y_i|$ (ppm)
- Range ratio: $RR_i = AE_i / R \times 100$ (%), R = 1,717.3 ppm (1,513.7 to −203.6 ppm)
- $F_q$ — relative error: $RE_i = |\hat{y}_i - y_i| / |y_i| \times 100$ (%)
- Avg and Max over the 3,450 test samples; mean ± std over three seeds

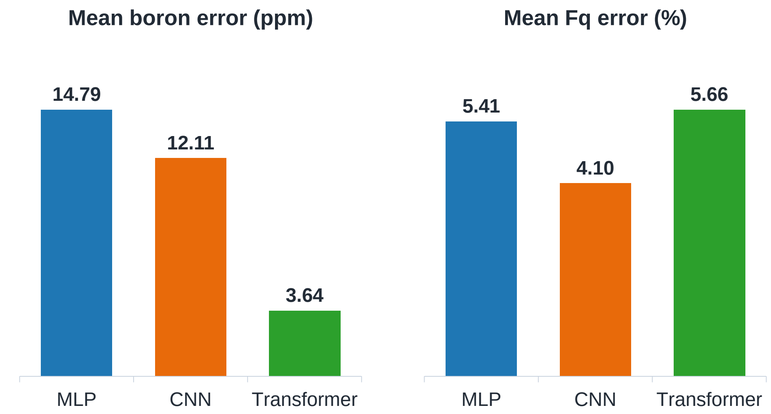
## 3 Results

**Tables II–III. Boron absolute error (ppm) and RR (%)**

| Model | Avg (ppm) | Max (ppm) | Avg RR | Max RR |
|---|---|---|---|---|
| MLP | 14.79 ± 0.62 | 79.67 ± 14.25 | 0.86 ± 0.04 | 4.64 ± 0.83 |
| CNN | 12.11 ± 1.12 | 74.82 ± 17.72 | 0.71 ± 0.07 | 4.36 ± 1.03 |
| Transformer | **3.64 ± 0.10** | **22.35 ± 2.27** | **0.21 ± 0.01** | **1.30 ± 0.13** |

**Table IV. Fq relative error (%)**

| Model | Avg (%) | Max (%) |
|---|---|---|
| MLP | 5.41 ± 0.16 | 29.35 ± 4.18 |
| CNN | **4.10 ± 0.09** | **22.44 ± 3.12** |
| Transformer | 5.66 ± 0.30 | 33.78 ± 3.16 |



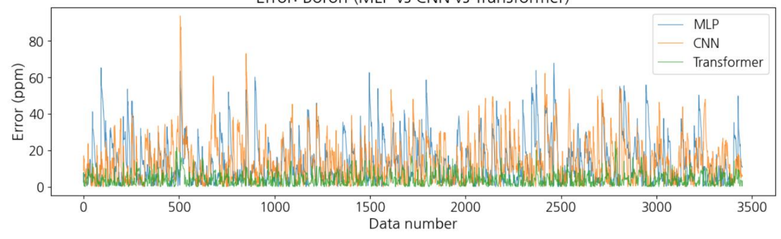




*Fig. 2. Boron absolute error per test sample (seed 0)*

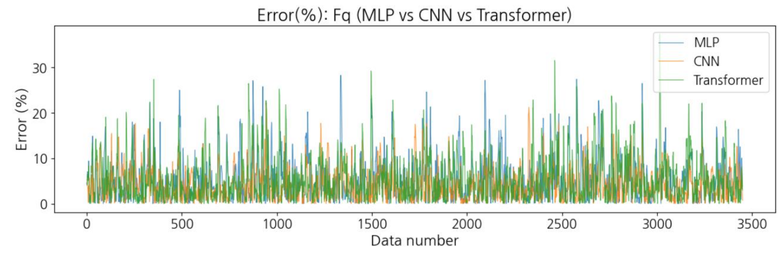



*Fig. 3. Fq relative error per test sample (seed 0)*

## 4 Discussion & Conclusion

- **Boron:** all models converged stably; mean error 3.64–14.79 ppm (0.21–0.86 % of range). The Transformer cut the error to ¼–⅓ of the others with the fewest parameters → an architectural, not a capacity, advantage.
- **$F_q$:** mean error looks acceptable (4.10–5.66 %), but max error reached 22.44–33.78 % and the three models perform alike. $F_q$ is a local quantity that also depends on the axial power distribution, which the 2D (k-inf, burnup) inputs do not carry.
- MLP overfits mildly; CNN and Transformer show large validation-loss oscillations — consistent with insufficient input information.
- **Future work:** add assembly-wise power distribution as input, compare $F_q$ with radial $F_r$ as the target, and extend the approach to SMR core design.

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