Heuristic Modeling of Material Properties in Nano/Angstrom-Scale Channels: Integrating Experimental Observations and MD Simulations

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Abstract

In this paper, we propose a unified framework to describe three key atomic-scale fluid properties—density, viscosity, and slip length—within nanoscale channels. These properties, which deviate significantly from bulk behavior, are expressed using simple power-law models as functions of the nanochannel height. The proposed framework accurately captures experimental and simulation data, providing a more flexible and interpretable alternative to existing complex or disparate models. The key advantage of our model lies in its mathematical properties. Continuity and a continuous derivative ensure seamless implementation into numerical simulations and theoretical predictions, leading to more understandable, stable, and accurate results. Additionally, the model adheres to physical principles, predicting convergence to bulk properties as channel size increases. Further, compared to existing exponential models, the unified power-law modeling approach provides several advantages. It offers flexibility by capturing nonlinear relationships and diverse data curvatures, interpretability with physically meaningful parameters, and adaptability to integrate with other functions for modeling complex phenomena. Its simplicity facilitates easy parameter estimation, model interpretation, and computational efficiency. Moreover, its robustness makes it less sensitive to outliers and noise while maintaining fewer parameters that directly relate to underlying physics and scaling laws. Hence, the proposed model's simplicity, smoothness, physical validity, and generality make it a significant heuristic model for efficient design and optimization of nanoscale devices using theory and simulations across a wide range of applications.

Keywords: Nanoconfined properties, nano/Angstrom-size channels, power-law models, modeling Density, modeling viscosity, modeling slip, nanochannel-based modeling, heuristic modeling, experimental observations, Molecular dynamics simulations.

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1 Introduction

The rapid advancement of nanoscale technology has led to a growing interest in understanding how fluids behave within these confined environments [1–7]. At the nanoscale, fluids exhibit unique behaviors that challenge traditional assumptions, such as uniform density, no-slip boundary conditions, and even the validity of the Navier-Stokes equations [6]. When the dimensions of confinement shrink to the scale of individual molecules, fluid behavior shifts significantly. Instead of behaving as a continuous medium, fluids begin to reveal the discrete movement of individual molecules. These nanoconfined fluids exhibit transport properties that differ from those of bulk fluids, highlighting the need for precise characterization to support a variety of applications [8–10].

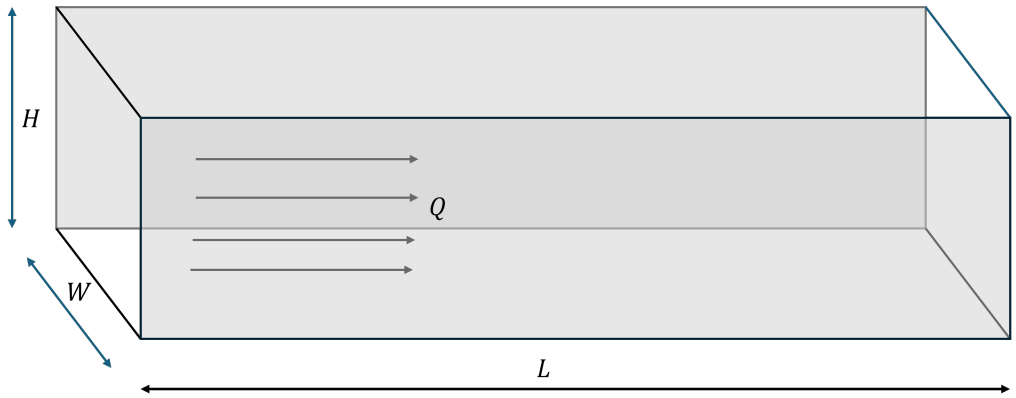

Figure 1: Schematic diagram of the flow Q in a nanochannel with length L and the height H.

The challenges of conducting atomic-level experiments have elevated molecular simulations to a critical role, complementing both theoretical and experimental approaches in studying nanoconfined fluids [11, 12]. Among the key findings is the significant impact of geometric dimensions—such as the height of a nanochannel (illustrated in Figure 1, showing fluid flow Q through a nanochannel of length L and height H)—on the material properties of confined fluids. Critical parameters like density (ρ), viscosity (η), and slip length (λ) are influenced by these dimensions [6, 7, 12, 13].

To better understand and predict these properties, it is essential to develop a consolidated modeling approach that links fluid properties to nanochannel dimensions. While Garg and Bishnoi [14] proposed a generic, user-friendly model for predicting fluid behavior in nanotubes, a comparable unified framework for nanochannels remains unavailable. Our review of existing literature reveals an intriguing discrepancy: in nanotubes, density and viscosity tend to increase with diameter, whereas in nanochannels, these properties often show an inverse relationship, decreasing as the channel size increases.

This contrast underscores the need for further research to create a simple, unified, and versatile model that accurately captures the behavior of fluids confined within nanochannels. Such a framework would significantly enhance our ability to understand and design nanofluidic systems.

This paper addresses these challenges by proposing a generic, unified power-law model for key nanoconfined fluid properties: density, viscosity, and slip length. The model's advantages include:

- Flexibility to describe non-linear relationships and diverse data trends.
- Simplicity for parameter estimation and computational implementation.
- Robustness against noise and outliers, ensuring reliable predictions.
- Adherence to physical principles, predicting convergence to bulk properties with increasing channel size.

1.1 Mathematical background

Various functional forms have been proposed and employed to model these material properties in the nanochannels. In one such modelling effort, Angelis et al. [15] employed a genetic programming-based method of symbolic regression, to obtain data-based mathematical relations based on existing molecular dynamics simulation data. They proposed a model for viscosity,

$$\eta = \eta_0 [e^{\epsilon_{wf}/\epsilon_{ff}(-u_1 F_{ext}+1)} e^{u_2}]^{1/H}, \tag{1}$$

where, η_0 is the bulk viscosity, the ratio $(\epsilon_{wf}/\epsilon_{ff})$ corresponds to flow between hydrophobic walls when it is closer to zero, and hydrophilic walls when it closer to unity. F_{ext} is the external force applied to every fluid particle to simulate the flow. u_1 and u_2 are constants with values of 1.6 and 0.39. Its evident that, the viscosity is strongly dependent on the channel height. In another modelling effort, Neek-Amal et al. [12] demonstrate the profound influence of the density and viscosity of water inside graphene nanocapillaries on the water flow rate, and proposed a channel height dependent model of viscosity

$$\eta = \eta_0 (1 + b e^{-H/\delta}), \tag{2}$$

where b and δ are the fitting parameters, η_0 is the bulk viscosity. The model was used to support the experimental findings of Radha et al. [6]. Their Molecular dynamics simulations consistently support the notion that water flow within nanochannels adheres to the slip-modified Hagen-Poiseuille relation. This finding is particularly interesting because it suggests higher flow rates compared to those predicted by the traditional no-slip Hagen-Poiseuille relation [16–20], which assumes water molecules stick to the channel walls. Also, Israelachvili [13] experimentally calculated the viscosity of tetradecane and water between two mica sheets placed at distances lower than 50 Å and proposed that the viscosity of water/tetradecane can be calculated using

$$\eta = \frac{KH}{\pi^2 r^2 \nu} [(A/A_0)^2 - 1]^{1/2}, \tag{3}$$

given the experimental parameters A_0, A, and ν are oscillation amplitudes and frequency used in experiment. The curve radius r is at which the plates are mounted in their experimental apparatus. The K is the spring constant from the apparatus and H is the separation

height between the two mica sheets. Further, Rudyak and Belkin [21] studied the viscosity of fluids in plane nanochannels using molecular dynamics method. They proposed the following model (equation 4) for viscosity variation of Argon in plane nanochannel made with carbon (increasing viscosity) and aluminium (decreasing viscosity) with increasing height of the nanochannel,

$$\eta = \eta_0 \left(1 \pm \frac{B}{H}\right), \tag{4}$$

in which the constant B depends on the properties of the fluid and the walls. Furthermore, Tu et al. [22] studied the viscosity of Argon between two platinum walls using Molecular dynamics simulations. They proposed a viscosity model dependent on the Knudsen number and channel-height ($Kn = k/H$, where k is the mean free path of Argon and H is the distance between the two platinum plates) as,

$$\eta = \eta_0 \left(\frac{H}{\alpha_\eta k}\right). \tag{5}$$

where, η_0 is the bulk viscosity and the α_η is a constant.

Similarly, the density in nanochannels changes depending on the height of the channel. Neek-Amal et al. [12], similar to their model for viscosity, proposed a model for density as given by

$$\rho = \rho_0(1 + a^{-H/\delta}). \tag{6}$$

where a and δ are constants obtained by fitting their Molecular dynamics simulations data and the experimental data by Radha et al. [6] in graphene nanochannels of heights H $\in$ [6.5 Å to 16 Å] and length 50 Å. The density behaves much in the same way as of viscosity as it increases as the channel height decreases and approached its bulk value as the channel height increases. Further, Shadloo-Jahromi et al. [23] calculated the density of water between two silicon sheets separated by distance H $\in$ [6 Å to 21 Å]. In their simulations, they used the following model density vs sheet separation height as,

$$\rho = \frac{(m_{\text{oxygen}} + 2 \times m_{\text{hydrogen}}) \times 10 \times N_w}{AB_a(H - t)}, \tag{7}$$

where, N_a is Avagadro's constant and $m_{\text{oxygen}} = 15.994$ and $m_{\text{hydrogen}} = 1.008$ are the molecular weight of oxygen and hydrogen, respectively. A is the cross-sectional area fixed in the study at 45.9165×38.264 Å^2. t is a constant to take care of the volume fraction covered by the silicon sheets, it's value is considered to be 1 Å.

Furthermore, similarly the slip length in nanoconfined channels changes depending on the height of the channel. Yen et al. [24] proposed that the slip length (λ) is given by

$$\frac{\lambda}{H} = 6.234 \left(\frac{H}{\sigma}\right)^{-1.033}, \tag{8}$$

where, $\sigma \approx 0.34$ nm is the molecular length scale. They used a hybrid molecular dynamics-continuum simulation with the principle of crude constrained Lagrangian dynamics for data

exchange between continuum and Molecular dynamics regions to resolve the Couette and Poiseuille flows with the channel heights falling in range H $\in$ [46σ to 400σ]. In another study, Yang and Zheng [25] investigated a wide range of cases of the channel flow problem by using either pure Molecular dynamics simulation or the hybrid molecular-continuum scheme. The focus of the study was on the influence of shear rate on the slip length and the channel scale effect on slip length under different shear rates. They proposed a log based direct relation between the slip length and the nanochannel height as

$$\log(\lambda/H) = -1.447\log(H/\sigma) + 1.79, \tag{9}$$

where, $\sigma \approx 0.34$ nm is the molecular length scale. For channel-height larger than 100σ, they proposed a similar relation with slightly modified coefficients as

$$\log(\lambda/H) = \log(H/\sigma) + 0.7. \tag{10}$$

Further, Kargar and Lohrasebi [26] studied the water flow in graphene-based channels using Molecular dynamics simulation and proposed that the slip length of water in the nanochannel is given by

$$\lambda = a\left(1 + \frac{a}{H}\right), \tag{11}$$

where a is a parameter also dependent on channel height to be obtained from the molecular simulation data. They studied graphene-based channels of sizes H $\in$ [10 Å to 15 Å]. The parameter a varied from 30 nm to 36 nm, respectively. Further, Kumar Kannam et al. [27] in an effort to understand the wide scatter in values of flow rates in nanopores aimed at precisely quantifying the characteristic slip length and flow rate of water flowing in a planar graphene nanochannels and proposed a slip length relation for Couette flow as

$$\lambda = \frac{mH}{1-2m}, \tag{12}$$

where m is the slope of slip velocity vs wall velocity plot. In the same study, they proposed another model for Poiseuille flow between two graphene sheets as

$$\lambda = \frac{2m\eta_0}{\rho H}, \tag{13}$$

where η_0 is bulk viscosity, ρ is density of the fluid and the m is the slope on the plot of slip velocity vs wall velocity. Further, Angelis et al. [15], similar to their model for viscosity, also proposed a model for slip length as

$$\lambda = \frac{w_2(m_w/m_f)^2 e^{-w_3(\epsilon_{wf}/\epsilon_{ff})^4}}{H}, \tag{14}$$

where m_w/m_f is the wall to fluid mass ratio, w_2 and w_3 are the constants with values of 1.3 and 4, respectively. The ratio $(\epsilon_{wf}/\epsilon_{ff})$ corresponds to flow between hydrophobic walls when it is closer to zero, and hydrophilic walls when it closer to unity.

The results and proposed models of various previous studies have shown that nanochannel height plays a crucial role in determining critical fluid properties. Additionally, researchers have utilized a range of models and equations to fit density, viscosity, and slip length, which has led to confusion and made it difficult to determine the most appropriate model to incorporate in numerical simulations. To address this issue, In this paper, we proposes a generic and simple power-law model for the material properties in the nanochannels that can be utilized to model all these properties such as density, viscosity, and the slip length of the fluids in nanoconfined channels.

The remainder of this paper is structured as follows: In Section 2, we provide the proposed methods and models for the power-law model, including equations for density, viscosity, and slip length. Section 3 presents the results of fitting experimental and Molecular dynamics simulation data using the proposed model, highlighting its accuracy and versatility. Finally, in section 4, the conclusions summarize the significance of the work and potential future directions.

2 Proposed methods and models

This section outlines the mathematical framework underpinning the proposed unified power-law model for density, viscosity, and slip length. The equations for density, viscosity, and slip length are derived through a combination of empirical understanding, scientific intuition, and insights gained from extensive studies of nanoconfined fluid [14] and non-Newtonian complex fluid [28] systems. These models are not the result of chance but rather the outcome of iterative refinement informed by data and observed trends. The parameters are further optimised based on the previous experimental and molecular dynamics simulation data. These models are derived to capture the dependence of material properties on the height of nanochannels (H), leveraging parameters with clear physical interpretations. The proposed equations are chosen not just because they fit the data well but also because they follow important physical principles. Power-law models are smooth and continuous, making them easy to use in computational simulations. They also behave correctly in extreme cases, such as predicting that fluid properties will return to their typical bulk values when the channel height becomes very large. Additionally, these models are reliable because they can handle noisy data and adapt to different systems, making them both practical and scientifically sound.

2.1 Density Model

The density of a nanoconfined fluid, $\rho(H)$, is modeled as:

$$\frac{\rho(H)}{\rho_0} = 1 + m_1 H^{-n_1}, \tag{15}$$

where ρ_0 represents the bulk density at $H \implies \infty$, and m_1, n_1 are fitting parameters. The power-law exponent n_1 quantifies the sensitivity of density to channel height, while m_1

scales the deviation from bulk behavior. We find that the proposed model's continuity and continuous derivative ensure its suitability for numerical simulations.

2.2 Viscosity Model

The viscosity of a nanoconfined fluid, $\eta(H)$, follows:

$$\frac{\eta(H)}{\eta_0} = 1 + m_2 H^{-n_2}, \tag{16}$$

where, $\eta(H)$ represents the channels's height-dependent viscosity of the fluid. The η_o is the bulk viscosity at $H \implies \infty$. m_2, n_2 are the free parameters. This model captures the non-linear dependence of viscosity on confinement dimensions. The power-law index n_2 shows the channel height dependence. The proposed model's key advantage for numerical simulations lies in its continuity and continuous derivative. These properties guarantee smooth and stable calculations. By possessing both continuity and a continuous derivative, the proposed model is well-suited for numerical simulations. This allows for efficient computations without encountering discontinuities that can hinder calculations.

2.3 Slip Length Model

The slip length $\lambda(H)$ is expressed as:

$$\lambda(H) = \lambda_0 + m_3 H^{-n_3}, \tag{17}$$

where, $\lambda(H)$ is the channel's height -dependent slip length of the fluid. The λ_o is the slip of the bulk at $H \implies \infty$. m_3 and n_3 are free parameter and captures the specific behavior of the fluid's slip in confinement. The power-law exponent (n_3) reflects the dependence of slip-length on the channel height (H). A key advantage of the proposed model for numerical simulations lies in its continuity and continuous derivative. These mathematical properties ensure smooth and efficient computations without encountering discontinuities that can disrupt calculations. In simpler terms, the model's inherent smoothness allows for stable and accurate numerical simulations.

The proposed power-law models are continuous and differentiable, ensuring compatibility with numerical simulations. Additionally, they are robust against data variability, allowing accurate predictions even for noisy or incomplete datasets. The simplicity of these models facilitates their integration into broader theoretical and computational frameworks.

3 Results and Discussion

Section 2 established the theoretical foundation for the unified power-law models. Here, we demonstrate their effectiveness by fitting experimental and molecular dynamics simulation data for density, viscosity, and slip length. The results validate the model's versatility, providing insights into fluid behavior across various nanoconfined systems. The power-law

model proposed in this study has several advantages over the exponential model proposed by Neek-Amal et al. [12] in various contexts. The power-law model provides more flexibility in describing a wide range of behaviors compared to the exponential model. It can capture nonlinear relationships and accommodate diverse datasets with varying degrees of curvature. Power-law relationships are often easier to interpret and understand intuitively, especially in scientific and engineering contexts. The parameters in the power-law model (e.g., exponent, coefficient) have clear physical meanings, making it easier to relate them to underlying mechanisms or phenomena. Power-law models can sometimes be combined with other functions to create more complex relationships. This allows for greater flexibility in describing real-world phenomena. On the other hand, exponential models are generally less adaptable for such modifications. Power-law relationships are prevalent in various natural and social phenomena, including fluid dynamics, material science, biology, economics, and sociology. The ubiquity of power-law behavior across different disciplines makes the power-law model a versatile tool for modeling and analysis. The mathematical form of the power-law model is relatively simple, involving straightforward algebraic operations such as multiplication and exponentiation. This simplicity facilitates parameter estimation, model interpretation, and computational efficiency compared to more complex models. Power-law models excel at capturing nonlinear dynamics and emergent phenomena in complex systems. They can describe scale-free behaviors, self-organization, and critical phenomena that are common in natural and social systems. Power-law relationships tend to be more robust against outliers and noise in the data compared to exponential relationships. This robustness makes the power-law model more reliable for fitting experimental or observational data, particularly in situations where data quality may be variable. Power-law models often involve just a few parameters, typically an exponent and a scaling factor. This makes them easier to interpret and relate to the underlying physical processes compared to exponential models which might require more complex parameterization.

By using our proposed simple, generic, single power-law model, we are able to fit a variety of experimental and molecular dynamics simulation data from the literature, even though for which multiple models had previously been used to model the same material property from the data. Our suggested model demonstrates excellent agreement with multiple independent datasets observed from both in the experimental observations and molecular dynamics simulations. Additionally, the model possesses the advantages of continuity and a continuous derivative, making it highly suitable for integration into numerical simulations [29]. Furthermore, our proposed model also adheres to far boundary conditions, meaning that when the channel height approaches infinity, the material properties tend to converge with the bulk properties of the fluid. Given the model's simplicity, smoothness, and versatility, this approach holds great potential for utilization in simulations and theory predictions. In section 3.1, we model the density. In section 3.2, we model the nanoconfined viscosity in the nanochannel. In section 3.3, we model the slip length.

3.1 Density of nanoconfined fluid in the nanochannel

In order to make the modelling effort simpler and more efficient, we need a consolidated model which can model all experimental or Molecular dynamics simulation data researchers obtained on fluid density in the nanochannels. For that, we propose a general nanochannel height-dependent power-law model with additional free parameters as earlier mentioned in equation (15) as $\frac{\rho(H)}{\rho_o} = 1 + m_1 H^{-n_1}$.

In figure 2(a-i), we show various previous density data of the fluid flowing in the nanochannels with blue circles, which are fitted with the proposed model equation (**??**) as shown with the red solid line. In figure 2(a), we show the data by Yousefi et al. [33] who employed equilibrium molecular dynamics simulation to explore the density and viscosity of hydrogen molecules (H_2) when subjected to extreme confinement within a nanochannel made by graphene sheets. The seperation between the graphene sheets was varied between 0.6 to 3 nm. Further, Barisik and Beskok [34] studied force driven isothermal flow of Argon gas. The cross section of the channel was kept constant at 54 $\times$ 54 nm^2. The height was varied between 5.4 nm to 54 nm at fixed Knudsen number and the density of the fluid is shown in figure 2(b). In figure 2(c), the Barisik and Beskok [35] studied force driven isothermal flow of Argon gas. Multiple cross sections of the channel like 27 $\times$ 27, 54 $\times$ 54, 108 $\times$ 108, 162 $\times$ 162, 216 $\times$ 216 nm^2 were used. The height was varied between 5.4 nm to 54 nm. Three different channel heights 10.8, 27, 54 nm were simulated at varied Knudsen number and the density data is shown.

Further, Wang et al. [30] studied water flow through graphene naochannels using Molecular dynamics simulations. The length and width of the channel were kept constant at 30 nm and 4.5 nm. The height was varied between 0.6 nm to 3.5 nm and the density data with blue circles are shown in figure 2(d). Also, Ghorbanian et al. [31] studied force driven flow of Argon through gold nanochannel. The height of the channel was varied from 1.63 nm to 35.89 nm with density data shown in figure 2(e). Furthermore, Mosaddeghi et al. [32] used molecular dynamics simulations to study the structure, dynamics, and transport properties of nano-confined water between parallel graphite plates with separation distances (H) from 7 to 20 Åwith density data shown in figure 2(f).

We also fitted the data by Kargar and Lohrasebi [26] in figure 2(g), who studied water flow through graphene nanochannels using Molecular dynamics simulations. The length of the channel was kept constant at 52 Å and height of the channel was varied between 10 Å to 15 Å. Neek-Amal et al. [12] studied water flow through graphene nanochannel using Molecular dynamics simulations. The length and width of the channel were kept constant at L = 50 Å and W = 20 Å. Height of the channel was varied between 6.5 Å to 16Å. The density data is shown in figure 2(h). Further, Radha et al. [6] studied water flow between two sheets of graphene experimentally. The channel width was kept constant at $W \approx$ 130 nm. The length was varied between 2 μm and 10 μm. The channel height was varied between 0.6 nm to 10 nm and the density data is shown in figure 2(i).

Table 1 summarizes the fitting process of all these density data for fluids flowing in nanochannels. The data were originally modeled using various approaches and different mod-

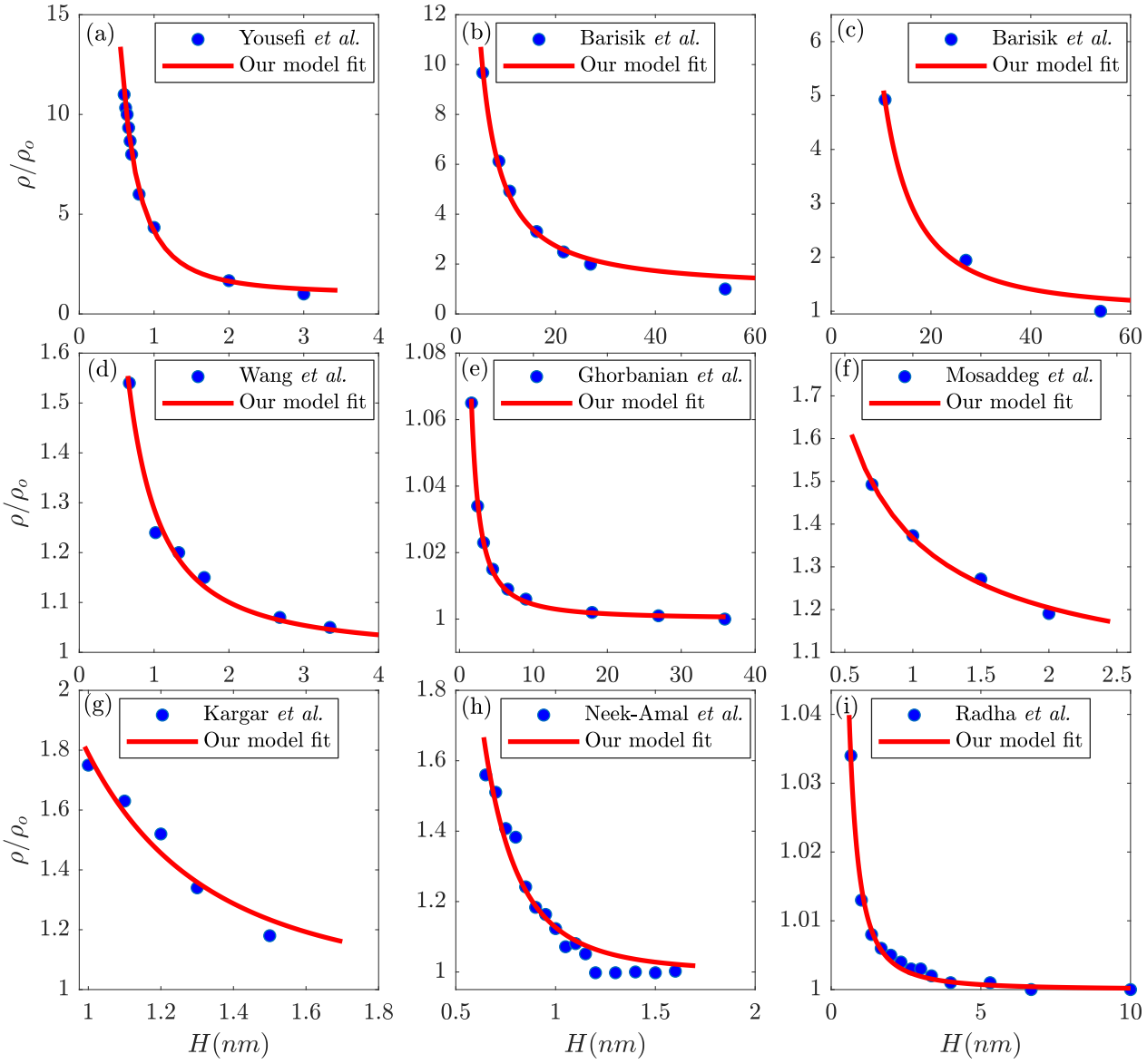

Figure 2: Comparison of the fitted density using our proposed model with the data in the literature by Kargar and Lohrasebi [26], [12], Radha et al. [6],Wang et al. [30], Ghorbanian et al. [31], Mosaddeghi et al. [32], Yousefi et al. [33], Barisik and Beskok [34], and Barisik and Beskok [35].

els in these study. We have re-evaluated this data predictions using our proposed model, resulting in the parameter values (m_1 and n_1) shown in the table. Additionally, we calculated the regression coefficient (R^2) for each fit, which is also included in the table. The R^2 values range from 0.95 to 0.99 for all studies, indicating an excellent fit of the proposed model to the entire data set. These results suggest the robustness of the proposed model, demonstrating its ability to effectively fit a wide range of fluid density data across various

S. No	Author	m_1	n_1	R^2
(a)	Yousefi et al. [33]	3.146	2.293	0.99
(b)	Barisik and Beskok [34], Fixed Knudsen Number = $(\sqrt{\pi}/2)$	71.89	1.244	0.99
(c)	Barisik and Beskok [35]	235.8	1.724	0.99
(d)	Wang et al. [30]	0.2881	1.519	0.98
(e)	Ghorbanian et al. [31]	0.1326	1.476	0.99
(f)	Mosaddeghi et al. [32]	0.3674	0.8464	0.99
(g)	Kargar and Lohrasebi [26]	0.7878	2.977	0.95
(h)	Neek-Amal et al. [12]	0.1267	3.721	0.95
(i)	Radha et al. [6]	0.0152	1.89	0.99

Table 1: Density data for fluids flowing in nanochannels and its fit with the proposed model

nanochannel configurations. Also, the excellent fit achieved across the data set implies the proposed model's generalizability. It can accurately capture the behavior of diverse fluid densities within nanochannels. In summary, the broad range of successfully fitted data highlights the robustness and generalizability of the proposed model for nanochannel fluid densities.

3.2 Viscosity of nanoconfined fluid in the nanochannel

Building upon the previously discussed nanochannel height-dependent models for nanoconfined viscosity (η) in the introduction, this section seeks a unified approach. These existing models attempt to capture the relationship between viscosity and channel height (H). Similar to the approach taken for nanoconfined density in the previous section, we propose a consolidated model for viscosity that encompasses a wider range of experimental and Molecular dynamics simulation data. This model leverages a power-law dependence on channel height (H) with additional free parameters to capture the specific behavior of different fluids. The proposed model is expressed as earlier mentioned in equation (16) as $\dfrac{\eta(H)}{\eta_o} = 1 + m_2\ H^{-n_2}$.

In figure 3(a-i), we show various previous viscosity data of the fluid flowing in the nanochannels with black circles, which are fitted with the proposed model equation (16) as shown with the magenta solid line. In figure 3(a-c), we show the data by Sofos et al. [38] who calculated the transport properties of liquid argon flowing through a nanochannel formed by krypton walls. Non-equilibrium molecular dynamics simulations are performed assuming flow conditions corresponding to the macroscopic equivalent of planar Poiseuille flow. They examined the effect of channel width and system temperature on diffusion coefficient, shear viscosity and thermal conductivity. The channel height was varied between 0.9 nm to 6.3 nm. Three different system temperatures of 100 K, 120 K, and 150 K as shown with the respective data in figures (a), (b), and (c), respectively, were employed in the study. Rudyak and Belkin [37] investigated the viscosity of Argon and Benzene in nanochannel made using carbon and aluminium using molecular dynamics simulation. The effective viscosity coefficient was determined using the nonequilibrium statistical theory. They found that the viscosity of argon

and benzene increases as the channel height decreases as shown in figure 3(d). However in carbon nanochannel, the viscosity of benzene decreases with decreasing channel height. They model the viscosity using equation (4). Further, Kargar and Lohrasebi [26] studied water flow through graphene naochannels using Molecular dynamics simulations. The length of the channel was kept constant at 52 Å and height of the channel was varied between 10 Å to 15 Åand the data is shown in figure 3(e). Also, Yousefi et al. [33] employed equilibrium molecular dynamics (EMD) simulation to explore the density and viscosity of hydrogen molecules

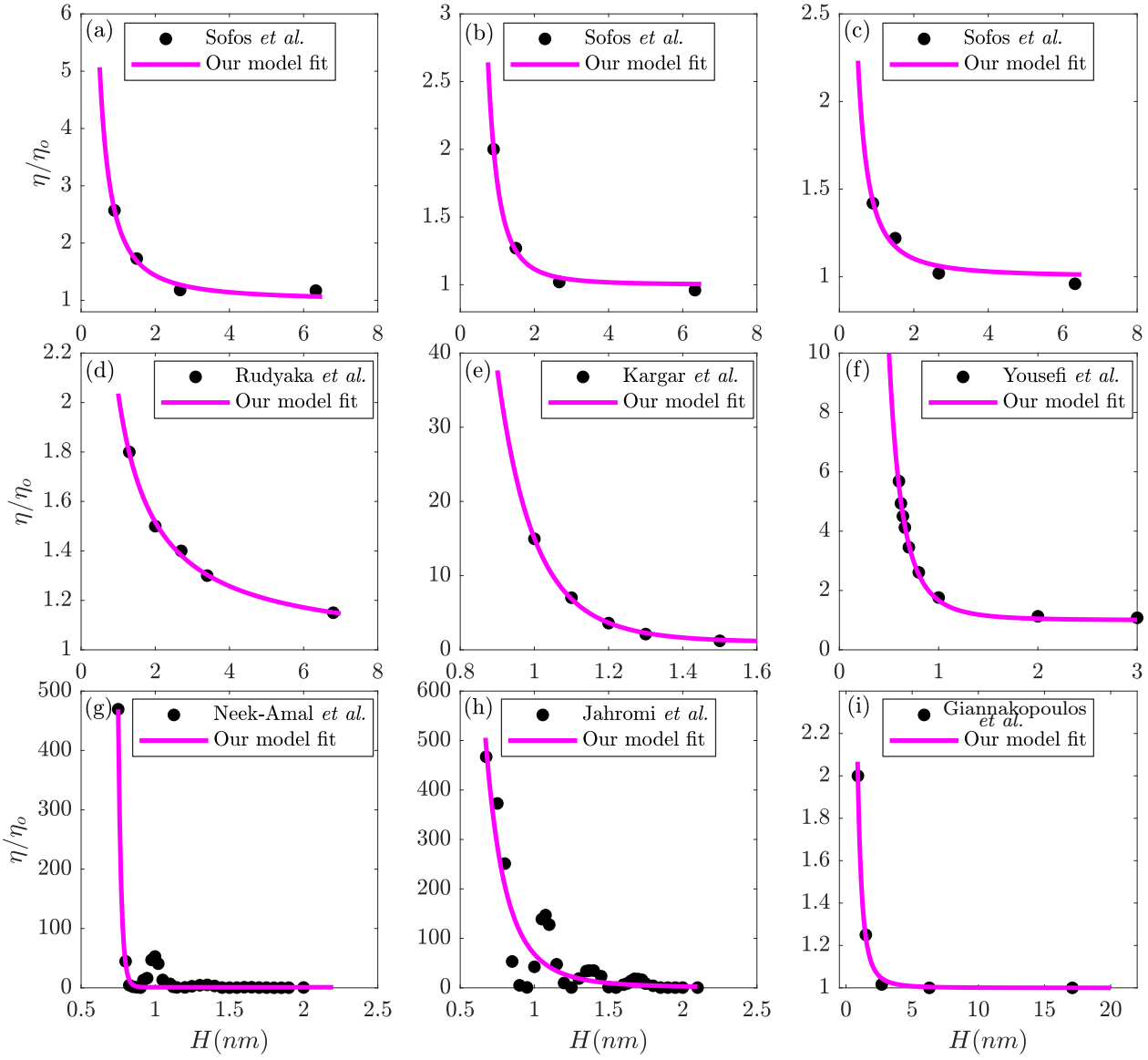

Figure 3: Comparison of the fitted viscosity using our proposed model with the data in the literature by [12], Shadloo-Jahromi et al. [23],Giannakopoulos et al. [36], Rudyak and Belkin [37], Kargar and Lohrasebi [26], Sofos et al. [38], and Yousefi et al. [33].

(H_2) when subjected to extreme confinement within a nanochannel made by graphene sheets. The seperation between the graphene sheets was varied between 0.6 to 3 nm and the data is shown in figure 3(f).

Furthermore, Neek-Amal et al. [11] employed equilibrium molecular dynamics simulations and investigated the effect of the channel size on the structure and shear viscosity of water confined between two graphene layers. They found that the shear viscosity oscillates as a function of the distance between the confining walls as shown in figure 3(g). The channel cross section was kept constant at 43 $\times$ 37.5 Å^2. The height of the channel was varied between 7.5 Å to 20 Å. Shadloo-Jahromi et al. [23] investigated the effect of sub-Angstrom variations of nanochannel size on the shear viscosity of water confined in a silicon wall by employing equilibrium molecular dynamics (EMD) simulations. Water molecules were confined between two infinite solid walls in the X and Y directions. The distance between the walls was varied between 6.25 Å to 21 Åand the data is shown in figure 3(h). Moreover, Giannakopoulos et al. [36] employed non-equilibrium molecular dynam- ics simulations of liquid argon flowing in a nanochannel formed by krypton walls, macroscopically equivalent to the planar Poiseuille flow, at constant temperature. The channel cross section was kept constant at 36.5 $\times$ 36.5 Å^2. The channel height was varied between 9 Å to 171.1 Å and the data is shown in figure 3(i) with black circle symbols.

Table 2 summarizes the fitting process of all these viscosity data for fluids flowing in nanochannels. The data were originally modeled using various approaches and different models in these study. We have re-evaluated this data predictions using our proposed model, resulting in the parameter values (m_2 and n_2) shown in the table. Additionally, we calculated the regression coefficient (R^2) for each fit, which is also included in the table. The R^2 values range from 0.95 to 0.99 except in one study where for data-set (h), $R^2 = 0.85$, otherwise indicating an excellent fit of the proposed model to the entire data set. These results suggest the robustness of the proposed model, demonstrating its ability to effectively fit a wide range of fluid viscosity data across various nanochannel configurations. Also, the excellent fit achieved across the data set implies the proposed model's generalizability. It can accurately capture the behavior of diverse fluid viscosities within nanochannels. In summary, the broad range of

S. No	Author	m_2	n_2	R^2
(a)	Sofos et al. [38] (Temperature = 100 K)	1.329	1.614	0.98
(b)	Sofos et al. [38] (Temperature = 120 K)	0.754	2.705	0.99
(c)	Sofos et al. [38] (Temperature = 150 K)	0.3572	1.787	0.95
(d)	Rudyak and Belkin [37]	1.036	1.004	0.99
(e)	Kargar and Lohrasebi [26]	14	9.136	0.99
(f)	Yousefi et al. [33]	0.6651	3.757	0.99
(g)	Neek-Amal et al. [11]	0.007634	38.32	0.97
(h)	Shadloo-Jahromi et al. [23]	67.14	5.036	0.85
(i)	Giannakopoulos et al. [36]	0.7444	2.816	0.99

Table 2: Viscosity data for fluids flowing in nanochannels and its fit with the proposed model

successfully fitted data highlights the robustness and generalizability of the proposed model for nanochannel fluid viscosities.

3.3 Slip length of nanoconfined fluid in the nanochannel

Analogous to nanoconfined density and the viscosity, numerous channel height-dependent models have been proposed for the slip length (λ) as discussed in the introduction of this paper. These models aim to capture the relationship between slip length and channel height (H). To streamline and enhance modeling efficiency for slip length, similar to the approach taken for nanoconfined density, we propose a unified model applicable to a broader range of experimental and Molecular dynamics simulation data. This model utilizes an power-law dependence on channel height (H) with additional free parameters to account for the unique behavior of various fluids. The proposed model as mentioned earlier in equation (17) is $\lambda(H) = \lambda_o + m_3\ H^{-n_3}$.

In figure 4(a-i), we show various previous slip-length data of the fluid flowing in the nanochannels with orange circles and red square symbols, which are fitted with the proposed model equation (17) as shown with the cyan solid line. In figure 4(a), we show the data by Sun et al. [41] who investigated fluid and heat transfer in a nanoscale channel by both Molecular dynamics simulations and the analytical solution of the continuum-based energy equation. Flow of liquid Argon was studied for channel height varying from 1.5 nm to 18 nm. In figure 4(b), we show the data by Atlaschian et al. [40] who employed molecular dynamics simulation to study flow of liquid Argon through nanochannels with height varying from 10 nm to 21 nm. Further, Sofos et al. [39] employed Non-equilibrium molecular dynamics simulation to study flow of Argon through nanochannel with height varying from 0.9 nm to 17.1 nm as shown the predicted data in figure 4(c).

Yang and Zheng [25] employed a hybrid scheme that coupled molecular dynamics simulation and a continuum solution to study of slip length behaviour in the Couette flow problem using liquid Argon. By varying the height of the channel across multiple length scales, the effect of channel scale on surface slip length was investigated. Additionally, by changing the velocity of the moving-solid wall, the influence of shear rate on the slip length was studied. The channel height was varied between 3.5 nm to 435 nm. The simulations were run for four different wall velocities i.e., 0, 1.5, 3, and 4.5 nm/s as the corresponding slip-length data is shown in figures 4(d) to 4(g), respectively. Also, Yen et al. [24] employed hybrid Molecular dynamics and continuum simulation to investigate Couette and Poiseuille flow for channel heights varying from 15 nm to 135 nm shown in figure 4(g) with red square symbols. Further, Wang et al. [30] employed Molecular Dynamics simulations to explore spontaneous capillary flow of water through graphene nanoslits. Temperature was kept constant at 300 K. By performing Non-equilibrium molecular dynamics for laminar flow in nanoslits with various channel widths, the slip length is found to decline with increasing H. The channel width was varied between 0.6 nm to 3.4 nm. Apart from Non-equilibrium molecular dynamics simulation, the slip length was also calculated using Washburn equation ([42]) and the obtained values are slightly higher, although the trend remained the same as shown in figures 4(h) and

4(i), respectively.

Table 3 summarizes the fitting process of all these slip length data for fluids flowing in nanochannels. The data were originally modeled using various approaches and different models in these study. We have re-evaluated this data predictions using our proposed model, resulting in the parameter values (m_3 and n_3) shown in the table. Additionally, we calculated the regression coefficient (R^2) for each fit, which is also included in the table. The R^2 values

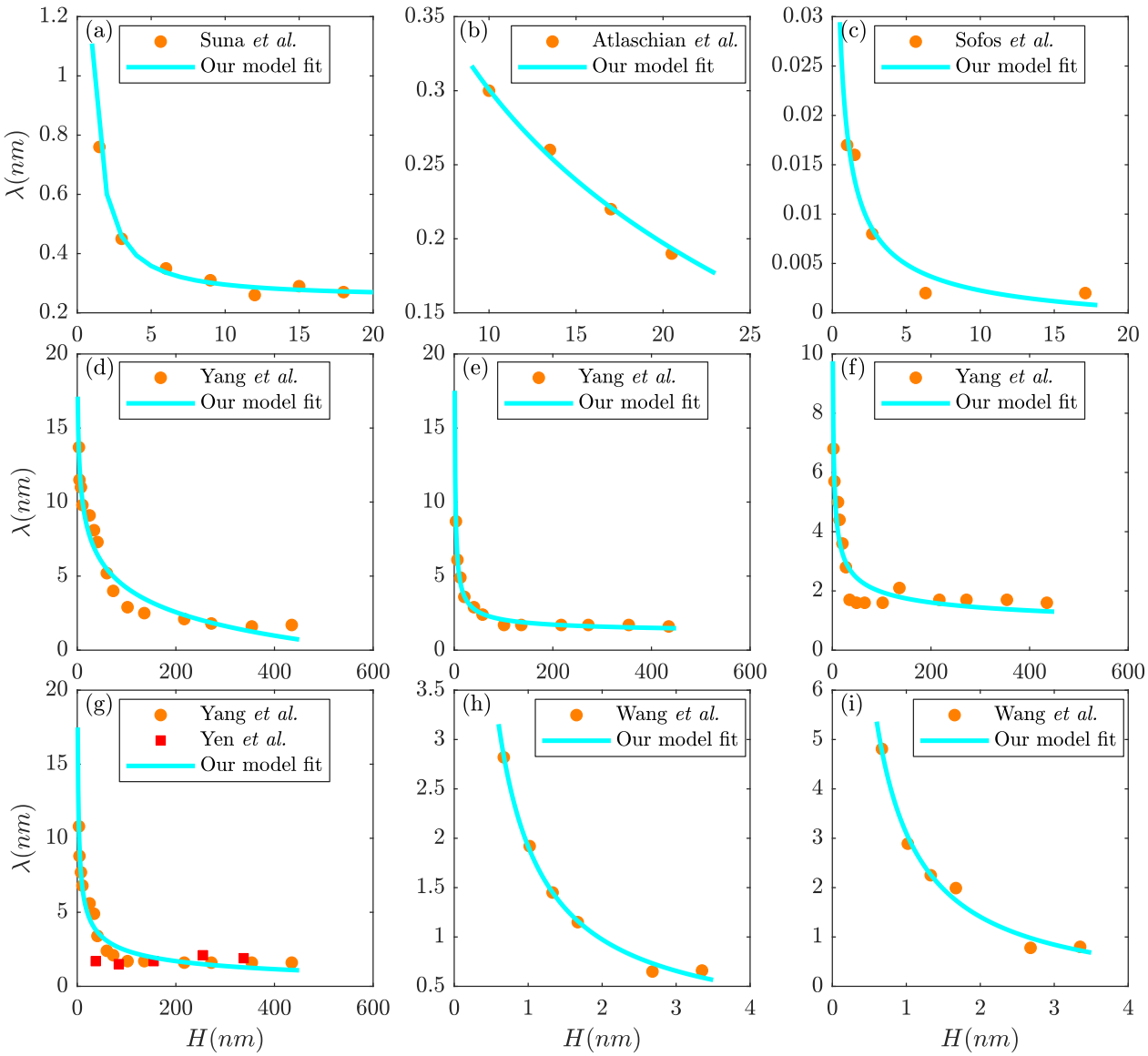

Figure 4: Comparison of the fitted slip-length using our proposed model with the data in the literature by [30], Yang and Zheng [25],Yen et al. [24], Sofos et al. [39], Atlaschian et al. [40], and Sun et al. [41].

S. No	Author	λ_0	m_3	n_3	R^2
(a)	Sun et al. [41]	0.252	1.297	0.8573	0.99
(b)	Atlaschian et al. [40]	-2.867	3.538	0.048	0.99
(c)	Sofos et al. [39]	-0.0025	0.02077	0.6394	0.94
(d)	Yang and Zheng [25] (Stationary wall)	-36.44	53.56	0.05985	0.96
(e)	Yang and Zheng [25] (Top wall moving at 1.5 nm/s)	-0.5949	18.08	0.3893	0.96
(f)	Yang and Zheng [25] (Top wall moving at 3 nm/s)	1.097	16.42	0.6161	0.99
(g)	Yang and Zheng [25] (Top wall moving at 4.5 nm/s), Yen et al. [24]	9.264	0.3993	0.492	0.91
(h)	Wang et al. [30] (NEMD Simulation)	0.00167	1.915	0.9769	0.99
(i)	Wang et al. [30] (Washburn Equation) [42]	-0.2831	3.386	1.001	0.99

Table 3: Slip length data for fluids flowing in nanochannels and its fit with the proposed model.

range from 0.91 to 0.99 for all studies, indicating an excellent fit of the proposed model to the entire data set. These results suggest the robustness of the proposed model, demonstrating its ability to effectively fit a wide range of fluid slip length data across various nanochannel configurations. Also, the excellent fit achieved across the data set implies the proposed model's generalizability. It can accurately capture the behavior of diverse fluid slip lengths within nanochannels. In summary, the broad range of successfully fitted data highlights the robustness and generalizability of the proposed model for nanochannel fluid slip-lengths in the nanochannels.

4 Conclusions

Nanofluidics has become an important area of research because of its many applications. Fluids confined in nanoscale channels—just a few nanometers to angstroms wide—show unique behaviors that are very different from their bulk properties. Key properties like density (ρ), viscosity (η), and slip length (λ) play a major role in controlling fluid flow, transport, and the performance of nanoscale devices. Understanding these properties is essential for designing effective nanofluidic systems and studying nanoscale phenomena.

One well-known factor affecting nanoconfined fluids is the height of the channel, which has a strong influence on density, viscosity, and slip length. Many models have been proposed to describe these effects, but they often use different equations for each property. This variety of approaches can make it difficult to choose the right model for numerical simulations. A simpler, unified method would help make these studies more efficient and accessible.

In this paper, we tried to propose a simple single power-law model for each nano confined material property such as for density $\rho(H)/\rho_o = 1 + m_1\ H^{-n_1}$, viscosity $\eta(H)/\eta_o = 1 + m_2\ H^{-n_2}$, and the slip length $\lambda(H) = \lambda_o + m_3\ H^{-n_3}$ (where $m_1,\ m_2,\ m_3,\ n_1,\ n_2,\ n_3,\ \lambda_o$ are the free fitting parameters) and their values depends on the fitting of various data sets from the experiments and Molecular dynamics simulations from the literature. We have discovered that a single proposed power-law equation for each material property, effectively captures and models all the data, even though many different models have been employed in the existing

literature to describe the same material property.

A significant advantage of our proposed model lies in its inherent mathematical properties. The model exhibits both continuity and a continuous derivative. These characteristics make it exceptionally well-suited for integration into numerical simulations. Numerical simulations rely heavily on smooth and continuous functions to achieve stable and accurate calculations. By seamlessly integrating into these simulations, our model avoids potential disruptions caused by discontinuities, leading to more reliable results. Furthermore, the proposed model adheres to established physical principles. As the nanochannel height (H) approaches infinity, the model predicts that the material properties of the confined fluid converge towards the bulk properties of the same fluid. This adherence to far-boundary conditions reinforces the model's physical accuracy and reflects a realistic representation of fluid behavior at different confinement scales. Further this unified power-law model for density, viscosity, and slip length compared to exponential models (for e.g., [12]), offers flexibility where it captures non-linear relationships and diverse data curvatures. Interpretability with clear physical meaning for parameters. Adaptability to combine with other functions for complex phenomena. Simplicity for easy parameter estimation, model interpretation, and computations. Robustness and less sensitive to outliers and noise in data and with fewer parameters to easy relate to underlying physics and scaling-laws.

Our proposed model presents a simple and significant leap forward in characterizing the intricate relationship between fluid properties at nanochannel dimensions with generic free parameter based power-law model. It also offers a unified and adaptable framework, replacing the current multitude of often-disparate, complex and sometimes mathematical singular current models. We can easily implement the proposed models in the theory and simulations which deepens our fundamental understanding of fluid behavior at the nanoscale and further unlocks exciting possibilities for advancements. Furthermore, the model's adaptability paves the way for future exploration. It can be readily extended to incorporate additional factors that might influence confined fluid behavior, such as surface chemistry or specific fluid-solid interactions. This adaptability allows researchers to continuously refine the model and gain a progressively more nuanced understanding of fluid dynamics at the nanoscale.

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References

[1] Zohreh Jalilvand, Farzin Zokaee Ashtiani, Amir Fouladitajar, and Hamid Rezaei. Computational fluid dynamics modeling and experimental study of continuous and pulsatile flow in flat sheet microfiltration membranes. *Journal of Membrane Science*, 450:207–214, 2014.

[2] Fatemeh Ebrahimi, Farzaneh Ramazani, and Muhammad Sahimi. Nanojunction effects on water flow in carbon nanotubes. *Scientific Reports*, 8(1):7752, 2018.

[3] Ashish Garg. Enhanced flow in deformable carbon nanotubes. *Journal of Applied Physics*, 135(7), 2024.

[4] Mainak Majumder, Nitin Chopra, Rodney Andrews, and Bruce J Hinds. Enhanced flow in carbon nanotubes. *Nature*, 438(7064):44–44, 2005.

[5] Ashish Garg. Modelling of enhanced water flow in deformable carbon nanotubes using a linear pressure-diameter relationship. *ChemRxiv- Nanoscience, DOI: 10.26434/chemrxiv-2023-k7mws*, pages 1–13, 2023.

[6] B Radha, A Esfandiar, FC Wang, AP Rooney, K Gopinadhan, A Keerthi, A Mishchenko, A Janardanan, P Blake, L Fumagalli, et al. Molecular transport through capillaries made with atomic-scale precision. *Nature*, 538(7624):222–225, 2016.

[7] Ashish Garg. Pulsatile pressure enhanced rapid water transport through flexible graphene nano/angstrom-size channels: a continuum modeling approach using the micro-structure of nanoconfined water. *New Journal of Physics*, 25(10), 2023.

[8] John A Thomas and Alan JH McGaughey. Reassessing fast water transport through carbon nanotubes. *Nano letters*, 8(9):2788–2793, 2008.

[9] Hongfei Ye, Hongwu Zhang, Zhongqiang Zhang, and Yonggang Zheng. Size and temperature effects on the viscosity of water inside carbon nanotubes. *Nanoscale research letters*, 6:1–5, 2011.

[10] Kerstin Falk, Felix Sedlmeier, Laurent Joly, Roland R Netz, and Lydéric Bocquet. Molecular origin of fast water transport in carbon nanotube membranes: superlubricity versus curvature dependent friction. *Nano letters*, 10(10):4067–4073, 2010.

[11] Mehdi Neek-Amal, Francois M Peeters, Irina V Grigorieva, and Andre K Geim. Commensurability effects in viscosity of nanoconfined water. *ACS nano*, 10(3):3685–3692, 2016.

[12] M Neek-Amal, A Lohrasebi, M Mousaei, F Shayeganfar, B Radha, and FM Peeters. Fast water flow through graphene nanocapillaries: A continuum model approach involving the microscopic structure of confined water. *Applied Physics Letters*, 113(8):083101, 2018.

[13] Jacob N Israelachvili. Measurement of the viscosity of liquids in very thin films. *Journal of colloid and interface science*, 110(1):263–271, 1986.

[14] Ashish Garg and Swati Bishnoi. An empirical experimental observations and md simulation data-based model for the material properties of confined fluids in nano/angstrom size tubes. *Nano Express*, 5(1), 2023. doi: 10.1088/2632-959X/ad2b83.

[15] Dimitrios Angelis, Filippos Sofos, Konstantinos Papastamatiou, and Theodoros E Karakasidis. Fluid properties extraction in confined nanochannels with molecular dynamics and symbolic regression methods. *Micromachines*, 14(7):1446, 2023.

[16] Ashish Garg and Pranjal Prasad. Yield–stress shear thinning and shear thickening fluid flows in deformable channels. *Physica Scripta*, 99(3), 2023. doi: 10.1088/1402-4896/ad2898.

[17] Ashish Garg, Nico Bergemann, Beccy Smith, Matthias Heil, and Anne Juel. Fluidisation of yield stress fluids under vibration. *Science Talks*, 3:100067, 2022.

[18] Ashish Garg. Scaling laws for optimal power-law fluid flow within converging–diverging dendritic networks of tubes and rectangular channels. *Physics of Fluids*, 36(7):073116, 07 2024. ISSN 1070-6631. doi: 10.1063/5.0217953. URL `https://doi.org/10.1063/5.0217953`.

[19] Ashish Garg, Himanshu Mishra, and Sudip K Pattanayek. Scaling laws for optimized power-law fluid flow in self-similar tree-like branching networks. *Journal of Applied Physics*, 135(20), 2024.

[20] Ashish Garg and Pranjal Prasad. Wall-slip effects on the yield-stress fluid flows in the rigid and deformable channel. *ChemRxiv-Polymer Science, DOI: 10.26434/chemrxiv-2023-l3knn*, pages 1–30, 2023.

[21] V Ya Rudyak and AA Belkin. Molecular dynamics simulation of fluid viscosity in nanochannels. *Nanosystems: Physics, Chemistry, Mathematics*, 9(3):349–355, 2018.

[22] Chengxu Tu, Lijuan Qian, Fubing Bao, and Weiwei Yan. Local effective viscosity of gas in nano-scale channels. *European Journal of Mechanics-B/Fluids*, 64:55–59, 2017.

[23] Alireza Shadloo-Jahromi, Masoud Kharati-Koopaee, and Rasoul Khaledialidusti. Shear viscosity calculation of water in nanochannel: molecular dynamics simulation. *Korea-Australia Rheology Journal*, 32:251–259, 2020.

[24] TH Yen, CY Soong, and PY Tzeng. Hybrid molecular dynamics-continuum simulation for nano/mesoscale channel flows. *Microfluidics and Nanofluidics*, 3:665–675, 2007.

[25] Xiaofan Yang and Zhongquan C Zheng. Effects of channel scale on slip length of flow in micro/nanochannels. 2010.

[26] Mahboubeh Kargar and Amir Lohrasebi. Water flow modeling through a graphene-based nanochannel: Theory and simulation. *Physical Chemistry Chemical Physics*, 21(6):3304–3309, 2019.

[27] Sridhar Kumar Kannam, BD Todd, Jesper Schmidt Hansen, and Peter J Daivis. Slip length of water on graphene: Limitations of non-equilibrium molecular dynamics simulations. *The Journal of chemical physics*, 136(2), 2012.

[28] WH Herschel and R. Bulkley. Measurement of consistency as applied to rubber-benzene solutions. *Proc ASTM Part II*, 26(82):621–633, 1926.

[29] Praveen Chandrashekar and Ashish Garg. Vertex-centroid finite volume scheme on tetrahedral grids for conservation laws. *Computers & Mathematics with Applications*, 65(1): 58–74, 2013.

[30] Ting-Ya Wang, Hsin-Yu Chang, Guan-Yu He, Heng-Kwong Tsao, and Yu-Jane Sheng. Anomalous spontaneous capillary flow of water through graphene nanoslits: Channel width-dependent density. *Journal of Molecular Liquids*, 352:118701, 2022.

[31] Jafar Ghorbanian, Alper T Celebi, and Ali Beskok. A phenomenological continuum model for force-driven nano-channel liquid flows. *The Journal of chemical physics*, 145(18), 2016.

[32] Hamid Mosaddeghi, Saman Alavi, MH Kowsari, and Bijan Najafi. Simulations of structural and dynamic anisotropy in nano-confined water between parallel graphite plates. *The Journal of chemical physics*, 137(18), 2012.

[33] Farrokh Yousefi, Omid Farzadian, and Mehdi Shafiee. Exploring the viscosity and structural behavior of confined hydrogen: A molecular dynamics approach. *Journal of Molecular Liquids*, 390:123028, 2023.

[34] Murat Barisik and Ali Beskok. "law of the nano-wall" in nano-channel gas flows. *Microfluidics and Nanofluidics*, 20:1–9, 2016.

[35] Murat Barisik and Ali Beskok. Molecular free paths in nanoscale gas flows. *Microfluidics and Nanofluidics*, 18:1365–1371, 2015.

[36] AE Giannakopoulos, F Sofos, TE Karakasidis, and A Liakopoulos. Unified description of size effects of transport properties of liquids flowing in nanochannels. *International journal of heat and mass transfer*, 55(19-20):5087–5092, 2012.

[37] V Ya Rudyak and AA Belkin. Fluid viscosity in nanochannels. In *AIP Conference Proceedings*, volume 2027. AIP Publishing, 2018.

[38] Filippos Sofos, Theodoros Karakasidis, and Antonios Liakopoulos. Transport properties of liquid argon in krypton nanochannels: anisotropy and non-homogeneity introduced by the solid walls. *International Journal of Heat and Mass Transfer*, 52(3-4):735–743, 2009.

[39] Filippos Sofos, Theodoros E Karakasidis, and Antonios Liakopoulos. Parameters affecting slip length at the nanoscale. *Journal of Computational and Theoretical Nanoscience*, 10 (3):648–650, 2013.

[40] Omid Atlaschian, Hamzeh Noorian, Ahmadreza Azimian, and Davood Toghraee. Effects of surface roughness periodicity and channel height in nano-channel flows. *HEFAT 2012*, 2012.

[41] Qiangqiang Sun, Yong Zhao, Kwing-So Choi, and Xuerui Mao. Molecular dynamics simulation of liquid argon flow in a nanoscale channel. *International Journal of Thermal Sciences*, 170:107166, 2021.

[42] Edward W Washburn. The dynamics of capillary flow. *Physical review*, 17(3):273, 1921.