Prediction of Surface Wettability with Water Droplet Placed on Smooth Surfaces Using Deep Learning

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Abstract

Surface wettability is the ability of a liquid to adhere to a solid surface, determined by the interaction between the liquid and the solid, primarily influenced by the liquid's surface tension and the solid's properties. The surface wettability can distinguish the surfaces into three categories, hydrophilic, hydrophobic, and superhydrophobic. Surface wettability plays various important roles in medical implants, drug delivery systems, and tissue engineering. It also plays an important role in microfluidics, textiles, surface coating materials, and solar panels. The conventional approaches to finding surface wettabilities using experiments may be costly and time-consuming. Hence in this work, we integrate the pseudo-potential lattice Boltzmann method and deep learning approach for analyzing and predicting surface wettability. First, we develop an LBM model for the collection of surface wettability data with various parameters. We consider the solid-fluid interaction parameter and droplet radius for analyzing the wettability. Then we develop deep learning models using LSTM and do various experiments to find the best models in terms of R2 score and Mean-Squared Error (MSE) for the performance evaluation. We provide detailed designs of models that could be advantageous for accelerating research in various engineering fields.

Keywords: Wettability; Contact angle; LBM, LSTM, R2 score

1. INTRODUCTION AND OBJECTIVE

The wettability of surfaces is an integral factor in many scientific, industrial, and technological contexts [1]. Fluid dynamics and material science processes are greatly influenced by it as they affect liquid's spreading and adhesion to solids. It is essential to understand how fluids interact with surfaces depending on their wettability. Fluid flows through pipes and channels are more frictionless and pressure drops are reduced when surfaces are hydrophobic [2]. Capillary action in porous materials and water purification are applications that benefit from hydrophilic surfaces. Recent developments in the field of time series modeling have been fueled by advances in neural network (NN) technology, which have made significant contributions to the prediction of Multiphase Flow Patterns (MPFs). Mi et al. (9) used self-organizing NNs to model a range of flow patterns, including vertical bubbly, slug, churn, and annular flows.

The main objective of this study is to integrate the lattice Boltzmann method and deep learning approach for the analysis and prediction of surface wettability of smooth surfaces using a water droplet placed at the center of the bottom surface in a domain of 200x200 µm especially using various Long-Short-Term Memory (LSTM) models.

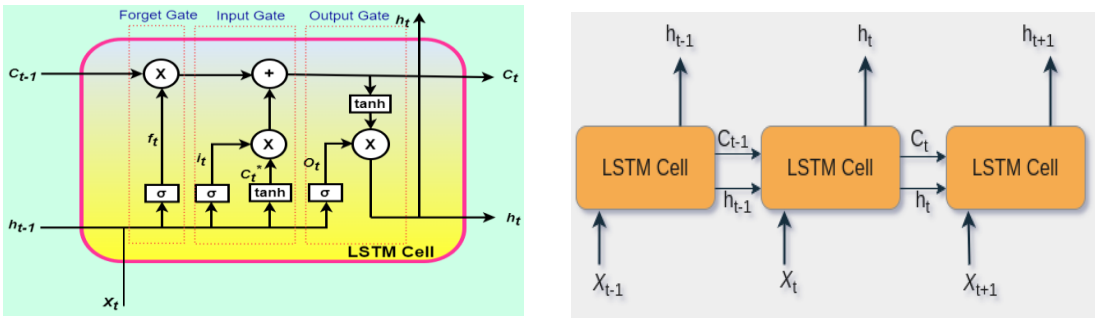

Figure. 1: The LSTM cell and an unfolded LSTM Network

2. RESULTS AND MAIN CONCLUSIONS

The study of surface wettability is crucial in modern material science, as it is vital for cell growth, biomolecule spotting, fluid microchips, microreactors, and metal rusting. An efficient method for determining wettability could lead to technological advancements in fields like cell growth, biomolecule spotting, fluid microchips, and microreactors.

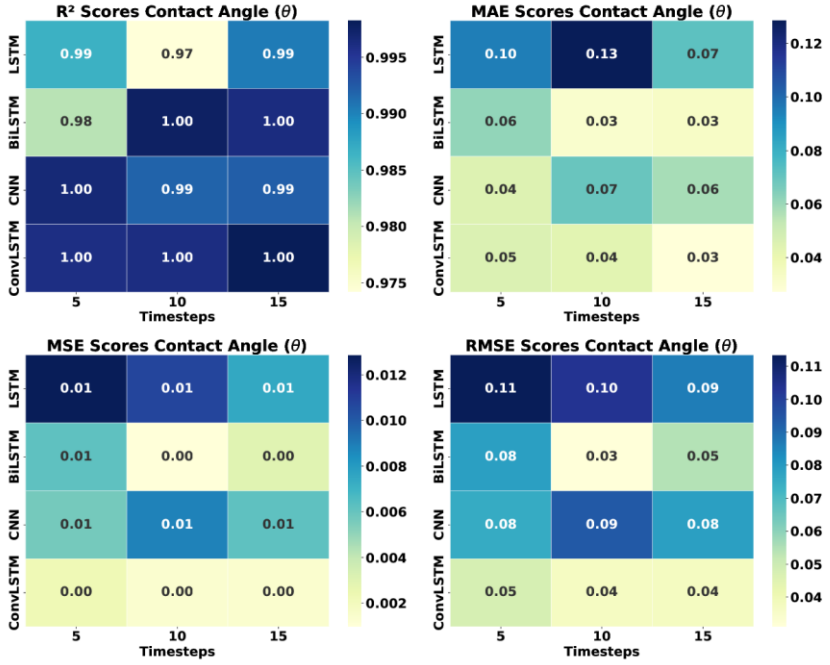

Figure. 2: Comparison of RMSE and R^2 for LSTM models

We have developed various LSTM models for the prediction of surface wettability using single water droplets. These models are been trained and tested on various datasets of contact angle with all models and from the optimations it has been found that the BiLSTM, CNN LSTM, and ConvLSTM models are predicting more accurate results than simple LSTM.

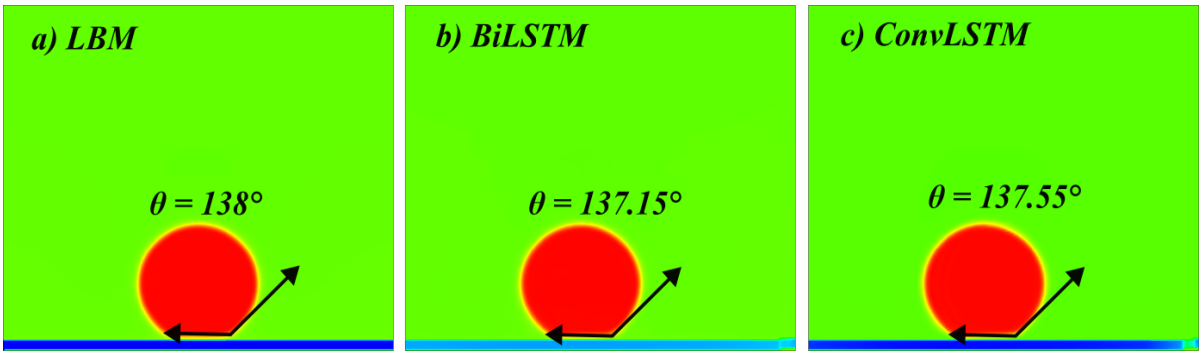

Figure. 2: Comparison of Wettability using LBM and LSTM models

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