Proceedings of the 1st international Symposium on AI and Fluid Mechanics
Abstract No S11 A6

Solve advection-diffusion-Langmuir adsorption processes in 2-D oscillatory flows using residual physics-informed neural networks

[1,2]Haobo Hua; [3]Bo Huang; [4]Sensen He; [5]Huan Han; [3]Zhigang Zuo*; [3]Shuhong Liu*

[1]*Department of Mathematics, Zhengzhou University of Aeronautics, Zhengzhou, 450046, China*

[2]*National Supercomputing Center in Zhengzhou, Zhengzhou University, Zhengzhou, 450001, China*

[3]*State Key Laboratory of Hydroscience and Engineering, and Department of Energy and Power Engineering, Tsinghua University, Beijing, 100084, China*

[4]*Baidu Inc., Beijing, 100085, China*

[5]*School of Energy and Environmental Engineering, University of Science and Technology Beijing, Beijing 100083, China*

**Corresponding authors*

Abstract

1. Problem Setup

The method of Physics-Informed Neural Networks (PINNs) has emerged as a powerful alternative to traditional numerical methods for solving partial differential equations, offering advantages such as mesh-free computation and efficient handling of complex boundary conditions. In a previous study, we performed computational investigations of the advection-diffusion-Langmuir adsorption (ADLA) process in Poiseuille flows in the 2-D plane with the finite difference method (FDM) [1]. Combined with theoretical analysis, an identification of dominant mass transfer processes was made under laminar flow conditions. Using PINNs in the following study, we revisited this ADLA process with a machine learning method [2]. The results indicated that PINNs can offer an efficient and accurate technique compared to FDM for solving ADLA equations.

This study applies PINNs to solve the ADLA equations in an oscillatory flow with the nondimensional form,

$$\frac{\partial c^*}{\partial t^*} = \lambda^2 \frac{\partial^2 c^*}{\partial x^{*2}} + \frac{\partial^2 c^*}{\partial y^{*2}} - \lambda \left[Pe_1\, y^*\left(1 - y^*\right) + Pe_2 \frac{1}{\alpha^2} f^*\left(\alpha, Sc, y^*, t^*\right) \right] \frac{\partial c^*}{\partial x^*}, \qquad (1)$$

$$\epsilon \frac{\partial c^*}{\partial y^*} = \frac{\partial \eta}{\partial t^*} = \epsilon Da [c_s^*(1-\eta) - \frac{1}{K_0}\eta], \qquad (2)$$

where c^*, η, and t^* are the normalized bulk concentration, the normalized surface concentration of the adsorbates, and the normalized time, respectively. In Eq.(2) that governs the adsorption process, c_s^* is the normalized concentration of free adsorbates in the bulk solution adjacent to the channel surface. Note that the oscillatory flow can be regarded as the superposition of a steady Poiseuille flow plus an additional flow oscillating around zero velocity [3]. Thus, there exist two Peclet numbers Pe_1 and Pe_2 that represent the ratio of convection to diffusion in the Poiseuille flow and the additional oscillatory components, respectively. Specifically, the Poiseuille flow is determined by a parabolic velocity distribution $y^*(1-y^*)$ with prime amplitude Pe_1. The oscillatory component is controlled by the oscillation amplitude Pe_2/α^2 and frequency coefficients α and Sc in $f^*(\alpha, Sc, y^*, t^*)$.

Let

$$ST = \sin\left(2\alpha^2\, Sc\, t^*\right), \qquad CT = \cos\left(2\alpha^2\, Sc\, t^*\right),$$

$$SN = \sin\left(\frac{\alpha(y^* - 0.5)}{0.5}\right), \qquad SH = \sinh\left(\frac{\alpha(y^* - 0.5)}{0.5}\right),$$
$$CS = \cos\left(\frac{\alpha(y^* - 0.5)}{0.5}\right), \qquad CH = \cosh\left(\frac{\alpha(y^* - 0.5)}{0.5}\right),$$ where Sc is the Schmidt number, defined as the ratio of momentum diffusivity (kinematic viscosity) and mass diffusivity, with α representing the ratio of the transient inertial force to the viscous force physically. Then, $f^*(\alpha, Sc, y^*, t^*)$ can be written in a brief form as:

$$\begin{aligned} f^*(\alpha, Sc, y^*, t^*) \quad &= \frac{1}{\cos(2\alpha) + \cosh(2\alpha)}[\cos(2\alpha) \cdot SN + \cosh(2\alpha) \cdot ST \\ &+ \sin(\alpha) \cdot \sinh(\alpha) \cdot CS \cdot CT \cdot CH - 2\sin(\alpha) \cdot SN \cdot ST \cdot SH \\ &- 2\cos(\alpha) \cdot \cosh(\alpha)(CS \cdot CH \cdot ST + CT \cdot SN \cdot SH)]. \end{aligned} \tag{3}$$

Figure 1 shows the schematic of the processes with geometric settings.

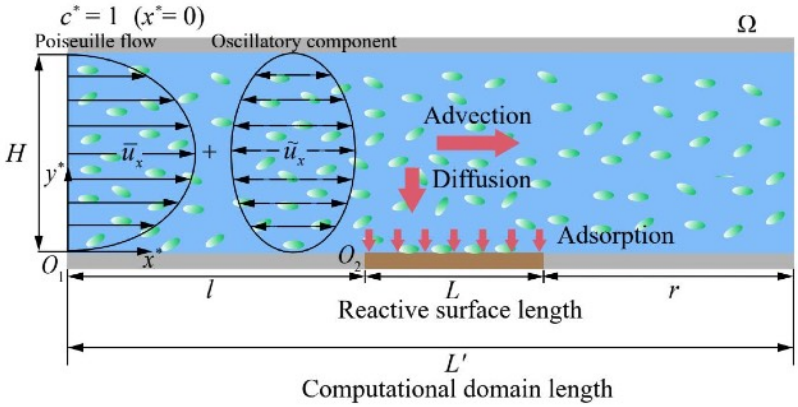

Fig. 1 Schematic and notation of the advection-diffusion-Langmuir adsorption processes in a two-dimensional oscillatory flow between two parallel planes. Adsorbates (molecules and particles) of concentration $c^* = 1$ at $x^* = 0$ are introduced from the inlet of the 2-D channel, i.e., $x^* = 0$, into the flow. When adsorbates are advected along with the fluids into the reactive surface area starting at O_2, the concentration of free adsorbates adjacent to the surface decreases due to the adsorption at the surface. Then the bulk adsorbates spontaneously diffuse toward the surface in response to the concentration gradient across the flow. In general, the coupling of these three processes of advection, diffusion, and adsorption modifies the concentration distribution of adsorbates in the flow.

2 Methods

The fourth term on the right-hand side of Eq. (1), which governs the mode of oscillation, makes the flows much more complicated. Our numerical tests indicate that the general PINNs method fails to handle these situations well. Here, we use the PirateNets, a novel adaptive residual connection architecture that is designed to facilitate stable and efficient training of deep PINNs models, allowing the networks to be initialized as shallow networks that progressively deepen during training [4].

We compare the results trained by PirateNets and simulated by the FDM we developed in Ref. [1] for Eqs.(1) and (2) of oscillatory flow conditions. The parameters for the simulations are listed in Tab. 1. It exhibits typical diffusion-dominant adsorption behavior in Poiseuille flows when $Pe_2 = 0$. We use a uniform mesh in FDM to facilitate the implementation of the numerical algorithm and conduct the mesh independence tests to ensure the computational accuracy in FDM.

Tab. 1: Parameters used in PirateNets and FDM simulations for ADLA processes in oscillatory flows.

Pe_1	Pe_2	α	ϵ	λ	Sc	Da	K_0
30.0	30.0	0.01	0.1	0.0333	16667	10.0	1.0

Let the computational domain be $\Omega = [0,L'] \times [0,H] = [0,30] \times [0,1]$. By denoting the reactive surface length as L, the length before L as l and after as l, the total length L' at the bottom of the computational domain (at axis $y^* = 0$) can be partitioned equally into three parts with $L' = l + L + r$, where $l = L = r = 10$, in the current case.

We implement two types of boundary conditions (B.C.) at the inlet of domain Ω:

$$(I)\quad \text{DirichletB.C.:}\quad c^* = 1, \quad \text{if } x^* = 0 \text{ and } y^* \in [0,H];$$
$$(II)\quad \text{NeumannB.C.:}\frac{\partial c^*}{\partial x^*} = 0, \quad \text{if } x^* = 0 \text{ and } y^* \in [0,H].$$

At the reactive surface, Eq.(2) can be embedded as a boundary condition in Eq. (1), and we have

$$\frac{\partial c^*}{\partial y^*} = Da\left[c_s^*(1-\eta) - \frac{1}{K_0}\eta\right], \quad \text{if } y^* = 0 \text{ and } x^* \in [l, l+L]. \qquad (4)$$

The initial condition of η is set as $\eta = 0$ for $t^* = 0$. Other boundary conditions for c^* are as follows:

$$\frac{\partial c^*}{\partial y^*} = 0, \quad \text{if} \begin{cases} y^* = H \text{ and } x^* \in [0,L'], \\ y^* = 0 \text{ and } x^* \in [0,l), \\ y^* = 0 \text{ and } x^* \in (l+L, L'], \end{cases} \qquad (5)$$

$$\frac{\partial c^*}{\partial x^*} = 0, \quad \text{if } x^* = L' \text{ and } y^* \in [0,H]. \qquad (6)$$

3. Results

Since the flow is oscillatory, the initial distribution of concentration c^* is put at the entry of the adsorption surface, i.e.,

$$c^* = \begin{cases} 1, & \text{if } x^* \in [0,l) \text{ and } t^* = 0, \\ 0, & \text{if } x^* \in [l, L'] \text{ and } t^* = 0. \end{cases} \qquad (7)$$

The aims of setting this initial condition for c^* are twofold: (1) to investigate the effect of the boundary conditions at the inlet on the changing of concentration c^* under steady oscillatory flows, and (2) to know if the PirateNets can capture the transient state of c^* and η as well as the FDM does.

3.1 Dirichlet B.C.

Under the Dirichlet boundary condition, the concentration continuously enters the flow channel at the inlet. We use the parameters listed in Tab. 1 for the demonstrations of c^* and η trained by PirateNets. Figure 2 shows its temporal comparisons with the FDM.

The results demonstrate that PINN training efficiently identifies the depletion zone in diffusion-dominated scenarios, subsequently enabling the prediction of the adsorption rate of adsorbates, denoted

$\partial\eta/\partial t$, at every moment. The concentration field generated by PINN training matches well with that computed by FDM, especially in the adsorption area we are interested in. The global maximum absolute error of c^* often occurs near the front edge and the end of the adsorption interval L, for which it is less than 20%.

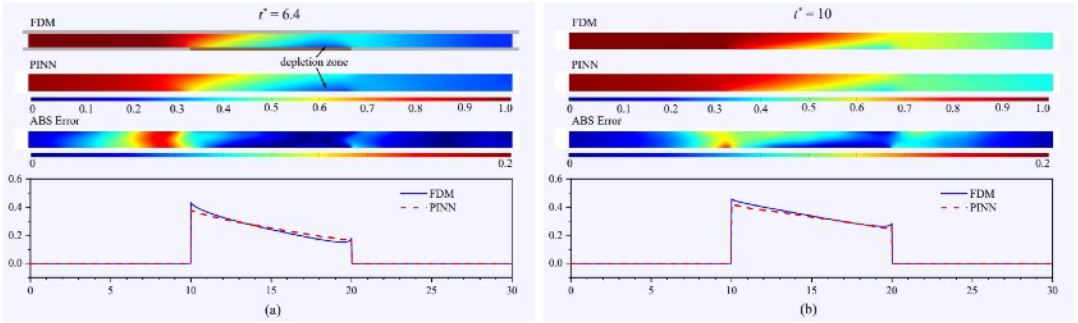

Fig. 2 Comparisons of c^* and η with temporal evolution for predictions by PINNs and computions by FDM. Dirichlet B.C. is applied with the parameters listed in Tab. 1.

3.2 Neumann B.C.

For the Neumann boundary condition, the concentration field c^* is conserved and determined by the initial c^* distribution, as described in Eq.(7). We still use the parameters listed in Tab. 1 for the demonstrations of c^* and η trained by PirateNets. Figure 3 shows its temporal comparisons with the FDM. Compared to Dirichlet B.C., the concentration field c^* with Nuemann B.C. is lower due to the absence of concentration input at the inlet ($x^* = 0$). Under the Nuemann B.C., the PINN method has likewise captured the depletion zone precisely during the time evolution process of c^*. The PINN results with Nuemann B.C. show lower absolute errors than that of FDM, with maximum values not exceeding 11%.

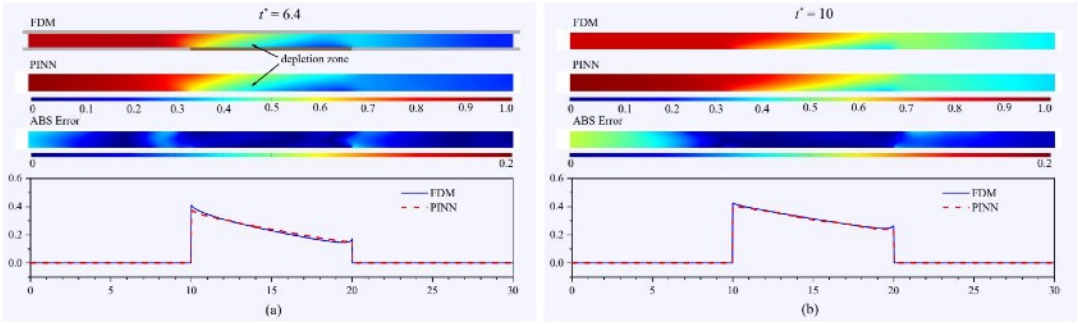

Fig. 3 Comparisons of c^* and η with temporal evolution for predictions by PINNs and computions by FDM. Neumnann B.C. is used with the parameters listed in Tab. 1.

4. Conclusion

By using the stable and training-efficient physics-informed neural networks PirateNets, we solved the advection-diffusion-Langmuir adsorption equations in two-dimensional oscillatory flows with two types of boundary conditions. Considering two kinds of boundary conditions, detailed numerical comparison in the case study shows that this kind of neural networks is highly suitable for such complex flow problems compared to the finite difference method we have developed in the case of diffusion.

This work demonstrates the ability of PINNs to model ADLA processes under dynamic flow conditions, providing an efficient framework for addressing challenges in chemical engineering, biomedical applications, and beyond.

References

[1] B. Huang, H. Hua, H. Han, Q. Wu, M. Zhang, Z. Zuo, S. Liu, Characteristics of advection–diffusion–Langmuir adsorption processes in two-dimensional plane Poiseuille flows, Phys. Fluids 35 (2) (2023) 021904. doi:10.1063/5.0133789.

[2] B. Huang, H. Hua, H. Han, S. He, Y. Zhou, S. Liu, Z. Zuo, Physics-informed neural networks for advection–diffusion–Langmuir adsorption processes, Phys. Fluids 36 (8) (2024) 081906. doi:10.1063/5.0221924.

[3] C. Thomas, A. P. Bassom, P. Blennerhassett, C. Davies, The linear stability of oscillatory Poiseuille flow in channels and pipes, Proc. R. Soc. A: Math. Phys. Eng. Sci. 467 (2133) (2011) 2643–2662.

[4] S. Wang, B. Li, Y. Chen, P. Perdikaris, PirateNets: Physics-informed deep learning with residual adaptive networks, https://doi.org/10.48550/ arXiv.2402.00326 (2024).

Keywords: oscillatory flows, PINNs, FDM, PirateNets, advection-diffusion-Langmuir adsorption