THERE'S PLENTY OF ROOM AT THE BOTTOM: UNDERSTANDING HOW THE NANOSCALE AND MACROSCALE CONNECT IN SUSPENSIONS

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BACKGROUND

C&B

LANGUAGE

English

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Introduction

Aggregation and breakage are fundamental phenomena in many processes involving concentrated suspensions (e.g. anaerobic digestion, food, blood circulation, building materials, pharmaceutical engineering, etc.). In turn, these phenomena are often controlled by a combination of hydrodynamic and molecular effects. Consequently, the emergent macroscopic behavior of these systems is the result of multi-scale interactions. As expected, empirical models are not able to adequately reproduce the intricacies usually found in suspensions of engineering and/or scientific interest. Advancing the fundamental understanding of the connections among scales is therefore very relevant.

Methodology

Molecular Dynamics is a valuable tool in the study of the nature of intermolecular interactions present in suspensions. These interactions are a key factor in determining whether particles will aggregate or break up under specific flow conditions. This information can be used to deduce how particle size distributions evolve at the mesoscopic scale, which subsequently determine macroscopic properties.

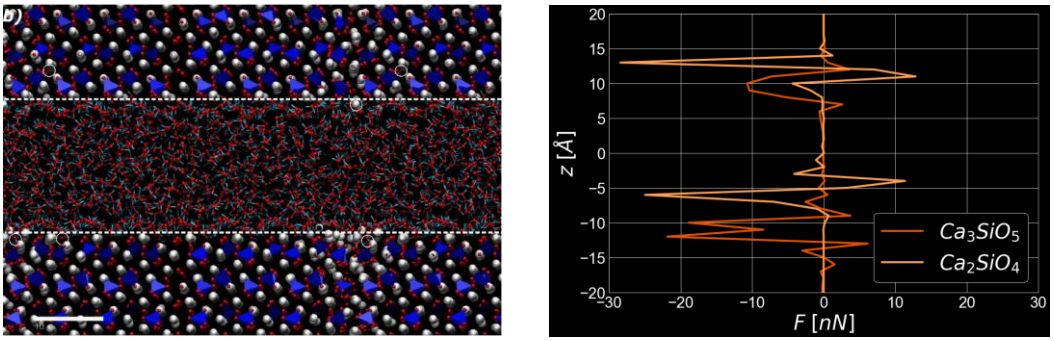
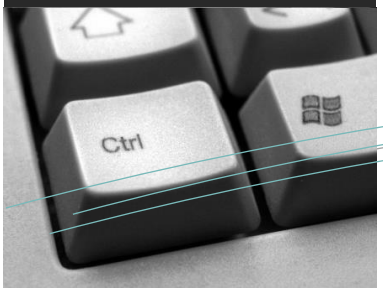


Figure 1 – The molecular structure of suspension granules (left) significantly affect their interaction forces (right).

Objectives of the thesis

This study aims to implement molecular dynamics models in order to further the knowledge of the influence of molecular interactions on the meso and macroscopic characteristics of suspensions.



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