Estimation of Xenon Oscillation with Physics Informed Neural Network

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1. Introduction

Xenon-135 (135 Xe) is produced by fission or by the decay of Iodine-135 (135 I), which is also produced by fission. It has a large thermal neutron absorption cross-section. This feature adversely affects both the reactor operation state and shutdown state. For example, it absorbs thermal neutrons instead of Uranium-235 (235 U) in operation, preventing the multiplication factor from being maintained as one [1]. In addition, it provides a greater negative reactivity than that of control rods for a period of time at shutdown, preventing the reactor from restarting [1]. As such, it is important to understand the amount of 135 Xe in a reactor since it has a lot of influence on the reactor during operation and after shutdown.

Actually, this phenomenon is well-known so there have been a lot of approaches to describe and estimate the decay chain of ¹³⁵Xe such as numerical analysis using a differential equation (PDE) solver, etc. Even though detailed models have been developed, this paper will use a simple form [1] to show the applicability of machine learning techniques in this area, particularly a physics-informed neural network (PINN) which does not require a large amount of training data. Instead of training data, it is driven by the laws of physics. Therefore, it can produce results more efficiently than other neural networks in complex physical phenomena, biological or engineering systems, and so on [2].

2. Background

This section describes the basic principles for PINN and differential equations for the production and destruction of 135 Xe.

2.1 Physics-informed neural networks (PINNs)

Nonlinear PDEs are used in many fields such as natural phenomena and laws of physics. A general nonlinear PDE is expressed in the following form.

$$u(x,t) + N_x[u] = 0, x \in \Omega, t \in [0,T]$$
(1)

where u(x, t) denotes the latent (hidden) solution, N_x is a nonlinear differential operator, x denotes a vector of space coordinates, and t denotes the time. The domain Ω of the nonlinear PDE is bounded based on the prior knowledge of the dynamic systems such as a length or a diameter of a pipe, and [0, T] is the time interval within which the system evolves [2]. In equation 1, the left side is defined as f. This f acts as a physical constraint in the process of approximating the nonlinear PDE with a neural network. The first term u in equation 1 is approximated by the neural network as learning proceeds. Meanwhile, the second term $N_x[u]$ of equation 1 is also derived with the same neural network. The loss function using mean square error (MSE) for approximating the solution of equation 1, which is denoted as L_{MSE} , is as follows [3, 4].

$$L_{MSE} = L^u_{MSE} + W \cdot L^f_{MSE} \tag{2}$$

where W is a factor denoting the weight associated with the loss term L_{MSE}^{f} ,

$$L_{MSE}^{u} = \frac{1}{N_{u}} \sum_{i=1}^{N_{u}} [u_{NN}(t_{u}^{i}, x_{u}^{i}; \theta) - u^{i}]^{2} \qquad (3)$$

$$L_{MSE}^{f} = \frac{1}{N_{f}} \sum_{i=1}^{N_{f}} [f(t_{f}^{i}, x_{f}^{i})]^{2}$$
(4)

where $\{t_u^i, x_u^i, u^i\}$ denotes the initial and boundary data points on u(x, t), $u_{NN}(x_u^i, t_u^i; \theta)$ denotes the prediction of the neural network on the inputs (x_u^i, t_u^i) , θ refers to the weights in the neural network, $\{x_u^i, t_u^i\}$ represents the collocation points for f(x, t), N_u and N_f represent the number of points generated for u(x, t) and f(x, t), respectively [2, 4].

In equation 3, L_{MSE}^u is the loss term for the initial value and the boundary value. It represents the difference between the initial, boundary value predicted by the learned neural network and the actual initial, boundary value. In equation 4, L_{MSE}^f is the loss term for the physical law of equation 1. It represents the difference between the physical values predicted by the learned neural network at the collocation point and the actual physical values.

Through L_{MSE}^{f} , solutions that violate the physics are immediately discarded, reducing the amount of solution space to be considered and significantly reducing the size of neural networks such as the number of nodes and layers [3]. Therefore, PINN can obtain the same level of solutions using relatively less computational cost compared to classical numerical analysis [2]. Purely data-driven models may fit observations very well, but predictions may be physically inconsistent or implausible, owing to extrapolation or observational biases that may lead to poor generalization performance. Compared to purely data-driven models, PINN is a physical law-based model that provides physically consistent predictions even when data is scarce [5].

2.2 Production and destruction of ^{135}Xe

There are two paths for the production of 135 Xe in a reactor. The first path is beta-decay of 135 I. 135 I is produced by the beta-decay of Tellurium-135 (135 Te) or fission of 235 U. 135 Te has a very short half-life (11 sec), so it can be assumed that 135 I is produced by only fission of 235 U. The second path for the production of 135 Xe is fission of 235 U [1].

There are also two destruction paths for 135 Xe in the reactor. The first path is for 135 Xe to absorb thermal neutrons. The second path is for 135 Xe to beta-decay to Cesium-135 (135 Cs).



Fig. 1. The process of production, destruction of ¹³⁵I, ¹³⁵Xe

According to the above production, destruction paths, in order to estimate the amount of 135 Xe, the differential equation for the amount of 135 I and of 135 Xe should be solved at the same time. Therefore, these differential equations appear in the form of a simultaneous equation as shown in equation 5, 6 [1].

$$\begin{pmatrix} \frac{dI}{dt} = \gamma_I \Sigma_f \phi_T - \lambda_I I & (5) \end{pmatrix}$$

$$\left(\frac{dX}{dt} = \gamma_X \Sigma_f \phi_T + \lambda_I I - \sigma_{a2}^X \phi_T X - \lambda_X X \right)$$
(6)

I is the number of ¹³⁵I *atoms/cm*³, γ_I is the effective yield of this isotope, and Σ_f is thermal fission cross-section. ϕ_T is the thermal neutron flux. λ_I is the decay constant of ¹³⁵I. *X* is the ¹³⁵Xe concentration in *atoms/cm*³. γ_X is the fission yield of the ¹³⁵Xe. σ_{a2}^X is the thermal absorption cross-section of ¹³⁵Xe and λ_X is the decay constant of ¹³⁵Xe.

3. Results

PINN requires differential equations and initial or boundary conditions instead of training data. Equation 5, 6 are f mentioned in Section 2.1 when the right side is moved to the left side or vice versa. Therefore, equation 5, 6 act as the physical law of PINN. The element necessary for learning of PINN is completed by additionally setting the initial or boundary condition. The conditions provide the loss function given in equation 3 in PINN. The following equation shows initial condition in equation 5 and 6.

$$I(0) = 10^{15} \, \#/cm^3, X(0) = 10^{14} \, \#/cm^3 \quad (7)$$

In addition, the condition that the ϕ_T in equations 5 and 6 is a step function was applied to observe the change in the amount of ¹³⁵Xe when the power of a reactor was 50% while maintaining the steady state in 100%.

$$\phi_T = \begin{cases} 10^{14} \, \#/cm^2 \cdot h &: t < 200h \\ 0.5 \times 10^{14} \, \#/cm^2 \cdot h : t \ge 200h \end{cases} \tag{8}$$

PINN consists of 4 hidden layers whose activation function is "RELU". The optimizer used ADAM with a learning rate of 0.001. The neural network was trained by making 20,000 collocation points for $t \in [0, 400]$. Figure 2 shows value of loss function of PINN for each iteration. Figure 3 is a graph showing the amount of 135I, 135Xe (blue, red dots) by time predicted by PINN and the analytic solution (gray, yellow line) of equation 5, 6.



Fig. 2. Loss function of PINN



Fig. 3. Amount of ¹³⁵I, ¹³⁵Xe using PINN and analytic solution

Figure 2 shows that as learning progresses, the loss value partially peaks, but converges to zero as a whole. Accordingly, it can be seen in Figure 3 that PINN predicts almost the same value as the analytic solution. Especially, the results of the PINN were predicted

similarly to the exact solution even around 200 hours, where the reactor power plunged from 100% to 50%.

4. Conclusions

 135 Xe is a representative poison which has a large thermal neutron absorption cross-section. Therefore, it is important to predict the amount of 135 Xe in a reactor during the operation of a nuclear power plant. This is because reactivity control, reactor dead time analysis, etc. can be properly performed only when the amount of 135 Xe in the reactor is known.

Differently from other artificial neural networks, PINN is able to accurately predict the amount of ¹³⁵Xe only with differential equations and initial conditions. Moreover, when the reactor power is in transient, it simulated the amount of ¹³⁵Xe similarly to the exact solution even at the boundary. In conclusion, if the governing equation is ready for a phenomenon with various variables or a case where data is difficult to obtain, PINN is expected to be one of the useful numerical approaches.

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