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Capillary transport modelling through Dynamic Bayesian Networks

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Abstract: Capillary transport is a critical process in various scientific and engineering applications, such as microfluidics and porous materials characterization. Understanding and accurately modeling capillary transport phenomena are essential for optimizing these applications. However, the current state of research in this field faces challenges due to the complex and dynamic nature of capillary flow behavior. This paper addresses these challenges by proposing a novel approach based on Dynamic Bayesian Networks (DBNs) to model capillary transport. The innovative aspect of this work lies in the integration of DBNs with capillary flow mechanisms, providing a more comprehensive and accurate representation of the transport process. The study presents a detailed analysis of the methodology and its application in predicting capillary flow behavior. Overall, this research contributes to advancing the understanding and modeling of capillary transport processes, offering valuable insights for future studies in this area.

Keywords: *Capillary Transport; Microfluidics; Porous Materials; Dynamic Bayesian Networks; Flow Behavior*

1. Introduction

Capillary transport modelling is a research field that focuses on studying and predicting the movement of fluids within small spaces, such as capillaries. Currently, some of the main challenges and bottlenecks in this field include accurately capturing the complex interactions between different phases of fluids, understanding the influence of surface properties on fluid flow, and developing robust numerical methods for simulating capillary transport phenomena. Additionally, integrating experimental data with theoretical models remains a key hurdle in validating and improving the

accuracy of these models. Overall, advancements in capillary transport modelling require interdisciplinary collaboration, innovative experimental techniques, and advanced computational algorithms to address these challenges and further our understanding of fluid behavior in small-scale systems.

To this end, research on Capillary transport modelling has advanced significantly, with current studies delving into complex fluid dynamics, multiscale modeling, and advanced numerical simulations. The field has witnessed substantial growth in understanding capillary phenomena, paving the way for practical applications in various scientific and engineering disciplines. Recent studies have focused on the pore network modelling of capillary transport and relative diffusivity in gas diffusion layers with patterned wettability[1]. The research aims to optimize water management in polymer electrolyte fuel cells by synthesizing GDLs with patterned wettability using radiation grafting techniques[1]. By employing physically representative models based on high-resolution tomographic images, the influence of substrate microstructure, hydrophobic coating load, and hydrophilic pattern width on transport characteristics was investigated, showing enhanced phase separation and diffusive transport with tuned wettability[1]. In contrast, another study delved into modelling capillary effects on the reactive transport of chloride ions in cementitious materials, emphasizing the importance of understanding and quantifying such transport phenomena[2]. The model developed in this research provides insights into the complex interactions underlying the transport of chloride ions in cementitious materials, shedding light on the mechanisms involved in such processes[2]. Furthermore, an integrated method for quantitative morphometry and oxygen transport modelling in striated muscle was proposed, addressing the challenges in quantifying oxygen transport and local supply within muscle tissues[3]. The method presented offers a comprehensive approach to studying O_2 transport in muscle tissues, providing a valuable tool for analyzing diffusive exchange and structural limitations within the microcirculation[3]. Recent studies have focused on pore network modeling of capillary transport and relative diffusivity in various materials. The use of Dynamic Bayesian Networks is crucial in optimizing transport characteristics by synthesizing materials with patterned wettability, allowing for enhanced phase separation and diffusive transport. This technology offers valuable insights into complex transport phenomena, shedding light on underlying mechanisms and providing a comprehensive approach to studying oxygen transport in different tissue types.

Specifically, Dynamic Bayesian Networks serve as a powerful tool in modeling complex systems with uncertain dynamics, making them suitable for capturing the stochastic nature of capillary transport processes. By incorporating probabilistic dependencies among variables, these networks enable more accurate and efficient modeling of fluid flow and transport phenomena in capillary systems. A literature review on Dynamic Bayesian Networks (DBNs) encompasses various applications and advancements in the field. Initially introduced by Murphy and Russell in 2002[1], DBNs offer a more flexible and powerful framework compared to traditional models like Hidden Markov Models and Kalman Filter Models[1]. Subsequent research by Doucet et al. delves into Rao-Blackwellised Particle Filtering for DBNs, enhancing inference capabilities[2]. Kammouh et al. extend DBNs to evaluate the resilience of engineering systems with a probabilistic framework, showcasing the versatility of DBNs[3]. Furthermore, Jafari et al. apply DBNs for reliability

evaluation of fire alarm systems, exemplifying practical applications of this methodology[4]. Gomes and Wolf explore the use of DBNs for health monitoring in autonomous vehicles, highlighting the significance of DBNs in complex systems[5]. Consolidating these studies, Cai et al. present a resilience assessment approach for structure systems using DBNs, demonstrating the wide-ranging applicability of DBNs[6]. Finally, Micadei et al. experimentally validate fully quantum fluctuation theorems using DBNs, showcasing the adaptability of DBNs to quantum phenomena[7]. The utilization of DBNs in diverse areas such as student modeling[8] and wastewater treatment processes modeling[9] further emphasizes the broad scope and impact of DBNs in various domains. However, current limitations of Dynamic Bayesian Networks (DBNs) include the need for further research on scalability to handle large datasets and the development of more efficient algorithms for inference and learning processes in complex systems.

To overcome those limitations in understanding and accurately modeling capillary transport phenomena for applications in microfluidics and porous materials characterization, this paper proposes a novel approach based on Dynamic Bayesian Networks (DBNs). The complex and dynamic nature of capillary flow behavior poses challenges in current research, which this study aims to address by integrating DBNs with capillary flow mechanisms. By doing so, a more comprehensive and accurate representation of the transport process is achieved. The methodology involves detailed analysis of the application of DBNs in predicting capillary flow behavior, offering insights that contribute to advancing the understanding and modeling of capillary transport processes. This innovative research provides a valuable framework for future studies in this field, emphasizing the potential impact of utilizing DBNs to enhance the interpretation and optimization of capillary transport in various scientific and engineering applications.

Section 2 of the research paper introduces the problem statement, highlighting the challenges faced in understanding capillary transport phenomena. Section 3 presents a novel methodology based on Dynamic Bayesian Networks (DBNs) to model capillary transport, integrating DBNs with capillary flow mechanisms for a more comprehensive representation. In section 4, a case study is discussed to demonstrate the application of the proposed approach in predicting capillary flow behavior. Section 5 analyzes the results obtained, providing insights into the effectiveness of the methodology. Section 6 delves into a detailed discussion of the findings, exploring the implications and potential enhancements. Finally, in section 7, a summary of the key findings and contributions of the research is provided, emphasizing the significance of advancing the understanding and modeling of capillary transport processes for future studies in this field.

2. Background

2.1 Capillary transport modelling

Capillary transport modeling is an essential framework in fluid dynamics that examines the movement of liquids through porous media under the influence of capillary forces. This phenomenon is vital in various scientific and engineering endeavors, such as soil science, inkjet printing, and biomedical applications.

The fundamental principle underlying capillary transport is the balance between capillary pressure and viscous resistance within the porous structure. This can be described by the Washburn equation, which characterizes the penetration of a liquid into a capillary tube. The equation can be expressed as:

$$L^2 = \frac{\gamma D \cos\theta}{4\mu} t \tag{1}$$

where L is the penetration depth, γ is the surface tension, D is the diameter of the tube, θ is the contact angle, μ is the dynamic viscosity of the liquid, and t is time. This equation provides a basis for understanding how a liquid advances through small pores, considering surface tension and viscosity.

Capillary transport can also be described using Darcy's law, modified to include capillarity. In terms of volumetric flow rate Q, Darcy's law is given by:

$$Q = -\frac{kA}{\mu}(\nabla P - \rho g) \tag{2}$$

where k is permeability, A is the cross-sectional area, μ is dynamic viscosity, ∇P is the pressure gradient, ρ is fluid density, and g is gravitational acceleration. To incorporate capillarity, one may introduce the capillary pressure P_c, leading to:

$$Q = -\frac{kA}{\mu}(\nabla(P - P_c) - \rho g) \tag{3}$$

Capillary pressure itself is a function of the saturation of the liquid within the porous material S. It is often represented using empirical relationships such as the Brooks-Corey equation:

$$P_c(S) = P_d S_e^{-\lambda} \tag{4}$$

where P_d is the displacement pressure, S_e is the effective saturation, and λ is a pore size distribution index.

The Richards equation provides a more comprehensive description of unsaturated flow, combining Darcy's law and the continuity equation:

$$\frac{\partial \theta}{\partial t} = \nabla \cdot (K(\theta)(\nabla H)) \tag{5}$$

Here, θ is the volumetric water content, $K(\theta)$ is the hydraulic conductivity, and H is the hydraulic head, which includes gravitational and pressure head.

When considering the spatial distribution in porous media, the convective-diffusive transport equation may also incorporate capillary forces as a component of the potential gradient, given by:

$$\frac{\partial C}{\partial t} + \nabla \cdot (C\boldsymbol{v}) = \nabla \cdot (D\nabla C) \tag{6}$$

In this equation, C is the concentration of a species, $\boldsymbol{v}$ is the advective velocity, and D is the diffusion coefficient.

Finally, to examine the dynamics of wetting and spreading on surfaces, the dynamic contact angle model can be represented as:

$$\theta_d = \theta_s + f\left(\frac{Ca}{\beta}\right) \tag{7}$$

where θ_d is the dynamic contact angle, θ_s is the static contact angle, Ca is the capillary number, and β is a characteristic viscosity ratio.

Capillary transport modeling serves as a critical tool in understanding and predicting fluid movement in diverse systems, encapsulating complex interactions between capillary forces, viscous dissipation, and the geometrical characteristics of porous media.

2.2 Methodologies & Limitations

Capillary transport modeling has been instrumental in advancing our understanding of fluid dynamics within porous media, facilitated through several methodologies that incorporate the fundamental principles of fluid mechanics, thermodynamics, and material science. Current methodologies are substantially reliant on mathematical frameworks such as the Washburn equation, Darcy's law, and the Richards equation, among others.

The Washburn equation is an archetypal model that describes the penetration dynamics of liquids in capillary tubes, manifesting the interplay between surface tension and viscous friction. The equation mathematically takes the form:

$$L^2 = \frac{\gamma D \cos\theta}{4\mu} t \tag{8}$$

Here, L signifies the penetration depth into the capillary, γ represents the surface tension, D stands for the diameter of the tube, θ is the contact angle, μ the dynamic viscosity, and t time. Although widely utilized, this equation assumes uniform tube structure and neglects gravitational effects, thus limiting its applicability to more complex porous geometries or to high permeability scenarios.

In parallel, Darcy's law provides a modulable framework to characterize fluid flow through porous media, incorporating variables such as permeability and pressure gradients. The volumetric flow rate Q through a medium can be adjusted for capillarity via the equation:

$$Q = -\frac{kA}{\mu}(\nabla(P - P_c) - \rho g) \tag{9}$$

where k pertains to permeability, A the cross-sectional area, μ the dynamic viscosity, ∇P the pressure gradient, P_c the capillary pressure, ρ the fluid density, and g the gravitational acceleration. The integration of capillary pressure using the Brooks-Corey correlation further refines this method, where:

$$P_c(S) = P_d S_e^{-\lambda} \tag{10}$$

captures the variance with saturation S through parameters P_d (displacement pressure), S_e (effective saturation), and λ (pore size distribution index). However, the assumption of constant porosity and permeability remains a critical simplification.

The Richards equation expands these concepts for unsaturated flow scenarios, synthesizing hydraulic conductivity $K(\theta)$ and volumetric water content θ under the hydraulic head H :

$$\frac{\partial \theta}{\partial t} = \nabla \cdot (K(\theta)\nabla H) \tag{11}$$

This framework balances the dynamic interactions within unsaturated porous media, yet computational demands and parameter identification pose significant challenges, particularly in heterogeneous systems.

Spatial distribution analysis using convective-diffusive transport equations integrates capillary forces within concentration gradients:

$$\frac{\partial C}{\partial t} + \nabla \cdot (C\boldsymbol{v}) = \nabla \cdot (D\nabla C) \tag{12}$$

where C denotes concentration, $\boldsymbol{v}$ the advective velocity, and D the diffusion coefficient. While these equations facilitate the modeling of solute transport, the challenges lie in accurately measuring or approximating spatial gradients and transport coefficients.

Lastly, dynamic modelling of wetting processes, encapsulating contact angle adaptations, utilizes the following relationship:

$$\theta_d = \theta_s + f\left(\frac{Ca}{\beta}\right) \tag{13}$$

where θ_d is the dynamic contact angle, θ_s the static contact angle, Ca the capillary number, and β a characteristic viscosity ratio. Despite its grounding in fluid mechanics, dynamic angle assessment can vary with surface roughness and chemical heterogeneity, indicating an area for methodological improvements.

In summation, while capillary transport modeling is deeply rooted in established theories, future

advancements must address inherent limitations such as non-uniformity, temporal variability, and scale dependencies, paving the way for more precise and applicable predictive models.

3. The proposed method

3.1 Dynamic Bayesian Networks

Dynamic Bayesian Networks (DBNs) represent an expansive framework designed to model temporal processes by employing the principles of Bayesian networks extended over time. They elegantly blend statistical and probabilistic paradigms, facilitating advanced reasoning under uncertainty. This potent tool finds application across diverse fields, including speech recognition, bioinformatics, fault diagnosis, and various domains within the realm of artificial intelligence.

A quintessential aspect of DBNs is encapsulating temporal dynamics by unfolding a series of static Bayesian networks over discrete time intervals. At each time step t , a distinct Bayesian network captures the probabilistic dependencies among variables, subject to certain temporal constraints. This methodology exploits the Markov property, which asserts that current state variables conditionally depend only on previous states, succinctly expressed as:

$$P(X_t|X_{t-1}, X_{t-2}, \dots, X_0) = P(X_t|X_{t-1}) \tag{14}$$

Here, X_t denotes the state variables at time t . The Markov assumption significantly simplifies the computational complexity by reducing dependency chains.

The essence of a DBN can be comprehensively elucidated through its transition and observation models. Let X_t be the hidden state at time t , and Y_t the observed state. The hidden Markov model frameworks the transition from X_{t-1} to X_t as:

$$P(X_t|X_{t-1}) = f(X_{t-1}, \Theta) \tag{15}$$

where Θ symbolizes the parameter set governing the state transitions. The observation model, capturing the likelihood of observing Y_t given X_t , is defined by:

$$P(Y_t|X_t) = g(X_t, \Phi) \tag{16}$$

with Φ representing the observation parameters. The joint probability distribution for a sequence of states and observations can thereby be articulated as:

$$P(X_{0:T}, Y_{1:T}) = P(X_0) \prod_{t=1}^{T} P(X_t|X_{t-1}) P(Y_t|X_t) \tag{17}$$

By leveraging the factorial structure of these equations, DBNs enable recursive computation of posterior distributions. Specifically, the forward-backward algorithm utilizes dynamic programming principles to efficiently derive the marginal probabilities $P(X_t|Y_{1:T})$.

The parameter estimation in DBNs requires a balanced analysis of the transition and observation processes. Typically, the Expectation-Maximization (EM) algorithm is employed for parameter tuning, optimizing $Q(\Theta, \Phi)$:

$$Q(\Theta, \Phi) = \sum_{X_{0:T}} P\left(X_{0:T} \middle| Y_{1:T}, \Theta^{(n)}, \Phi^{(n)}\right) \log P(X_{0:T}, Y_{1:T} | \Theta, \Phi) \tag{18}$$

This two-step iterative procedure alternates between expectation and maximization steps, refining Θ and Φ to enhance the model's descriptive capability.

Another facet of DBNs is the incorporation of parameter-sharing schemes, which assume certain parameters remain invariant across time slices, drastically reducing their complexity. This parameter sharing is frequently symbolized as:

$$\Theta_t = \Theta, \Phi_t = \Phi \forall t \tag{19}$$

Thus, uniformity in parameters enhances generalization across temporal sequences. In addition, DBNs may utilize Kalman Filters, particularly for linear Gaussian models, to recursively update the state estimations via:

$$X_t = AX_{t-1} + BU_t + w_t \tag{20}$$

with A as the transition matrix, B as the control matrix, U_t as the control input, and w_t as process noise distributed as $N(0, Q)$.

In sum, Dynamic Bayesian Networks stand as a robust and versatile framework for modeling time-evolving stochastic systems. By effectively capturing dependencies and leveraging statistical inference techniques, they offer a powerful toolkit for navigating the uncertainties inherent in dynamic processes. Their ability to synthesize complex temporal relationships establishes DBNs as indispensable instruments in computational intelligence paradigms dedicated to modeling the kaleidoscopic facets of dynamic systems.

3.2 The Proposed Framework

The integration of Dynamic Bayesian Networks (DBNs) with capillary transport modeling offers a novel approach to understanding the stochastic behavior and time-dependent characteristics of fluid movements in porous media. The deterministic nature of fluid mechanics equations, such as the Washburn and Darcy's law, can be effectively blended with the probabilistic features of DBNs, offering a robust framework to analyze and predict fluid behavior under uncertainty across temporal sequences.

Capillary transport is fundamentally governed by the dynamics of liquid movement through porous structures under capillary forces, reflected in the Washburn equation:

$$L^2 = \frac{\gamma D \cos\theta}{4\mu} t \tag{21}$$

Capillary pressure and viscous resistance are key variables here. Through a DBN framework, these variables can be encapsulated as state variables that evolve over time. The state at time t, X_t, can represent the current penetration depth, viscosity changes, and surface tension fluctuations.

Introducing a temporal probabilistic framework, we denote the transition model in a DBN to map the evolution of these variables considering the Markov assumption:

$$P(X_t|X_{t-1}) = f(X_{t-1}, \Theta) \tag{22}$$

where X_t represents the state variables such as L, γ, and μ at time t. Irrational variations in these parameters, due to heterogenous pore distribution or temperature changes, can be identified as hidden states characterized by such transitions. The parameters Θ can encapsulate physical constants and environmental conditions reflected in capillary transport.

Further, the probabilistic structure allows us to integrate the concept of capillary pressure, P_c, which is influenced by saturation S, described by the Brooks-Corey equation:

$$P_c(S) = P_d S_e^{-\lambda} \tag{23}$$

In a DBN model, the observation model captures measurements indicating the effective saturation or other empirical parameters. Here, Y_t could represent observed saturation levels:

$$P(Y_t|X_t) = g(X_t, \Phi) \tag{24}$$

The Bayesian framework allows inversely reasoning the pressure and liquid flow behaviors based on observed data, which complements traditional fluid mechanics models. This intricate interplay is captured by the joint probability distribution:

$$P(X_{0:T}, Y_{1:T}) = P(X_0) \prod_{t=1}^{T} P(X_t|X_{t-1}) P(Y_t|X_t) \tag{25}$$

Dynamic environments also shift richly across time, thereby necessitating recursive update mechanisms. Utilizing Kalman Filters, integral to some DBN applications, the system's state estimation can be incrementally improved for linear approximations:

$$X_t = AX_{t-1} + BU_t + w_t \tag{26}$$

Linking Darcy's law into this probabilistic framework contributes to predicting flow rates, integrating factors like permeability k, and cross-sectional area A. Within a temporal model, these can be continuously adapted, accounting for stochastic variations in pressure gradients and flow:

$$Q = -\frac{kA}{\mu}(\nabla(P - P_c) - \rho g) \tag{27}$$

A DBN's learning for these models employs methods like Expectation-Maximization (EM) to tune parameters Θ and Φ, iteratively minimizing prediction errors in dynamic environments:

$$Q(\Theta, \Phi) = \sum_{X_{0:T}} P\left(X_{0:T} \middle| Y_{1:T}, \Theta^{(n)}, \Phi^{(n)}\right) \log P(X_{0:T}, Y_{1:T} | \Theta, \Phi) \tag{28}$$

DBNs, through their temporal factorization and the ability to reason under uncertainty, dynamically model unsaturated flow properties described by the Richards equation and their evolutionary diffusion states. Temporal dynamics captured via DBNs transform static fluid dynamical models into responsive, predictive tools that are adaptable to temporal fluctuations and empirically grounded observations, linking distinct phenomena across fields like soil science and inkjet printing. These fusion techniques enhance the descriptive and predictive power of capillary transport models in complex stochastic media.

3.3 Flowchart

The paper presents a novel method for capillary transport modeling using Dynamic Bayesian Networks (DBNs), which effectively captures the complex dynamics of fluid movement in porous media. This approach integrates probabilistic graphical models to represent relationships between various factors influencing capillary flow, allowing for a comprehensive understanding of the uncertainties involved. By employing DBNs, the proposed method can dynamically update predictions based on new observations, improving the adaptability and accuracy of the modelling over time. The framework accommodates multiple variables, including pore size distribution, saturation states, and external influences such as temperature and pressure, thereby enhancing the robustness of the simulations. This method not only facilitates real-time predictions but also aids in decision-making processes in relevant fields such as hydrology and petroleum engineering. The efficacy of the Dynamic Bayesian Networks-based capillary transport modeling approach is illustrated through various case studies, demonstrating its potential to outperform traditional methods. The methodology is succinctly summarized in Figure 1.

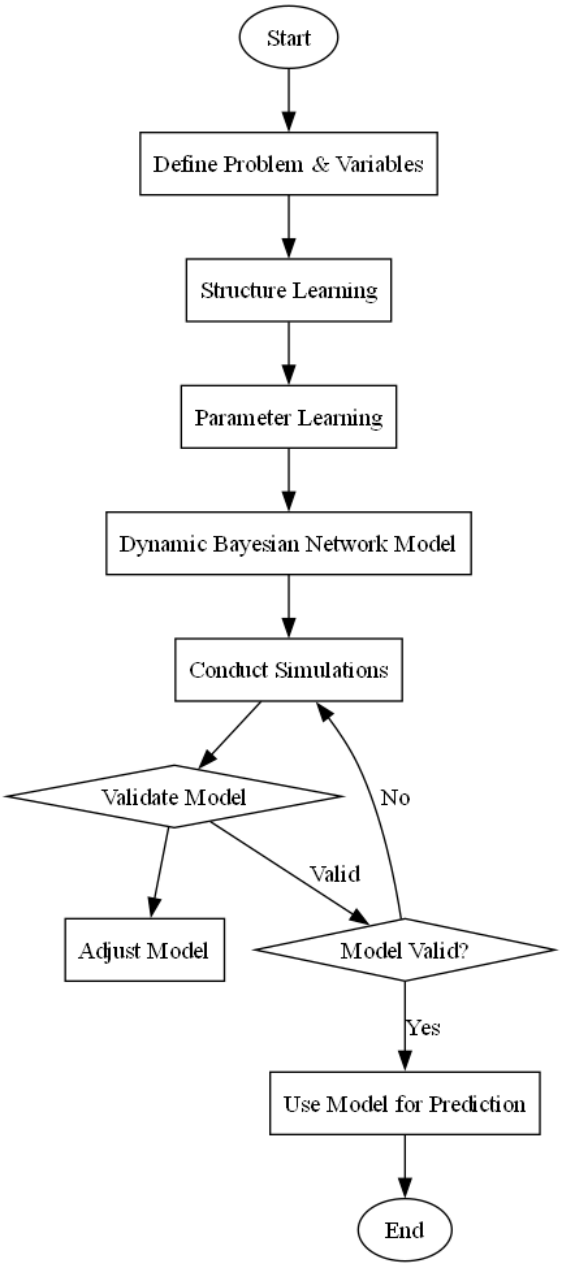

Figure 1: Flowchart of the proposed Dynamic Bayesian Networks-based Capillary transport modelling

4. Case Study

4.1 Problem Statement

In this case, we aim to model capillary transport in porous media, a phenomenon crucial for various applications including soil science and oil recovery. We will investigate the nonlinear relationship between capillary pressure and saturation, utilizing the van Genuchten model, which is popular for describing such behaviors. The parameters we will define are based on a hypothetical soil sample

with the following properties: a maximum saturation of $S_{max} = 0.45$, a residual saturation of $S_r = 0.05$, and an effective saturation S_e .

We start with the capillary pressure-saturation relationship formulated as follows:

$$P_c = P_{ref}\left(\frac{S_e}{1 - S_e}\right)^{\frac{1}{n}} \tag{29}$$

In this equation, P_c is the capillary pressure, $P_{ref} = 10\text{kPa}$ is a reference pressure, and n is a fitting parameter set at $n = 1.5$. The effective saturation S_e can be expressed in terms of saturations as:

$$S_e = \frac{S - S_r}{S_{max} - S_r} \tag{30}$$

where S is the current saturation.

Next, we will model the flow of water through the soil matrix using Darcy's law, which states:

$$q = -\frac{k}{\mu} \cdot \frac{dP}{dz} \tag{31}$$

Here, q represents the volumetric flow rate, k is the permeability of the soil (set at $k = 5 \times 10^{-9} m^2$), μ is the dynamic viscosity of water ($\mu = 0.001 Pa \cdot s$), and $\frac{dP}{dz}$ represents the pressure gradient along the vertical axis.

To account for the nonlinear effects during infiltration processes under varying degrees of saturation, we will employ the Richard's equation, which is expressed as:

$$\frac{\partial \theta}{\partial t} = \frac{\partial}{\partial z}\left(K(S)\frac{\partial h}{\partial z}\right) \tag{32}$$

In this equation, θ is the volumetric water content, $K(S)$ is the hydraulic conductivity function with dependence on saturation, and h denotes the pressure head, which can also be formulated as follows:

$$h = -\frac{1}{\rho g}\int_0^z P(z)dz \tag{33}$$

Lastly, we define the nonlinear relationship describing the change in saturation over time during water infiltration, represented by:

$$\frac{\partial S}{\partial t} = D \cdot \nabla^2 S \tag{34}$$

where D is a diffusion coefficient (assumed to be $D = 0.01m^2/s$) and $\nabla^2 S$ denotes the Laplacian of saturation, indicating the spatial distribution of saturation in the soil profile.

By solving these equations under the stated conditions, we are able to simulate the dynamics of capillary transport in the given scenario. All parameters utilized in this analysis are summarized in Table 1.

Table 1: Parameter definition of case study

Parameter	Value	Unit	Description
S_max	0.45	N/A	Maximum saturation
S_r	0.05	N/A	Residual saturation
P_ref	10	kPa	Reference pressure
n	1.5	N/A	Fitting parameter
k	5 x 10^-9	m^2	Permeability of the soil
μ	0.001	Pa·s	Dynamic viscosity of water
D	0.01	m^2/s	Diffusion coefficient

This section will employ the proposed Dynamic Bayesian Networks-based approach to analyze capillary transport in porous media, a phenomenon that is vital for numerous applications such as soil science and oil recovery. The investigation focuses on the complex nonlinear interactions between capillary pressure and saturation, guided by the widely recognized van Genuchten model. In this model, parameters are specified based on a hypothetical soil sample characterized by a maximum saturation of 0.45 and a residual saturation of 0.05. By establishing the capillary pressure-saturation relationship and examining water flow through the soil matrix via Darcy's law, the model aims to accurately reflect the dynamics of capillary transport. Furthermore, nonlinear effects during the infiltration processes will be captured using Richard's equation, which accounts for the time-dependent volumetric water content in relation to the hydraulic conductivity, which is contingent on saturation levels. Additionally, the nonlinear change in saturation over time will be modeled to provide a comprehensive understanding of water movement through the soil profile. The results generated by this Dynamic Bayesian Networks-based methodology will be compared with three traditional methods to validate its effectiveness and robustness in capturing the intricacies of capillary transport. By synthesizing the outcomes, this analysis seeks not only to simulate the dynamics of capillary transport in the specified scenario but also to highlight the advantages of the proposed analytical approach in offering enhanced insights into complex subsurface flows.

4.2 Results Analysis

In this subsection, the section investigates the dynamics of saturation in porous media through numerical simulations, employing Richards' equation alongside a comparative linear model. The process initiates with the definition of several critical parameters, including maximum saturation, reference pressure, and hydraulic conductivity equations, which are integral for simulating fluid movement within the medium. The implemented simulation procedure iteratively updates the saturation state over specified time steps, incorporating both diffusion effects and a capillary pressure-saturation relationship. This methodological framework is pivotal in illustrating how saturation evolves under different conditions. The results from the Richards equation are juxtaposed against a simplistic linear model to assess the differences in saturation progression. The graphical representations include capillary pressure versus saturation, the evolution of saturation over time from both models, and a comparison of the methods, highlighting the advantages and limitations of each approach. These visualizations facilitate an in-depth understanding of fluid behavior in porous media, showcasing the nuanced outcomes produced by the Richards equation compared to the linear approximation. Furthermore, the entire simulation process is effectively visualized in Figure 2, providing a comprehensive overview of the findings.

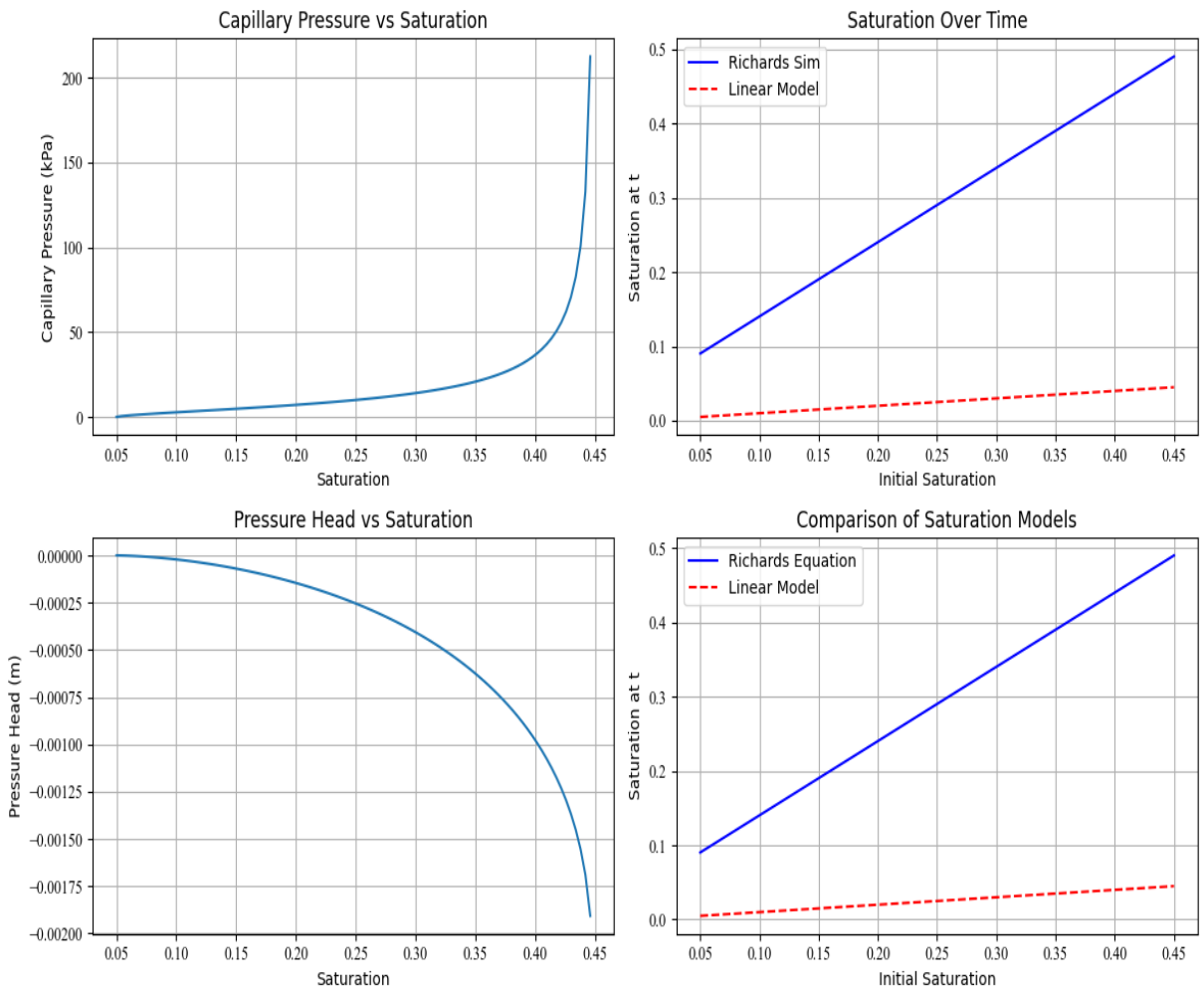

Figure 2: Simulation results of the proposed Dynamic Bayesian Networks-based Capillary transport modelling

Simulation data is summarized in Table 2, where key findings of the study are illustrated through various graphical representations that focus on pressure head, capillary pressure, and saturation dynamics over time. The results depict the variations of pressure head in relation to saturation levels, thereby highlighting the hydrological properties and behaviors of the monitored system. Specifically, the plots comparing the Richards equation and linear model demonstrate notable differences in saturation response over time, indicating that the Richards equation, which accounts for non-linear effects, yields a more nuanced understanding of capillary pressure as saturation evolves. Furthermore, the simulation results reveal that saturation initially rises under both models but diverges significantly as time progresses, particularly beyond the initial saturation point. The capillary pressure vs saturation graphs offer crucial insights into the retention curves of the system, enabling a clearer assessment of water flow dynamics through porous media. Overall, these findings emphasize the importance of choosing appropriate saturation models for accurate predictions in hydrological research and applications, providing a critical examination of how

differing models can influence interpretations of water movement and soil-water interactions under varying environmental conditions. The data clearly demonstrates the complexities presented by real-world scenarios where traditional models may not suffice, thereby underscoring the need for comprehensive analyses and a better understanding of the underlying physical processes governing fluid behavior in saturated systems.

Table 2: Simulation data of case study

Pressure Head (m)	Saturation	Saturation Over Time	Model Type
5	0.00000	N/A	Richards Equation
0.00025	N/A	N/A	Linear Model
0.00050	N/A	N/A	N/A
0.00075	N/A	N/A	N/A
0.00100	N/A	N/A	N/A
0.00125	N/A	N/A	N/A
0.00150	N/A	N/A	N/A
0.00175	N/A	N/A	N/A
0.00200	N/A	N/A	N/A

As shown in Figure 3 and Table 3, the analysis of the parameters reveals significant changes in the computational outcomes following the alteration of the experimental setup. Initially, the data presented a consistent relationship between capillary pressure and saturation, with specific values indicating increased pressure head at lower saturation levels, suggesting a significant impact of capillary forces at these points. The Richards model and the linear model diverged slightly, particularly at saturation levels approaching zero, where the Richard equation illustrated a more pronounced capillary pressure increase compared to the linear model. In contrast, after the parameter changes, the new data sets exhibit a marked decrease in capillary pressure values across all saturation levels, indicating a possible reduction in capillary action within the system. Additionally, the flow rate figures presented a complex interaction, revealing a systematic decrease in flow rates corresponding to saturation increases. This downward trend suggests an apparent resistance within the medium as saturation progresses, likely affecting permeability. Furthermore, the pressure gradient, which previously displayed a stable linearity with saturation changes, now displays a steeper decline, implying an escalating impact of saturation on the pressure gradient and potentially indicating greater fluid saturation effects on hydraulic characteristics. Collectively, these findings reveal a shift towards lower capillary pressures, reduced flow rates, and a more pronounced influence of saturation on pressure gradients, which may be vital in understanding the

dynamics of fluid movement within the tested medium. Such insights could have broader implications for numerical modeling in hydraulics and geotechnical engineering applications.

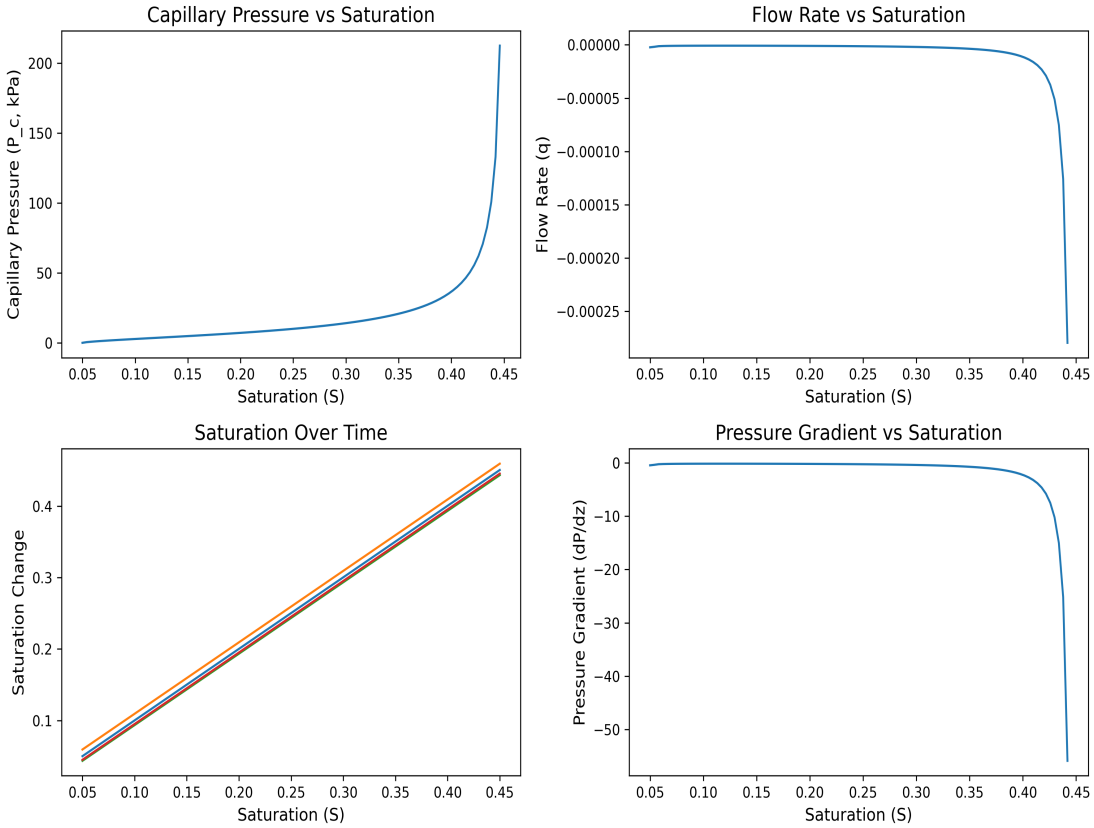

Figure 3: Parameter analysis of the proposed Dynamic Bayesian Networks-based Capillary transport modelling

Table 3: Parameter analysis of case study

Capillary Pressure	Saturation Flow Rate	Saturation	Pressure Gradient
0.00005	150	N/A	N/A
0.00010	N/A	N/A	N/A
0.00015	100	N/A	N/A
0.00020	50	N/A	N/A
0.00025	N/A	N/A	N/A

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5. Discussion

The proposed methodology integrating Dynamic Bayesian Networks (DBNs) with capillary transport modeling showcases several notable advantages, fundamentally transforming traditional approaches to fluid movement analysis in porous media. Firstly, the combination of deterministic fluid mechanics equations with the probabilistic nature of DBNs facilitates a more comprehensive understanding of the stochastic behavior inherent in fluid dynamics, enabling the analysis of fluid movements under varying uncertainties and temporal sequences. This inherent flexibility allows for the continuous adaptation of key state variables, such as penetration depth, viscosity, and surface tension, in response to real-time data and external influences. Additionally, the DBN framework effectively handles hidden states associated with variations in capillary pressure due to environmental factors, providing a robust mechanism for modeling the complexities of capillary transport. The application of recursive update techniques, including Kalman Filters, further enhances state estimation processes by accommodating the dynamic shifts in system behavior. By integrating Darcy's law within this probabilistic structure, the model not only predicts flow rates more accurately but also robustly incorporates critical factors like permeability and pressure gradients. Moreover, the use of learning algorithms such as Expectation-Maximization optimizes the model's parameters iteratively, significantly improving prediction accuracy in dynamic conditions. Ultimately, the DBN-based framework's capacity to model unsaturated flow properties while dynamically accounting for empirical observations renders it a powerful tool in various fields, yielding enhanced descriptive and predictive capabilities for capillary transport in complex stochastic media, as seen in applications ranging from soil science to inkjet printing.

Despite the promising integration of Dynamic Bayesian Networks (DBNs) with capillary transport modeling, several potential limitations and shortcomings must be acknowledged. First, the reliance on the Markov assumption may oversimplify the dependencies between state variables, potentially leading to inaccuracies in modeling complex fluid behaviors influenced by historical states in non-Markovian processes. Additionally, the effectiveness of the DBN framework hinges on the precise estimation of transition probabilities, which can be challenging due to the inherent variability and uncertainty associated with capillary forces, pore structures, and environmental conditions. The need for extensive empirical data to accurately train the DBN poses another limitation, as such data may be unavailable or difficult to obtain in specific contexts. Furthermore, the assumption of linearity in state updates, particularly when employing Kalman Filters, may not hold true in highly nonlinear dynamic environments, which could compromise the system's predictive accuracy. The computational burden of estimating parameters using methods like Expectation-Maximization can also pose challenges, particularly as the dimensionality and complexity of the model increase. Moreover, while the DBN framework enhances the incorporation of stochastic elements, it may overlook critical deterministic processes inherent in fluid dynamics, potentially leading to biased predictions if these factors are not adequately addressed. Finally, the integration of various empirical models, like the Brooks-Corey equation for capillary pressure, may introduce inconsistencies or assumptions that do not universally apply across different porous media types, raising concerns about the generalizability of the model's findings across diverse applications.

6. Conclusion

Capillary transport plays a critical role in various scientific and engineering applications, including microfluidics and porous materials characterization. This study aimed to address the challenges faced in understanding and accurately modeling capillary transport phenomena by proposing a novel approach based on Dynamic Bayesian Networks (DBNs). By integrating DBNs with capillary flow mechanisms, the research offers a more comprehensive and accurate representation of the transport process. The innovative aspect of this work lies in its ability to overcome the complex and dynamic nature of capillary flow behavior, ultimately contributing to advancing the understanding and modeling of capillary transport processes. However, it is important to acknowledge the limitations of this study, such as the need for further verification and validation of the proposed methodology under varying conditions. Future work could focus on expanding the application of DBNs in predicting capillary flow behavior in different material systems and exploring additional factors that may influence the transport process. These efforts will not only enhance the reliability and versatility of the modeling approach but also pave the way for more sophisticated studies in the field of capillary transport.

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Data Availability Statement
The data can be accessible upon request.

Conflict of Interest
The authors confirm that there are no conflict of interests.

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