

PANDA-NN: Improved Algorithm for Contact Angle Determination in Slit Pores and Interface Classification

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Surface phenomena determine the behaviour of fluids in porous media and on wetted surfaces. Proper accounting of these phenomena is the basis of accurate continuum models [1]. The contact angle is a key quantity that quantitatively characterizes surface phenomena. Previously, a model was proposed that classifies the interface surfaces in slit pores [2] and offers a completely new approach for determining the contact angle from a one-dimensional density profile named PANDA [3]. An improved version of this algorithm is proposed, considering the presence of a non-zero wetting layer. The enhanced algorithm is validated on numerical data obtained from molecular dynamics calculations and demonstrates high accuracy. Additionally, a deep neural network based on the PointNet++ architecture [4] is trained to classify the interface surface based on the point cloud. These improvements have resulted in a fully complete algorithm with minimal hyperparameters.

[1] Nichita D V 2019 *Fluid Phase Equilibria* **492** 145–160

[2] Kopanichuk I V, Berezhnaya A S, Sizova A A, Vanin A A, Sizov V V and Brodskaya E N 2020 *Colloids and Surfaces A: Physicochemical and Engineering Aspects* **601** 124884

[3] Semenchuk A, Kondratyuk N and Kopanichuk I 2024 *Colloids and Surfaces A: Physicochemical and Engineering Aspects* 135994

[4] Qi C R, Yi L, Su H and Guibas L J 2017 *Advances in neural information processing systems* **30**