

Computational Interface Verification of Selective Wetting in a Functionalized CSCP Sponge for Oil–Water Separation

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Abstract—Oil–water separation requires materials that preferentially interact with oil while minimizing water uptake. This work presents a computational interface-verification study of a functionalized CSCP sponge framework. The interface was analyzed along a 4.0 nm coordinate grid perpendicular to the solid barrier, with the reference boundary at $Z = 1.0$ nm. Water and hexane were considered as representative polar and non-polar liquid phases, respectively. The water profile exhibited an exclusion gap characterized by zero density near the investigated boundary, whereas the hexane profile showed a sharp accumulation peak. The corresponding thermodynamic interpretation indicated that water was repelled from the surface while hexane was absorbed into the matrix. These contrasting behaviors provide preliminary computational evidence of selective wetting relevant to oil–water separation. Quantitative molecular-dynamics analyses are required for definitive assessment of separation performance.

Index Terms—CSCP sponge; oil–water separation; selective wetting; silica; water; hexane; molecular simulation; interface analysis.

I. INTRODUCTION

Oil contamination in water is an important environmental and industrial problem. Efficient separation materials should preferentially capture oil while limiting water uptake. Surface wettability strongly influences interactions between a separation material and different liquid phases.

A computational approach can examine liquid behavior near an engineered surface before experimental fabrication. This study focuses on computational verification of selective wetting in a

functionalized CSCP sponge framework by comparing representative water and hexane systems.

II. PROJECT OBJECTIVE

The main objective is:

To computationally verify whether a functionalized CSCP sponge framework exhibits water-repellent and oil-attracting behavior suitable for oil–water separation.

The specific objectives are:

- To construct a computational representation of the solid interface.
- To analyze liquid behavior perpendicular to the solid surface.
- To compare the water and hexane interface profiles.
- To identify water exclusion behavior.
- To identify hexane accumulation behavior.
- To determine whether the contrasting liquid behavior supports selective wetting.

III. TRAJECTORY PROFILE ANALYSIS

The liquid distributions were examined along the direction perpendicular to the solid interface.

The analysis considered:

- liquid exclusion,
- liquid accumulation,
- interface density behavior,
- surface interaction,
- qualitative thermodynamic behavior.

The supplied report identifies the analysis as a trajectory-profile visualization and provides a

boundary numerical comparison between the two liquid systems.

IV. COMPUTATIONAL METHODOLOGY

The computational interface was evaluated along a 4.0 nm coordinate grid perpendicular to the solid barrier. The reference boundary was defined at $Z = 1.0$ nm. Two independent liquid systems were considered: water as the aqueous phase and hexane as a representative non-polar hydrocarbon phase. Trajectory profiles were examined along the direction normal to the interface. The analysis focused on exclusion, accumulation, density behavior, and qualitative thermodynamic interaction with the surface.

V. RESULTS

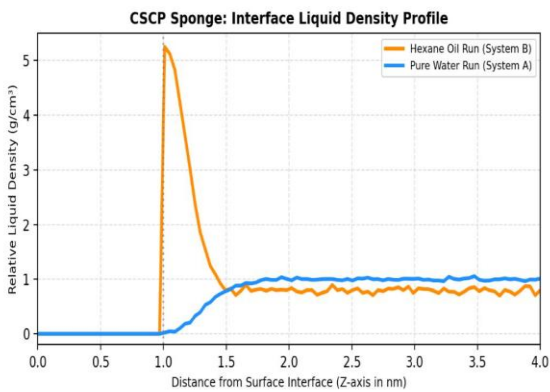


Fig. 1. Interface liquid density profile for water and hexane relative to the functionalized CSCP sponge surface.

A. Water Phase

The water phase exhibited an exclusion gap with zero density at the investigated boundary region. This indicates that water did not preferentially accumulate near the functionalized interface under the investigated computational conditions. The thermodynamic interpretation reported for the water system was:

Repelled from surface

Therefore, the calculated water profile is consistent with water-repellent behavior of the modeled interface.

B. Hexane Phase

The hexane phase showed a sharp accumulation peak near the investigated interface.

This indicates preferential accumulation of the non-polar hydrocarbon phase near the matrix.

The thermodynamic interpretation reported for the hexane system was:

Absorbed into matrix

Thus, the hexane profile indicates a stronger tendency of the modeled interface to interact with the hydrocarbon phase compared with water.

The contrasting profiles indicate different surface affinities for the two liquid phases. The result is consistent with a water-repellent and hydrocarbon-preferring interface under the investigated computational conditions.

TABLE I. SUMMARY OF INTERFACE BEHAVIOR

Property	Water	Hexane
Interface behavior	Exclusion gap	Sharp accumulation peak
Density behavior	Density = 0	Accumulation near interface
Thermodynamic path	Repelled from surface	Absorbed into matrix

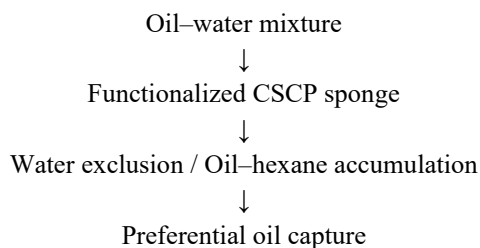
VI. DISCUSSION

The contrasting behavior of water and hexane is relevant to the proposed oil–water separation mechanism. Water exclusion suggests reduced water affinity, while hexane accumulation suggests preferential interaction of the non-polar phase with the modeled matrix.

These observations support the concept of selective wetting. However, the current result should be interpreted as computational interface verification rather than a direct measurement of experimental separation efficiency.

This difference suggests that the functionalized interface has selective wetting characteristics.

The proposed mechanism can therefore be represented as:



This behavior is desirable for an oil-selective sponge because the material should preferentially interact with the oil phase while resisting water uptake.

VII. SIGNIFICANCE OF THE RESULT

The present computational observation provides preliminary evidence that surface functionalization can produce different responses toward polar and non-polar liquids.

The observed water exclusion and hexane accumulation are particularly relevant to oil–water separation because they represent the two desired characteristics:

- i. Water repellency
- ii. Oil affinity

Therefore, the computational interface result supports the feasibility of using a suitably functionalized CSCP sponge as a selective oil-uptake material.

However, the present result should be interpreted as computational interface verification, rather than as a direct measurement of experimental oil–water separation efficiency.

VIII. LIMITATIONS AND FUTURE WORK

The present analysis does not provide quantitative diffusion coefficients, contact angles, adsorption energies, or experimental separation efficiencies. Water and hexane were also evaluated as separate systems. Future work should include validated force-field parameters, equilibrated molecular-dynamics simulations, a competitive water–hexane system, density profiles, interaction energies, diffusion coefficients, and wetting analysis.

The computational model should also be extended toward a realistic porous sponge geometry and compared with experimental oil-uptake or separation measurements.

IX. CONCLUSION

A computational interface-verification study demonstrated contrasting wetting behavior for water and hexane at a functionalized CSCP sponge framework. The water system exhibited an exclusion gap and was characterized as repelled from the surface, whereas hexane showed a sharp accumulation peak and was characterized as absorbed into the matrix. These observations provide preliminary support for selective wetting relevant to oil–water separation. Further quantitative molecular-dynamics and experimental validation are required before claiming separation efficiency.

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