

Preliminary Assessment of Indicator-Based Hybrid CFD-GNN Acceleration for T-Junction Thermal Mixing

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1. Introduction

In the primary circuit piping of nuclear reactors, thermal mixing at T-junctions generates high-cycle temperature fluctuations on the pipe wall when two fluid streams at different temperatures merge. Thermal fatigue cracking driven by these fluctuations has been reported at operating plants [1, 2], and accurate analysis of this phenomenon requires three-dimensional unsteady CFD simulations. However, high-resolution 3D analyses on fine meshes demand hundreds of computational hours, limiting their applicability to iterative design studies and real-time monitoring.

Hybrid methods that couple machine-learning surrogates with CFD solvers have been proposed to reduce computational cost. XRePIT [3] decides whether to fall back to the CFD solver by comparing the continuity-equation residual of the surrogate prediction against a threshold (τ), and its validity has been demonstrated for two-dimensional natural convection problems. Existing XRePIT cases, however, targeted 2D structured-mesh problems; extension to the 3D unstructured-mesh environment considered here requires further examination. This study examines the applicability of a solver-surrogate hybrid approach to a 3D T-junction thermal-mixing problem. A graph-based surrogate is employed within the hybrid control loop framework, and the accuracy-speedup trade-off is assessed under OECD/NEA-Vattenfall T-junction benchmark [1] conditions using a velocity-based switching indicator.

2. Methods

2.1 CFD baseline setup

The geometry follows the benchmark of Smith et al. [1] (Table I, Fig. 1). Simulations were performed in OpenFOAM v13 with the $k-\omega$ SST turbulence model [4] and the Boussinesq approximation on a ~ 3.5 M cell mesh (snappyHexMesh), run in parallel on 32 MPI cores over 0–8 s ($\Delta t = 0.01$ s), yielding 801 snapshots of T , U_x , U_y , U_z .

Table I. Flow conditions for the OECD/NEA-Vattenfall T-junction benchmark.

Parameter	Cold inlet	Hot inlet
Inner diameter	140 mm	100 mm
Temperature	19°C (292.15 K)	36°C (309.15 K)
Flow rate	9.0 L/s	6.0 L/s
Mean velocity	0.585 m/s	0.764 m/s
Reynolds number	$\sim 79,400$	$\sim 107,000$

2.2 GNN Surrogate Design

The original FVMN surrogate is structurally incompatible with 3D unstructured meshes because it assumes a fixed neighbor count, whereas the present mesh has 3–21 neighbors per cell. A graph-based surrogate (GraphSAGE [5]) was therefore employed, treating each cell as a node and face-sharing relationships as edges. Key model settings are listed in Table II. Following the training strategy of the original XRePIT framework, only the first three time steps ($t = 0, 0.01, 0.02$ s; two training pairs) were used, which kept training feasible but constrained surrogate generalizability.

Table II. GNN surrogate model configuration.

Parameter	Setting
Architecture	SAGEConv 3-layer (GraphSAGE)
Input / Output	$[T, U_x, U_y, U_z] \rightarrow \Delta[T, U_x, U_y, U_z]$
Training data	First 3 time steps (2 pairs)
Best loss	0.01233 (epoch 624 / 1000)
Time per epoch	~ 0.4 min

2.3 Indicator-Based Hybrid Loop

As illustrated in Fig. 2, at each time step the GNN predicts the next state as a delta, and the mean absolute velocity discontinuity between neighboring cells is computed as a switching indicator R . If $R \leq \tau$, the prediction is accepted; if $R > \tau$, the simulation falls back to OpenFOAM, which corrects the result, and the GNN weights are updated via transfer learning. The speedup factor ψ is defined as

$$(1) \quad \psi = t_{\text{CFD-only}} / t_{\text{hybrid}}$$

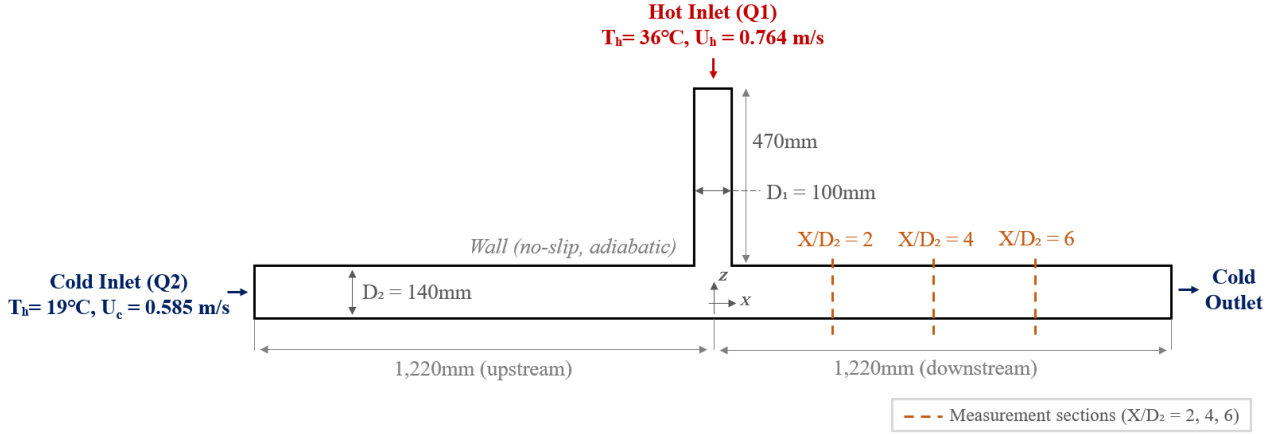


Fig. 1. T-junction geometry and boundary conditions. Dashed lines indicate cross-sectional measurement positions.

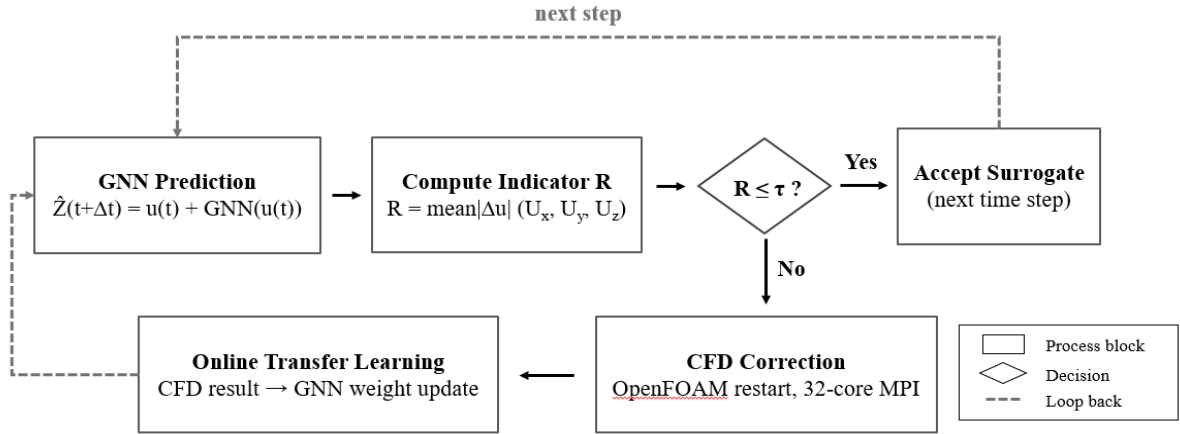


Fig. 2. Hybrid CFD-GNN experimental pipeline. After establishing the CFD baseline and training the GNN, the hybrid loop alternates between surrogate prediction and CFD fallback based on the switching indicator

The CFD-only reference time (163.6 min) covers the same 3–8 s window as the hybrid runs. The switching indicator used here differs structurally from the original XRePIT indicator, which normalizes the continuity-equation residual ($\nabla \cdot \mathbf{U}$) by the CFD baseline residual to form a dimensionless quantity. The present indicator is a velocity-based approximation computed directly from surrogate outputs; the quantitative effect of this difference on switching behavior remains to be examined.

3. Results and Discussion

3.1 Surrogate-Only Error Accumulation

When the GNN surrogate alone was used to predict 3–8 s without any CFD fallback, MAE_t accumulated linearly over time, reaching 11.10 K at $t = 8.0$ s (Fig. 3), suggesting that CFD fallback plays an important role in suppressing error accumulation over long prediction horizons.

3.2 Hybrid Loop Results

Three cases with different τ and indicator direction were run over 3–8 s (500 time steps). Results are summarized in Table III, with the MAE_t time series shown in Fig. 3 and the MAE_t - ψ trade-off in Fig. 4.

In all three cases, CFD fallback suppressed error accumulation relative to the surrogate-only baseline. MAE_t was reduced from 11.10 K to 0.214–1.061 K depending on the switching condition (Table III, Fig. 3).

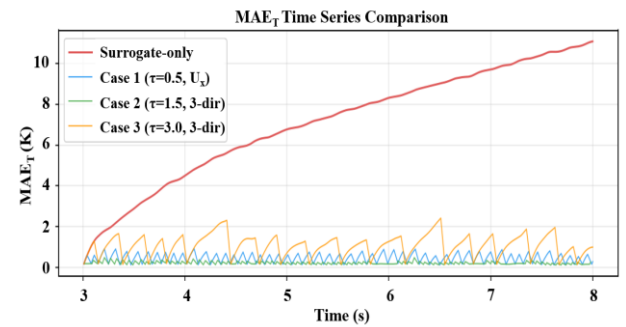


Fig. 3. Temperature MAE_t over time. Error accumulates linearly in the surrogate-only run, whereas all three hybrid cases suppress error growth.

Table III. Hybrid loop experiment results (3–8 s, CFD-only baseline: 163.6 min).

Parameter	Case 1	Case 2	Case 3
Threshold τ	0.5	1.5	3.0
Indicator direction	U_x only	3-dir. sum	3-dir. sum
GNN step fraction	69.4%	40.2%	89.2%
CFD fallback count	51	100	18
MAE_t [K]	0.458	0.214	1.061
Wall-clock time [min]	109.1	199.8	45.7
Speedup ψ	1.500	0.819	3.574

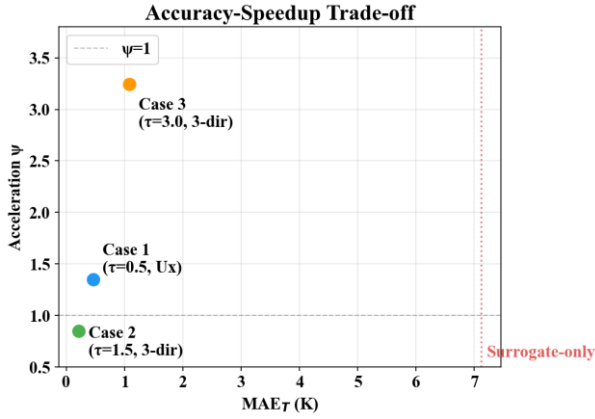


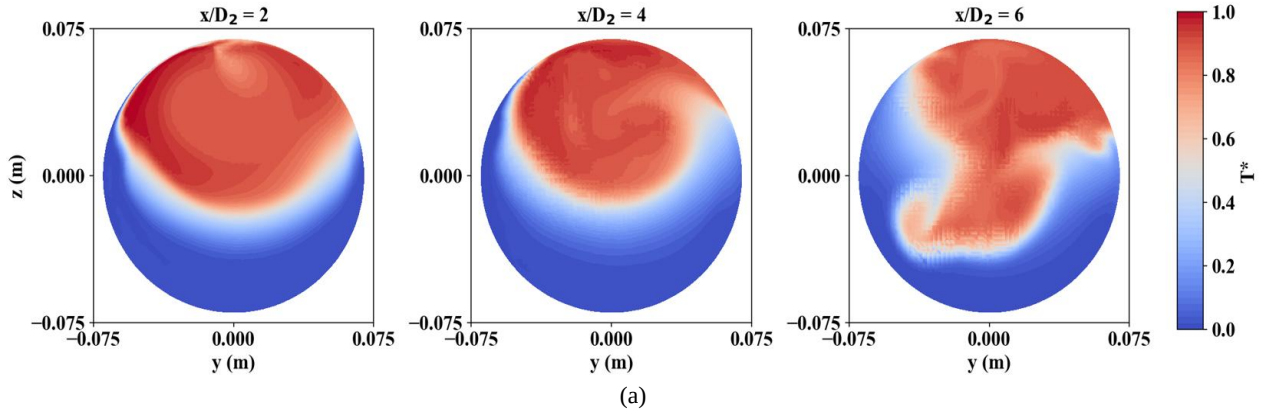
Fig. 4. MAE_t -speedup ψ trade-off. Higher τ tends to increase ψ . Case 2 ($\psi = 0.819$) did not achieve speedup relative to the CFD-only baseline.

The switching threshold τ governed a trade-off between accuracy and wall-clock time: higher τ increased the GNN step fraction and reduced computation time, at the cost of higher MAE_t (Fig. 4, Table III). However, excessively frequent fallback eliminated the speedup benefit. Case 2 (100 fallbacks, $\psi = 0.819$) was slower than the CFD-only baseline, as each fallback incurred a fixed overhead of approximately 70–120 s (estimated from wall-clock logs). This indicates that switching frequency has a direct effect on achievable speedup in 3D geometries where fallback cost is substantial.

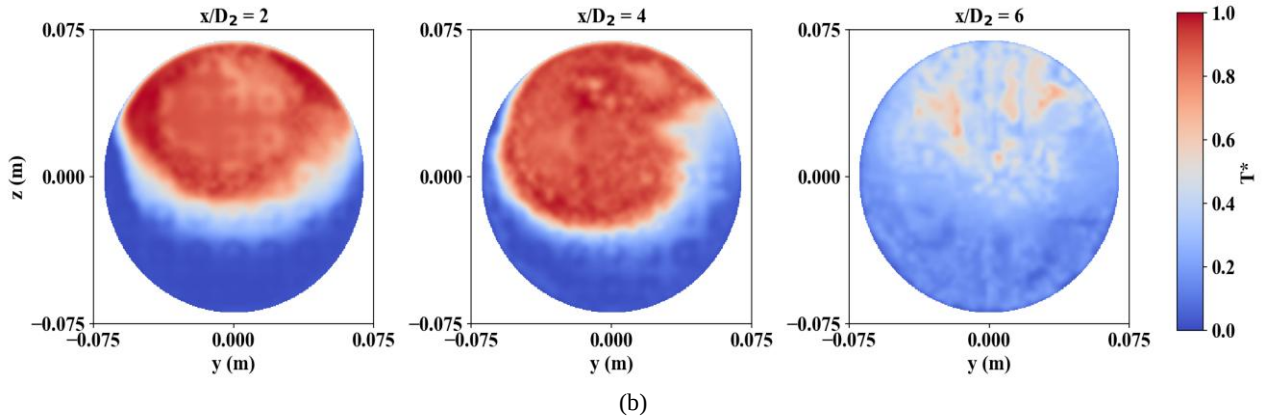
Comparing Case 1 ($\tau = 0.5$, U_x only) with Case 2 ($\tau = 1.5$, 3-direction), despite the higher threshold in Case 2, MAE_t was lower (0.214 K vs. 0.458 K). Because both τ and the indicator direction changed simultaneously, their individual effects cannot be separated; whether the indicator definition influences switching accuracy requires a controlled experiment in which each factor is varied independently.

As seen in Fig. 5, surrogate prediction error is relatively small near the junction ($x/D_2 = 2$) and increases downstream ($x/D_2 = 6$). This spatial pattern suggests that surrogate accuracy degrades in the more complex mixing region, and the effect of training data composition and indicator definition on this spatial error distribution requires further investigation.

CFD Temperature Field at $x/D_2=2,4,6$ ($t=8s$)



Hybrid (Case 3, $\tau=3.0$) at $x/D_2=2,4,6$ ($t=8.00s$)



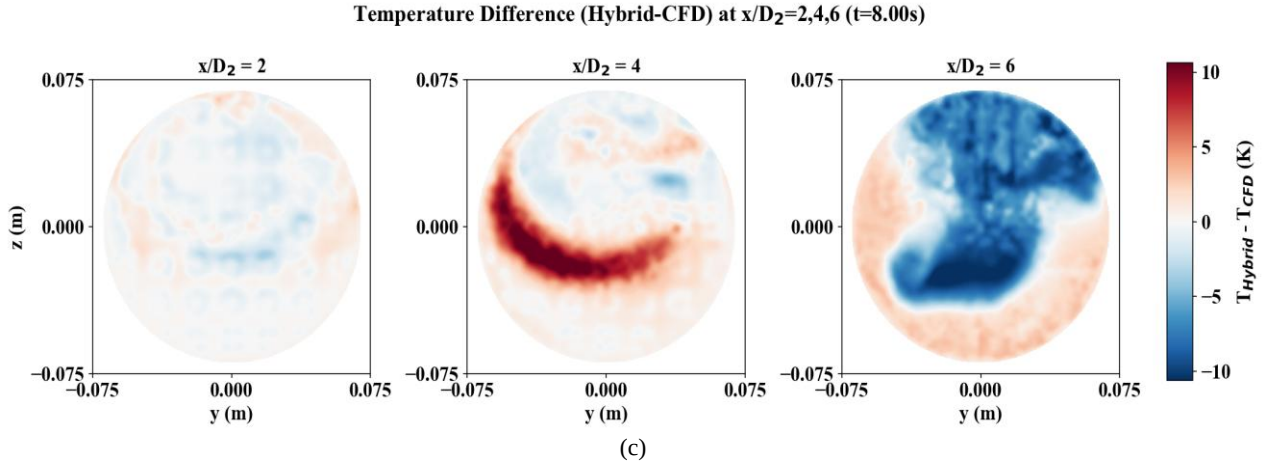


Fig. 5. Dimensionless temperature field T^* and error field at cross-sections $x/D_2 = 2, 4, 6$ ($t = 8$ s, Case 3, $\tau = 3.0$). (a) CFD results (b) Hybrid prediction (Gaussian smoothing applied; $T^* = (T - T_c)/(T_h - T_c)$). (c) Absolute error field $T_{Hybrid} - T_{CFD}$. Prediction error is smaller near the junction ($x/D_2 = 2$) and larger further downstream ($x/D_2 = 6$).

4. Conclusions

This study provided a preliminary assessment of a solver-surrogate hybrid approach for 3D T-junction thermal mixing under benchmark conditions. The main findings are as follows.

(1) The original FVMN surrogate was found to be structurally incompatible with the 3D unstructured mesh due to variable cell connectivity (3–21 neighbors per cell). A graph-based surrogate (GraphSAGE) was employed as a practical alternative to handle variable neighbor counts. Training time per epoch was reduced from ~33 min to ~0.4 min in this setup.

(2) Surrogate-only prediction accumulated MAE_t of 11.10 K by $t = 8$ s, which was suppressed to 0.214–1.061 K by indicator-based CFD fallback. In the Case 1 vs. Case 2 comparison, the case with the higher τ showed lower MAE_t , suggesting that the indicator definition affects switching behavior, though causal separation is not possible under the current experimental design. Case 2 ($\psi = 0.819$) failed to achieve speedup, as the high CFD fallback count drove total runtime above the baseline.

The spatial error pattern in Fig. 5 (smaller near the junction, larger downstream) suggests that surrogate accuracy degrades in the more complex mixing region.

Future work will focus on systematic refinement of the indicator design and switching strategy, architectural improvement of the graph-based surrogate, expansion of training data for improved generalizability, and validation across a broader range of thermal-hydraulic conditions.

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