Abstract of master's thesis

Topic: «**Water *filtration by use of molybdenum disulfide MoS_2 nano-membrane***»

According to a report by the World Health Organisation (WHO) in 2017, 2.1 billion people do not have access to drinking water at home, while 4.4 billion people do not have adequate sanitation. According to projections by the World Resources Institute, the situation could be even more critical by 2040. These freshwater shortages are affecting certain parts of the world, including large parts of North Africa, the Middle East, parts of Southern Europe, the United States and certain Asian countries such as China and India. According to recent figures from the Food and Agriculture Organization of the United Nations (FAO), 45 countries around the world are suffering from water shortages as defined by the United Nations through the Falkenmark indicator (water stress index). These water shortages are due in particular to the overuse of surface water, the galloping growth of the world's population, but also to clumsy water governance in certain regions and countries, the sharp increase in groundwater extraction, and in the future the effect of climate change will further affect water availability.

In fact, around 70% of the earth's surface is covered by water. However, 97% of this water is salty, as it comes from the seas and oceans. Only 3% of the earth's water is fresh water. Freshwater is water containing less than one gram per litre of salts, metals and nutrients. According to recent estimates, 39% of the world's population lives less than 100 km from the sea, which is why desalination has become a major new source of fresh water.

Desalination of seawater and brackish water is one possible response to water crises and shortages. In our work we have explored one of the desalination methods based on Reverse Osmosis, using a layer of a two-dimensional material as a membrane in the filtration process of this fluid. Our work deals in particular with one of the aspects in the salty fluid (water) that is filtration of the salt ions present in the water by taking into account certain physico-chemical aspects of the material. The choice of material used is based on certain properties such as a two-dimensional nanoporous material, mechanical resistivity, thickness, composition and insolubility in water. These criteria led us to choose a material from the Transition Metal Dichalcogenide (TMD) family, the chosen material being molybdenum disulphide.

Given the size of the particles and the simulation time required, the ideal method is based on molecular dynamics. The simulation will therefore describe the system on an atomic scale by

describing the movement of the atoms (chlorine and sodium) and molecules (water) that make up our system. We used the Lenard Jones and Coulombian potentials to describe the interactions between the water molecules and the chlorine and sodium atoms respectively. The hardware we used to model our system was VESTA (Visualization for Electronic and Structural Analysis) and Packmol, and for the simulation code we used LAMMPS (Large-Scale Atomic/Molecular Massively Parallel Simulator) and some basic tools for representing the results. For the simulations we chose pressures of 50MPa, 100MPa, 150MPa, 200MPa, 250MPa and 1000MPa respectively and simulation times ranging from 0ns to 10ns with a composition of 900 water molecules and 32 salt ions (16 chlorine and sodium atoms). The simulation was carried out on a molybdenum disulphide monolayer with a pore size of 1nm.

The results obtained in this study were based on the following parameters: the number of water molecules filtered, the permeability of molybdenum disulphide to water and the salt rejection rate. For the first parameter studied (number of water molecules filtered), our results indicate that the rate of molecule passage is relatively low and constant, and that the yield is below average. For low pressures (<50MPa) and for a pressure range of 100MPa to 250MPa, our results show a better yield for the passage of water molecules, ranging from 77% to 88%, and when the pressure is 1000MPa, the yield is almost perfect at 99%, illustrating the fact that the passage of molecules is better than for high applied pressures. Our results on the study of the water permeability of a molybdenum disulphide monolayer indicate a very high permeability through the nanopores of the material and the yield is better for fairly low linearity times (1.8ns and 2ns) over a pressure range of 100MPa to 250MPa these compared with the other materials studied previously. The last parameter studied was the salt rejection rate. The pore sizes we achieved on the molybdenum disulphide monolayer indicate much better performance at low applied pressures. A perfect yield of 100% for pressures less than or equal to 50MPa this yield decreases with increasing pressure. For pressures ranging from 100MPa to 250MPa, the yield indicates a slight variation in salt rejection of 65% to 90% and for a pressure of 1000MPa the salt rejection is very low at 40%.

In short, our study shows that molybdenum disulphide is a very good material for the water desalination process. The results obtained in the study of a monolayer of this material are highly relevant, as the performance of molybdenum disulphide allows us to predict that this study could well be developed on a large industrial scale to solve the problem of access to drinking water for a large proportion of the world's population.

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