

Employing Machine Learning in the Study of Differential Equations Related to Nuclear Engineering



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ABSTRACT

Most of differential equations that describe the real-world phenomena cannot be solved exactly and one must utilize an approximation method to obtain a solution, such as finite difference, finite volume, finite element numerical method, etc. The goal of this project is to utilize machine/deep learning methods in study of conservation laws that model multi-phase flows. Our project's emphasis is on relatively recent methods for solving differential equations that utilize machine learning and, specifically, neural networks, motivated by the universal approximation theorem.

Our approach consists of proposing a trial solution consisting of two parts – the first part, satisfying the initial/boundary conditions, with no adjustable parameters, and the second part consists of a neural network that is trained to satisfy the differential equation by minimizing the squared error loss. We have found that the machine learning approximation methods yield more accurate and faster results than typical approximation methods.

BACKGROUND

Differential equations model a variety of phenomena in sciences and engineering. The main focus of this project is on time-dependent partial differential equations known as conservation laws that are used to model multiphase flows. In particular, these equations are of interest to engineers who design nuclear reactor pipes to ensure the optimal flow of gasses and liquids.

We consider the differential equations stated in [3]. They are a simplified model for the flow of gasses and liquids in vertical pipes and are expressed as time-dependent one-dimensional conservation of mass laws in terms of volume fractions for the liquid and gas (α_l and α_g). Since $\alpha_l + \alpha_g = 1$, we state only the equation for α_l and for simplicity of notation, we drop the subscript l:

$$\partial_t \alpha + h'(\alpha) \partial_x \alpha = 0$$

where $\alpha(x, t)$ is the unknown function denoting the fractional volume of liquid, t and x denote the temporal and spatial variables and h is the flux given by:

$$h(\alpha) = -\frac{\alpha \cdot (1 - \alpha)^2}{\alpha \cdot (1 - \alpha) \cdot I_g \cdot \mu_g + (1 - \alpha)^2 \cdot I_l \cdot \mu_l + II \cdot \mu_l} \cdot \Delta \gamma$$

We consider the physical variables posed in [3] table 5.1:

$$h(\alpha) = -\frac{\alpha \cdot (1 - \alpha)^2}{\alpha \cdot (1 - \alpha) \cdot 30,000 + (1 - \alpha)^2 \cdot 7.2 + 720} \cdot 9,800.19$$

as well as the initial and boundary conditions,

$$\alpha(x, 0) = \begin{cases} \alpha_{left}, & x = 0, \\ f(x), & 0 < x < 1, \\ \alpha_{right}, & x = 1, \end{cases}$$

Typically, these PDE solutions are approximated using numerical methods such as finite differences, finite volumes or finite elements [6]. However, we utilize the above stated background to generate solutions using neural network method stated in [5].

SOLUTION APPROXIMATION

Method discussed in [5] results in an approximating solution that is given in a differentiable, closed analytic form. The main idea is to consider a trial solution written as a sum of two parts. The first part is constructed to satisfy the initial/boundary conditions, while the second part is given in terms of a neural network whose parameters are learned by minimizing the squared error loss function that imposes the governing differential equation. The trial solution is defined by

$$\alpha_{trial}(x, t) = A(x, t) + xt(1 - x)N(x, t, \vec{p})$$

where the first term $A(x, t)$ will be defined to incorporate initial and boundary conditions and the second term involves neural network with set of parameters denoted by \vec{p} that will incorporate the differential equation. The appropriate choice for $A(x, t)$ is

$$A(x, t) = (1 - x) \cdot \alpha_{left} + x \cdot \alpha_{right} + (1 - t) \cdot [f(x) - (1 - x)f(0) - xf(1)]$$

The boundary conditions state what the fractional volume of liquid is at the entry of the pipe (when $x = 0$) and at the exit of the pipe (when $x = 1$), while the initial condition (when $t = 0$) specifies the initial distribution of liquid inside the pipe. Here, α_{left} and α_{right} are constants given in advance and $f(x)$ will be a function that is given in advance. In our case, $\alpha_{left} = 1$, $\alpha_{right} = 0$, and $f(x)$ which is compatible with α_{left} and α_{right} is a piecewise constant function as in [3].

Next, we need to define the neural network. We have two input variables x and t , one hidden layer with 20 nodes, and output N . Each node in the hidden layer is of the form,

$$z_i = w_{1i}x + w_{2i}t + u_i$$

We utilize the sigmoid activation function. Therefore our neural network is defined as follows.

$$\sigma(z) = \frac{1}{1 + e^{-z}}, \quad N(x, t) = \sum_{i=1}^{20} v_i \sigma(z_i)$$

In defining the minimization problem we consider 400 points from the domain $[0, 1] \times [0, 1]$, obtained by considering 20 equidistant points in the interval $[0, 1]$ in each variable t and x . We want to minimize the error by finding the optimal parameter set \vec{p} satisfying

$$\min_{\vec{p}} \sum_{m,n} (\partial_t \alpha_{trial}(x_m, t^n) + h'(\alpha_{trial}(x_m, t^n)) \cdot \partial_x \alpha_{trial}(x_m, t^n))^2.$$

RESULTS

Our results yield accurate results, consistent to traditional methods, such as finite differences at a faster rate. This allowed for us to generate a surface as displayed in Figure 2, without computationally burdening our system. We are confident machine learning methods are also successful in approximating equations describing the multiphase flows.

Following the accuracy results utilizing the methods in [5], we wish to now implement a physics informed deep neural network approximation method discussed in [8]. This would allow for a more detailed and fine-tuned surface generation.

FIGURES

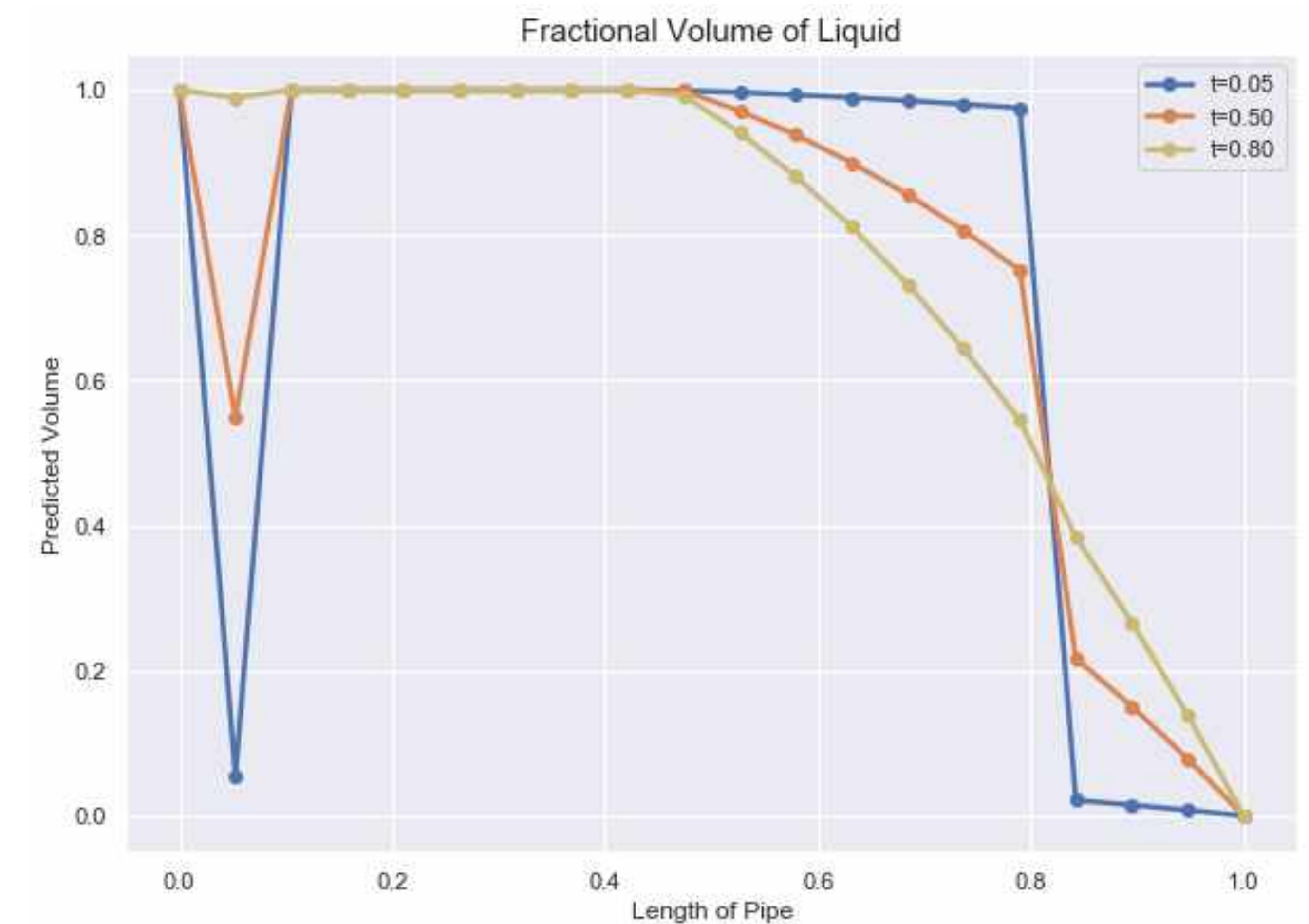


Figure 1. Neural Network's Predicted volume in relation to length of pipe, for fixed times $t = 0.05$, $t = 0.50$, $t = 0.80$.

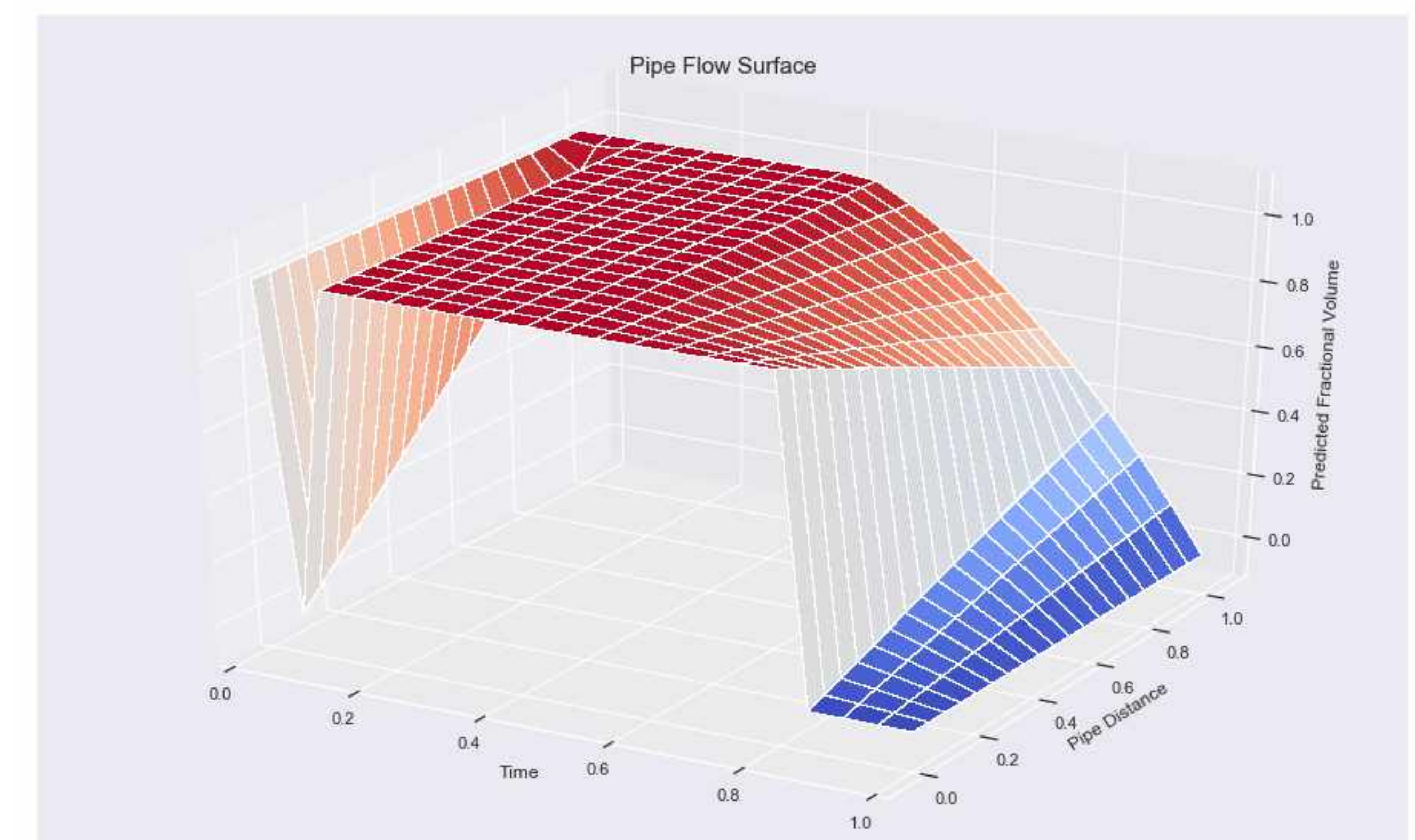


Figure 2. Neural Network's Surface generation in relation to time, length of pipe (distance) and predicted fractional volume.

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