

MODELING OF FILTRATION PROCESS IN COMPLEX FILTER STRUCTURES USING A PHYSICS-INFORMED NEURAL NETWORK COUPLED WITH SMOOTHED PARTICLE HYDRODYNAMIC

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ABSTRACT

Fiber-based structures play a crucial role in technical filtration applications. These structures are inherently complex, characterized by randomly oriented fibres with varying diameters and porosities. Accurately modelling particle deposition within such intricate geometries is challenging—not only due to the irregular structure but also because of the computational effort required for mesh generation. To overcome these limitations, this study introduces an alternative framework that integrates Physics-Informed Neural Networks (PINNs) as flow solvers with Smoothed Particle Hydrodynamics (SPH) for simulating particle interactions within the fibre network. This combined approach allows for the modelling of complex processes such as particle deposition, liquid film formation, and re-entrainment, providing a robust alternative to conventional CFD techniques. PINNs have recently gained significant traction in the fluid mechanics community. Their appeal lies in their unique loss formulation, which embeds governing physical equations (such as the Navier–Stokes equations) and boundary conditions directly into the optimization process without the need for extensive training data. The SPH method, on the other hand, is a mesh-free CFD technique that represents fluids as discrete particles. To accurately capture the filtration process in complex fibre geometries, this work couples the PINN and SPH methods into an integrated framework. This coupling is crucial for handling dynamic domain changes such as local blockages caused by extensive film deposition. Although initial PINN training can be computationally demanding, subsequent time steps benefit from transfer learning, enabling rapid adaptation to geometric updates (including new film layers on fibres). This hybrid PINN–SPH framework provides an efficient and scalable approach for simulating drop-let deposition in three-dimensional fibre structures. The proposed numerical model has been validated against data from single-fibre filtration experiments. The simulation results for complex multi-fibre configurations are presented and analysed in detail, demonstrating the capability and accuracy of the coupled PINN–SPH approach.

KEYWORDS:

physics-informed neural network, smoothed particle hydrodynamic, filtration process, meshless method

Introduction

Since the early development of numerical methods, numerical modelling has become an established alternative to experimental measurements. Computational models offer greater flexibility for parametric studies without requiring modifications to the experimental setup, are generally more cost-effective, and—most importantly—provide reproducible results as well as deeper insights into flow behaviour. Early numerical studies employed simplified models to describe the deposition of solid particles and dendritic growth on a single fibre [1,2] or within small arrays of parallel fibres [3]. With the advancement of more sophisticated CFD techniques, simulations have become increasingly detailed, investigating these processes at the single-fibre level using the finite volume method (FVM) [4], the lattice Boltzmann method [5], and the immersed boundary approach [6,7], as well as within fibre assemblies [8–10]. Research on the filtration of liquid droplets is considerably less extensive because droplets—unlike solid particles—exhibit complex behaviours such as coalescence, breakup, and drainage, which complicate modelling. Consequently, most studies focus on experimental observations [11–13]. Limited numerical investigations include studies of droplet dynamics on a vibrating fibre using the volume-of-fluid method [14,15] and the phase-field approach [16] within the FVM framework, as well as phase-field methods in lattice Boltzmann simulations [17]. Due to this complexity, the investigation of droplet deposition in randomly oriented fibre assemblies remains an open research problem. Conventional CFD methods face important limitations in this context, particularly due to the extensive preprocessing required (e.g., mesh generation for complex filter geometries) and extremely small timesteps imposed by the small length scales of droplets and fibres, which lead to prohibitively long computational times. Machine-learning (ML)-assisted approaches offer an alternative to classical numerical methods and have the potential to address challenges such as high computational cost. Voss et al. [18] employed a U-Net model [19] trained on two-dimensional low-Reynolds-number (Re) flow simulations around arbitrarily shaped cylinders and coupled it with a Lagrangian particle solver. The U-Net predicted the flow field, while the Lagrangian solver computed particle trajectories. This combined approach enables efficient prediction of particle deposition on cylindrical surfaces while accounting for deposition mechanisms such as interception, inertial impaction, and Brownian motion. Other studies have used convolutional neural networks (CNNs), for example for bubble detection and shape reconstruction [20], reconstruction of droplet history from deposition patterns [21], and recognition of liquid–liquid flow regimes [22]. Despite their flexibility and accuracy, these approaches rely on labelled training datasets derived from experimental measurements or numerical simulations. They are therefore particularly suitable as powerful complementary tools for detailed flow analysis or post-processing techniques, but less so as standalone predictive models. Moreover, such models learn flow patterns solely from the training data and do not inherently enforce physical laws, such as conservation equations. This limitation can be critical in many applications. Physics-informed neural networks (PINNs) [23,24] represent a recently developed class of scientific ML algorithms that embed physical constraints—such as the governing equations and the associated boundary and initial conditions—directly into the loss function of a neural network. This integration offers several advantages, particularly in fluid mechanics. By incorporating the Navier–Stokes (N–S) equations into the loss function, PINNs inherently enforce conservation of mass, momentum, energy, and other relevant quantities. Related studies include PINNs trained on sparse clinical data to predict cardiovascular flows [25], PINNs trained on CFD data for a continuously stirred tank reactor [26], and inverse PINNs applied to tomographic background-oriented schlieren (TomoBOS) imaging to reconstruct three-dimensional flow around a hot espresso cup [27]. Modelling filtration processes requires not only resolving the flow field but also tracking particle trajectories and their interactions with each other and with the filter structure. For solid particles, Lagrangian particle tracking is sufficient; however, it does not capture the complex mechanisms of liquid droplet filtration. Smoothed particle hydrodynamics (SPH), in contrast, can represent

droplet dynamics as well as the potential formation of thin liquid films following deposition. Previous studies have demonstrated the effectiveness of SPH for modelling droplet dynamics and thin-film formation [28–30].

In this work, we present a surrogate modelling framework that combines a data-free PINN with SPH to simulate filtration processes based on the work of Zargaran et al. [31]. The PINN computes incompressible three-dimensional flow through complex, randomly oriented fibre assemblies with varying diameters, while SPH resolves droplet dynamics and their interaction with the medium.

Methods and Materials

The modelling strategy and simulation tools employed in this study are described in detail in the following sections.

Simulation methodology

The geometrical complexity of filter elements—including fibres, inter-fibre pores, and deposited droplets or particles—presents significant challenges for conventional mesh-based simulation approaches. These difficulties, together with the need for extremely small time steps to resolve fine-scale interactions, can be efficiently addressed through a surrogate modelling framework, as illustrated in Figure 1. In this framework, a physics-informed neural network (PINN) is initially employed to learn the steady-state flow field based on the filter geometry, provided in the Standard Tessellation Language (STL) format. The computed flow field is subsequently used by a Smoothed Particle Hydrodynamics (SPH) solver to track droplet motion and capture their interactions with the fibres, including phenomena such as drainage and re-entrainment. Time integration within the SPH solver proceeds under the assumption that the droplets do not substantially perturb the background flow (internal loop). When droplet-induced disturbances become significant, the framework triggers an external loop: the updated droplet geometry is extracted from the SPH solver in STL format and incorporated back into the PINN model. Transfer learning is then applied to fine-tune the network over a limited number of epochs—typically 10%–30% of those required for the initial training—since the pre-trained network already provides a close approximation and only minor adjustments are needed. As both PINN and SPH are mesh-free methods, geometric and field information is exchanged seamlessly, eliminating the overhead associated with mesh generation.

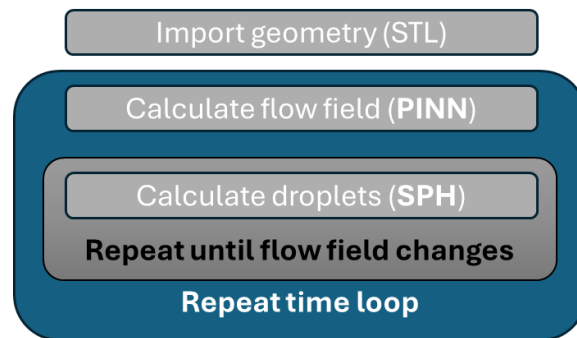


Figure 1: Coupled modelling approach of PINN and SPH

Simulation model

The simulation domain is shown in Figure 2 (left). The channel has dimensions of $100\ \mu\text{m} \times 30\ \mu\text{m} \times 30\ \mu\text{m}$. In this study a gradient of the filter structure is applied consisting of three distinct regions with increasing mean diameters of the fibres in flow direction ranging from 1.5

– 2.25 – 3 μm , The corresponding normal distribution of each of the three classes can be seen as well in Figure 2 (right). Since the channel represents a representative volume element of a larger filter, the surrounding channel walls are assigned a free-slip velocity boundary condition. Specifically, the normal component of the velocity vector ($\mathbf{u}_n$) and the normal gradient of the tangential velocity components ($\partial \mathbf{u}_t / \partial n$) are set to zero at these boundaries. At the inlet, a uniform gas velocity of $u_{\text{inlet}} = 0.35 \text{ m/s}$ is prescribed. Due to the open channel configuration, the flow profile at the inlet remains unaffected by wall interactions. At the outlet, a reference pressure of $p_{\text{outlet}} = 0 \text{ Pa}$ is imposed, with the gas flowing along the positive x -direction. No-slip boundary conditions are enforced on the fibre surfaces. Hydrogen is used as the carrier gas and oil as the dispersed droplet phase, reflecting conditions relevant to gas transport in hydrogen pipelines and potential lubricant contamination. Both phases are treated as Newtonian, incompressible, and isothermal, with constant properties for oil, $\rho_{\text{oil}} = 900 \text{ kg}\cdot\text{m}^{-3}$ and $\mu_{\text{oil}} = 9\cdot 10^{-2} \text{ Pa}\cdot\text{s}$; for hydrogen, $\rho_{\text{hydrogen}} = 0.0826 \text{ kg}\cdot\text{m}^{-3}$ and $\mu_{\text{hydrogen}} = 8.788\cdot 10^{-6} \text{ Pa}\cdot\text{s}$. The SPH solver captures the principal mechanisms governing droplet–fibre interactions, including coalescence, thin-film formation, and drainage. Evaporation effects are neglected in the present simulations.

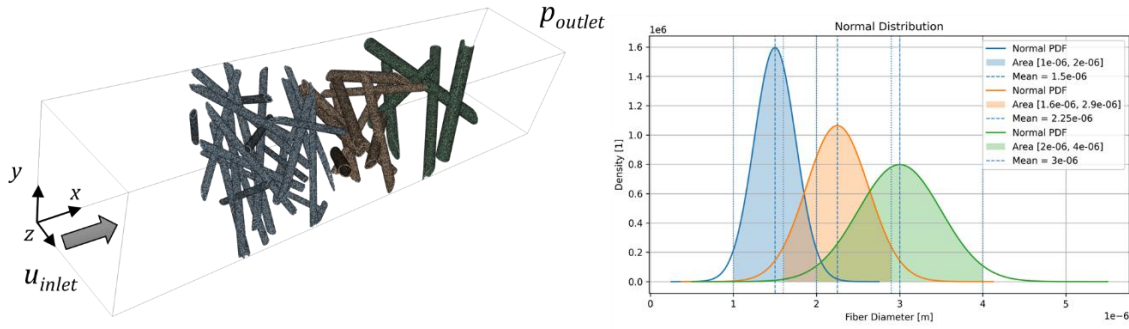


Figure 2: Left: Simulation model of a filter structure with a changing gradient of the fibre diameter in flow direction, right: Normal distribution of the fibre diameter in the three distinct regions

The flow is assumed to be isothermal, incompressible as well as steady-state, leading to the mass and momentum balances for the three-dimensional flow field $\mathbf{u}$:

$$\nabla \cdot \mathbf{u} = 0 \quad \text{Eq. 1}$$

$$\mathbf{u} \cdot \nabla \mathbf{u} = -\frac{1}{\rho} \nabla p + \nu \Delta \mathbf{u} \quad \text{Eq. 2}$$

with the pressure p , and the kinematic viscosity ν of the gas.

Physics-Informed Neural Network

The Physics-Informed Neural Network (PINN) architecture employed in this study is designed to take as input the spatial coordinates of collocation points distributed throughout the simulation domain and to predict the corresponding velocity components and pressure field. Boundary conditions (BCs) are enforced in a soft manner: Rather than applying transformations to strictly satisfy BCs (commonly referred to as hard BCs), these conditions are incorporated into the network's loss function as additional penalty terms ($\mathcal{L}_{\text{BC}}$), alongside the residuals of the governing Navier–Stokes equations ($\mathcal{L}_{\text{PDE}}$). Soft enforcement provides substantial flexibility, allowing the network to approximately satisfy boundary constraints while maintaining a balance between accuracy and training stability. For domains with a single inlet and outlet, mass conservation requires that the mass flow rate across any cross section perpendicular to the x -axis

remains equal to the inlet flow rate. Under the incompressibility assumption, this condition reduces to a constant volumetric flow-rate constraint. To incorporate this requirement, volumetric flow-rate constraints were imposed at multiple cross sections, and their contributions ($\mathcal{L}_{\text{VFR}}$) were included in the total loss function. Prior work has demonstrated that such constraints enhance training performance and reduce the risk of convergence to suboptimal solutions [34]. The overall training objective is thus defined as a composite loss function:

$$\mathcal{L}_{\text{PINN}}(\theta) = \mathcal{L}_{\text{PDE}}(\theta) + \mathcal{L}_{\text{BC}}(\theta) + \mathcal{L}_{\text{VFR}}(\theta) \quad \text{Eq. 3}$$

While a standard PINN is theoretically capable of capturing the general characteristics of the flow considered here, it may exhibit limited accuracy in regions with complex geometric features, such as narrow pores between fibres. This limitation is commonly attributed to the spectral bias of neural networks [35], which describes the tendency of networks to learn low-frequency components of a target function more efficiently than high-frequency components. As a result, accurate convergence to high-frequency features is not guaranteed, even when deeper architectures or extended training are employed. A well-established strategy to mitigate spectral bias is input encoding, wherein input variables are transformed into a higher-dimensional feature space using high-frequency functions. This Fourier feature embedding allows the network to more accurately capture high-frequency variations in the target solution [32]. For fluid flow through densely packed filters, where local accelerations and steep velocity gradients are prevalent due to variable pore sizes, FF-NNs enhance predictive accuracy by effectively resolving these high-frequency flow features. Figure 3 schematically illustrates the architecture of a physics-informed model employing a FF-NN as the function approximator for steady-state three-dimensional flow, trained using the physics-informed loss formulation described above [31].

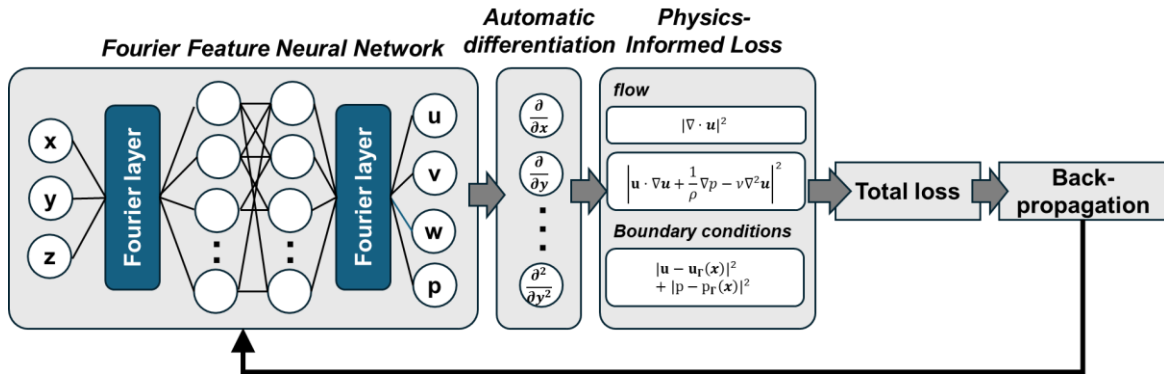


Figure 3: Schematic representation of Physics-Informed Neural Network architecture

Smoothed-Particle Hydrodynamics

Droplet motion is modelled using a mesh-free smoothed particle hydrodynamics (SPH) approach [33]. Within this framework, a field variable A is initially represented as a continuous integral approximation using a smoothing kernel with smoothing length h , which defines the spatial extent of each particle's influence (Eq. (4)). This continuous formulation is subsequently discretized by summation over neighbouring particles, yielding a particle-based approximation (Eq. (5)), where m_j and ρ_j denote the mass and density of particle j , and $\mathbf{r}_i$ and $\mathbf{r}_j$ represent the positions of particles i and j , respectively.

$$\langle A(\mathbf{r}) \rangle = \int A(\mathbf{r}') \mathcal{W}(\mathbf{r} - \mathbf{r}', h) d\mathbf{r}' \quad \text{Eq. 4}$$

$$\langle A(\mathbf{r}_i) \rangle = \sum_j \frac{m_j}{\rho_j} A_j \mathcal{W}(\mathbf{r}_i - \mathbf{r}_j, h)$$

Eq. 5

Results and discussion

The flow velocities and the pressure in the filter without particle loading is shown in Fig. 4 for a cross section in the middle of the filter.

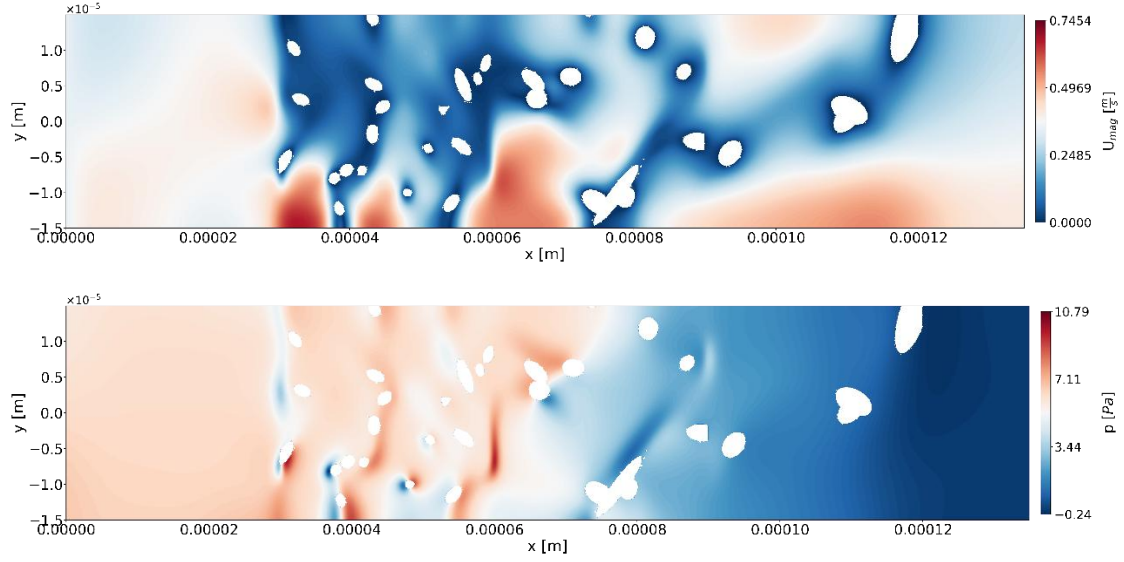


Figure 4: Magnitude of the velocity (top) and the pressure (bottom) in a cross section in the middle of the filter media before loading. Flow direction is from left to right

After the loading of the filter, Fig. 5 shows the filter structure with 33 particles. The diameters of the droplets have a diameter between 0.7 to 1.3 times the diameter of the fibres.

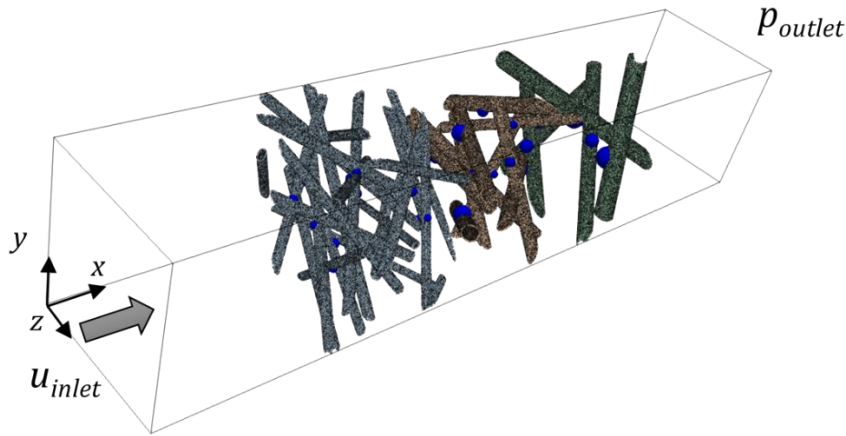


Figure 5: Simulation model of the filter geometry with deposited droplets.

Fig. 6 shows the corresponding flow field (velocity magnitude and pressure) in the filter media for a cross section in the middle of the filter media. Compared to Fig. 4, one can see the increase of the maximum velocity as well as for the pressure drop (approx. 2 Pa) for the loaded filter media although the small number of particles in the filter media.

A detailed validation of the PINN model for a constant diameter of the fibres can be found in Zargaran et al. [31].

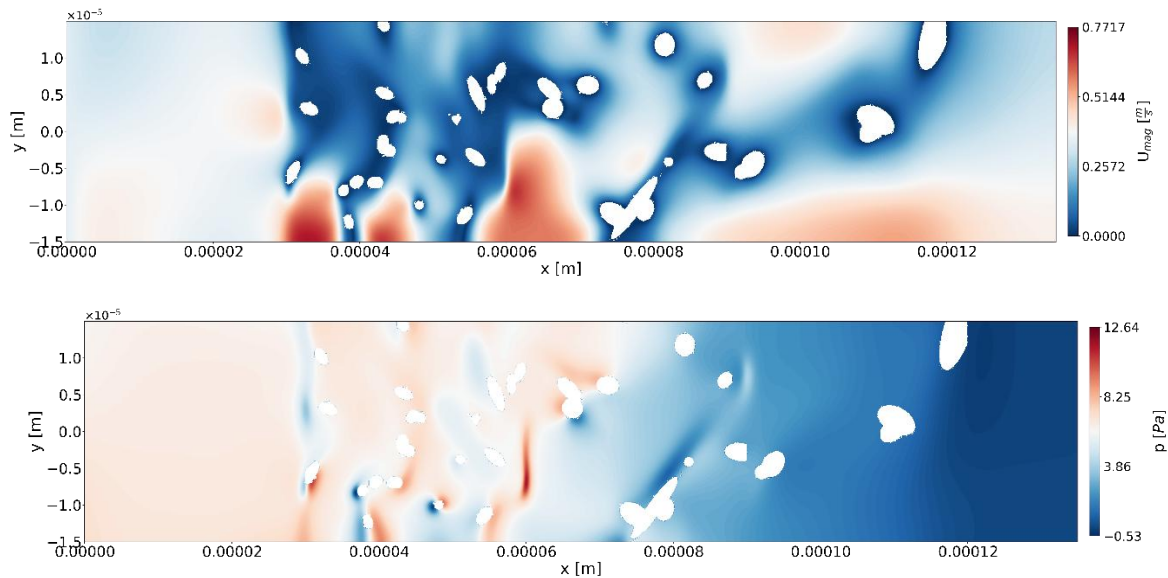


Figure 6: Magnitude of the velocity (top) and the pressure (bottom) in a cross section in the middle of the loaded filter media. Flow direction is from left to right

Conclusion and outlook

A surrogate modelling framework for simulating gas–liquid filtration was developed, coupling a physics-informed neural network (PINN) with smoothed particle hydrodynamics (SPH). Within this framework, a modified Fourier feature neural network (FFNN) is employed to learn the steady-state three-dimensional velocity and pressure fields within complex fibrous structures directly from the Navier–Stokes equations, without reliance on labelled training data. The present study demonstrates the capability of PINNs to accurately represent both the flow field and droplet deposition in gradient-based fibre assemblies.

Future work will extend this approach to filters of greater depth, with the aim of providing more comprehensive insights into particle transport and capture mechanisms in deep filtration systems.

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