A FDM-PINN Hybrid Approach for MELCOR CVH/FL Module

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1. Introduction

Severe accident (SA) analysis is a key element in ensuring the safety of nuclear power plants, and system codes such as MELCOR are commonly employed to simulate accident progression [1]. MELCOR represents complex thermal-hydraulic behaviors—such as core degradation, coolant depletion, and hydrogen combustion—within a control volume (CV)-based framework. While this approach is widely used, it faces significant challenges regarding computational efficiency and numerical stability, particularly in long-term transient simulations. MELCOR's numerical solution scheme heavily relies on traditional finite-difference methods (FDM). Although FDM is considerably less expensive than full-scale computational fluid dynamics (CFD), it remains computationally demanding for large-scale probabilistic safety assessment (PSA) applications that require numerous iterative calculations over extended periods. Furthermore, ensuring numerical stability in such FDM-based simulations often necessitates strict constraints on time-step sizes, which further exacerbates the computational burden during the long-term progression of severe accidents. These limitations highlight a critical need for an alternative methodology that can significantly accelerate computation while maintaining the rigorous numerical stability required for long-term transient analyses

Recently, machine learning methods have been actively investigated to address the computational cost issues associated with conventional numerical techniques [2]. Among these, Physics-Informed Neural Networks (PINNs) have emerged as a promising alternative because, unlike traditional data-driven approaches, they do not require large labeled datasets and instead obtain solutions by directly enforcing physical laws [3]. By leveraging automatic differentiation while satisfying physical constraints, PINNs have been successfully applied to approximate the solutions of partial differential equations (PDEs) in fluid dynamics and heat transfer [4]. Furthermore, various surrogate PINN approaches have been developed to accommodate changes in boundary conditions or variations in parameters [5]. However, they still fail to resolve the problem of error accumulation in long-term predictions [6]. Therefore, existing PINN frameworks are not yet directly suitable as drop-in replacements for system codes like MELCOR in realistic SA scenarios.

To address both the error accumulation issue and the high computational cost, this study introduces Mini-PINN, a novel hybrid approach that integrates a surrogate PINN within the traditional FDM framework. Rather than completely replacing the numerical scheme, Mini-PINN strategically employs the surrogate PINN to rapidly evaluate the complex flow transfers and interactions between system components. The overall system state is then updated using the conventional FDM scheme based on these PINN predictions. Because this FDM update step naturally enforces strict physical conservation laws and error tolerances before advancing to the next time step, this coupled mechanism effectively resolves the error accumulation problem typical of standalone PINNs. Consequently, while the Mini-PINN framework incurs a slightly higher computational cost than a pure surrogate PINN, it bypasses the most demanding iterative calculations required by conventional FDM, substantially decreasing the overall computational burden. Notably, the efficiency and robustness of this approach will be further amplified as the complexity of the accident scenarios increases.

2. Surrogate PINN Formulation

2.1 Scenario Description

The MELCOR code represents thermal-hydraulic behavior during severe accidents using a network of control volumes (CVs) and flow paths (FLs). In this study, we analyze a simplified gravity-driven draining problem consisting of six control volumes linked by a single flow path, as shown in Fig. 1. At the initial state, the upper control volume (CV01) is completely filled with water and the lower volume (CV02) is empty. Both volumes are exposed to the atmosphere, so pressure effects are neglected. Each control volume has a height of 2 m and a cross-sectional area of 50 m², and they are connected through a flow path with a diameter of 0.2 m and a length of 0.1 m. Water drains from CV01 to CV06 under gravity alone, and the calculation is carried out until the water levels reach equilibrium.

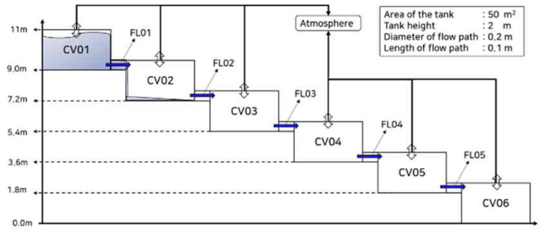

Fig. 1. Nodalization for the scenario model

2.2 Governing Equations

The physical behavior of the described scenario can be represented by two fundamental conservation equations, derived from the MELCOR CVH/FL module, governing mass and momentum conservation.

The mass conservation equation describes the temporal evolution of water height within each control volume. The inflow and outflow velocities through the connected flow paths, together with the relevant geometric parameters, determine the rate of change in water height over time, as expressed in Eq. (1).

$$A_i \rho^d_{j,m} \frac{\partial H_{i,m}}{\partial t} = \sum_j \sigma_{ij} \, \alpha_{j,\phi} \rho^d_{j,m} v_{j,\phi} F_j A_j \qquad (1)$$

In this equation, $H_{i,m}$ represents the water height within control volume i, and A_i is the cross-sectional area of the control volume. $\rho^d_{j,m}$ denotes the density of the fluid within the flow path, which is assumed to be constant. Additionally, $v_{j,\phi}$ represents the velocity within flow path j.

The momentum conservation equation governs the velocity dynamics within each flow path, where temporal changes in velocity are primarily driven by gravitational forces and opposed by frictional losses, as shown in Eq. (2).

$$L_j \frac{\partial v_{j,\phi}}{\partial t} = g\Delta z - \frac{1}{2} K^*_{j,\phi} |v_{j,\phi}| v_{j,\phi} \qquad (2)$$

Here, L_j represents the inertial length of the flow path j, and $v_{j,\phi}$ denotes the new velocity within the flow path. Δzcorresponds to the water height, while $K^*_{j,\phi}$ represents the net form and wall-loss coefficient.

In MELCOR, these conservation equations are solved in a discretized form, whereas PINNs directly use the governing equations in their original continuous form.

2.3 Surrogate Physics-Informed Neural Network (PINN) Formulation

PINNs incorporate governing equations directly into the neural network training process so that the solution consistently satisfies physical laws. Among them, surrogate PINNs take parameters—such as material properties or state variables—as additional network inputs, enabling the model to serve as a flexible surrogate even when these parameters vary. Fig. 2 shows the surrogate PINN architecture used in this study. The proposed model consists of a sub-network that takes the one-dimensional temporal input (t) and a separate sub-network that takes *the height difference* (Δh) as input. The outputs of the final layers of these two sub-networks are concatenated and passed to a decoder network that predicts the FP velocity (v). With this design, the network can predict the FP velocity without retraining, even when Δz changes across scenarios.

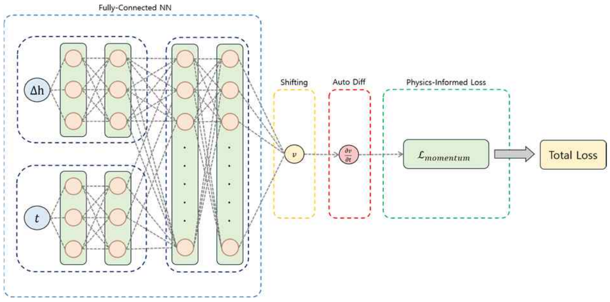

Fig. 2. Architecture of the proposed surrogate PINN

2.4 Surrogate PINN Training Results

The training results of the surrogate PINN are illustrated in Fig. 3. As shown, the surrogate PINN was trained to predict the velocity within the prescribed ranges of (Δh) and (t). Therefore, for any input values within these ranges, the surrogate PINN can respond flexibly by providing velocity predictions. Validation of this capability is presented later in Chapter 3.

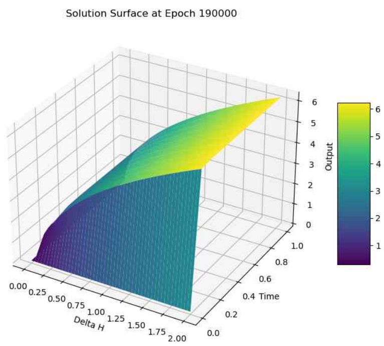

Fig. 3. Training results of the surrogate PINN

Fig. 4 shows the training loss history of the surrogate PINN. Because the surrogate PINN generally exhibits a more complex loss landscape than a standard PINN, the model appeared to experience difficulty converging during the early stages of training. However, after a sufficient number of epochs, the loss was observed to converge stably.

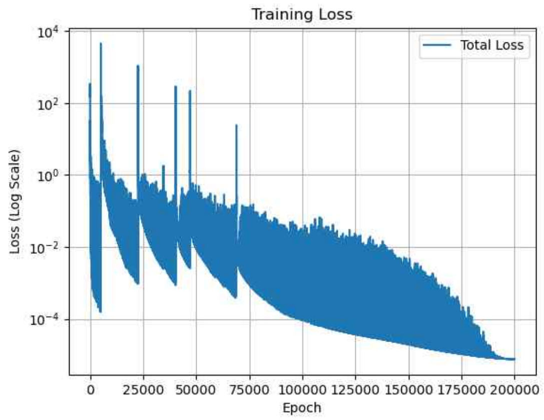

Fig. 4. Training loss histories of the surrogate PINN

One important point is that oscillations or occasional spikes in the loss curve do not necessarily indicate convergence failure. In general, PINN loss functions are known to be non-convex, and oscillatory behavior is expected due to the characteristics of gradient-descent-based optimization. Thus, rather than focusing solely on the shape of the loss curve, it is more important to confirm that the loss decreases to sufficiently small values and that the resulting predictions are physically reasonable. As seen in Figs. 3 and 4, the surrogate PINN achieves plausible results while maintaining a sufficiently low loss level.

3. Mini-PINN Framework and Evaluation

3.1 Hybrid Mini-PINN Algorithm

In general, system codes such as MELCOR are designed to predict long-term transient behavior using purely numerical schemes. In contrast, standalone surrogate PINNs do not effectively resolve the error-accumulation issue over long time horizons. To overcome this limitation, this study develops a Mini-PINN architecture, a fundamentally hybrid framework that deeply couples neural network predictions with traditional numerical solvers.

In the present scenario, the CV water level governed by Eq. (1) is computed using the FDM whereas the FP velocity governed by Eq. (2) is predicted by the surrogate PINN. Fig. 5 illustrates the Mini-PINN algorithm. At the current time step (t^n), the water-level difference between CVs is first calculated. A pre-trained surrogate PINN is then used to predict the velocity (v) at the next time step (t^{n+1}). Using the predicted velocity (v), the CV water level is subsequently updated via FDM.

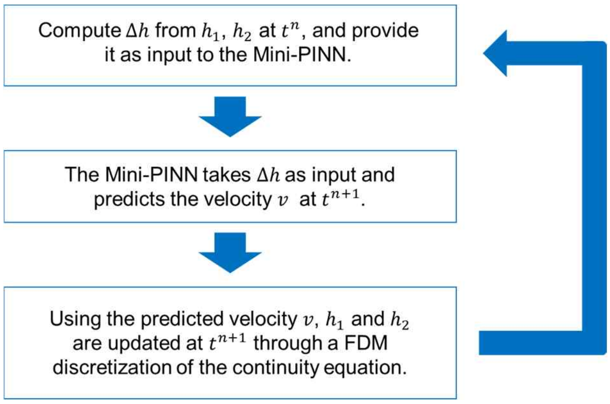

Fig. 5. Mini-PINN Algorithm

This approach offers the following advantages. First, once trained, a PINN can provide near–real-time predictions, and Mini-PINN can effectively leverage this strength. Although Mini-PINN may be somewhat slower than using a surrogate PINN alone due to the inclusion of the FDM update, it can offer clear computational benefits compared with an FDM-only approach as the problem complexity increases.

Second, coupling with FDM helps mitigate error accumulation. In general, FDM performs computations using small time steps (typically 1.0). Because the surrogate PINN in Mini-PINN follows the same time-step size to remain consistent with the FDM update, it does not need to predict the entire long-time evolution in a single shot. As a result, error accumulation in long-term predictions can be effectively controlled.

3.2 Mini-pinn verification

The performance of the Mini-PINN was evaluated by comparing its results with the solution values obtained from the FDM. Fig. 6 illustrates the comparison between the FP velocity, which was exclusively predicted by the surrogate PINN module within the hybrid architecture (solid line), and the reference solution (dotted line). The Mini-PINN predicted the pipe velocity during the transient with high accuracy, demonstrating that the Surrogate PINN described in Chapter 2 was effectively trained. Furthermore, the model achieved remarkably low error, with a Mean Absolute Error (MAE) of 6.71e-3 and a Mean Squared Error (MSE) of 1.62e-4, indicating its high precision and reliability in numerical estimation.

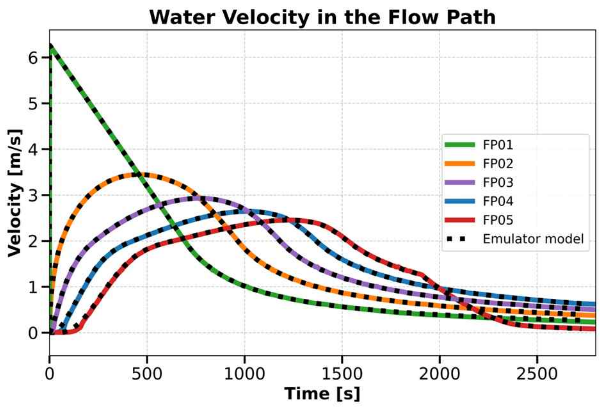

Fig. 6. Comparison of predicted water velocity in the FPs

Fig. 7 illustrates the comparison between the CV water level, which was updated by the FDM module based on the PINN's prior velocity predictions (solid line), and the reference solution (dotted line). Similar to the velocity results, the FDM module accurately calculated the water level within the CVs. This outcome confirms that the Surrogate PINN's precise estimation of FP velocity directly and accurately drives the FDM's state updates. The performance is further substantiated by the remarkably low error metrics, with a MAE of 1.09e-3 and a MSE of 3.25e-6. These results effectively validate the robustness and efficiency of the proposed Mini-PINN framework in capturing complex fluid dynamics.

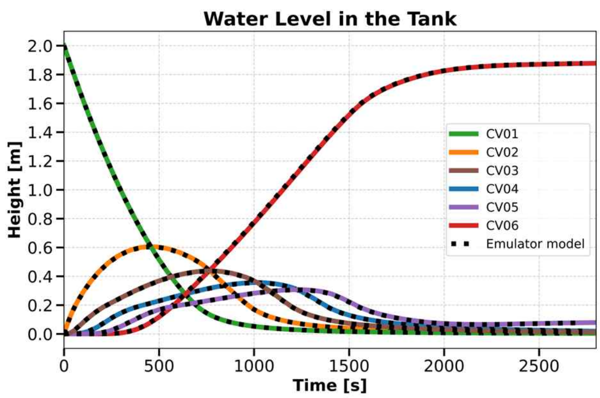

Fig. 7. Comparison of predicted water level in the CVs

4. Conclusion

In this study, the feasibility of applying a surrogate PINN to the CVH/FL module of MELCOR was investigated. To address the inherent limitation of error accumulation in long-term transient predictions common in traditional PINN frameworks, a Mini-PINN framework was proposed. This architecture integrates a surrogate PINN for flow path velocity predictions with the conventional FDM for updating CV water levels. By alternating these calculation schemes, the proposed framework successfully demonstrated numerical stability throughout the transient conditions.

The verification results indicated that the Mini-PINN provides high precision and reliability compared to reference solutions. The model achieved remarkably low error metrics, with a MAE of 6.71e-3 for velocity predictions and 1.09e-3 for water level calculations. These findings suggest that the Mini-PINN effectively maintains physical consistency while mitigating the instability issues typically associated with long-term deep learning-based fluid simulations.

While the current implementation of Mini-PINN is somewhat slower than an FDM-only approach in the simplified gravity-driven draining scenario, the ultimate objective of this architecture is to achieve significant computational acceleration as the problem complexity increases. Future research will focus on validating this acceleration potential by applying the Mini-PINN framework to more complex scenarios involving multi-physics interactions. Specifically, further studies will evaluate the performance of the model when integrated with additional MELCOR modules, such as Heat Structure (HS) and RadioNuclide (RN), which are essential for capturing comprehensive severe accident behaviors.

Ultimately, the Mini-PINN framework offers a promising foundation for real-time prediction and computational efficiency in large-scale nuclear system safety assessments

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