UNIVERSITI TEKNOLOGI MARA

WATER-SURFACTANT-SILICA NANOPARTICLES MOLECULAR INTERACTION USING MOLECULAR DYNAMIC TECHNIQUE

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ABSTRACT

Enhance oil recovery (EOR) using surfactant flooding has challenge in maintaining the foam during the process. Application of nanotechnology and silica have been found can play a role in helping to EOR but its molecular dynamic interface abilities and interactions behavior not widely known. The molecular dynamic is prediction tool for researchers to predict the output process. It is necessary to simulate the interface of water, Alpha Olefin Sulfonate (AOS) surfactant and silica nanoparticle using molecular dynamics simulations and to study the molecular interactions behaviours and understanding the structural and dynamic information from diffusivity and surface tension. The silica nanoparticles were constructed into a ring shape as to study the interaction in terms of two-dimensional. From the molecular dynamic simulation, the mean square displacement (MSD) graph was plotted to find the diffusivity of the AOS into the system. The cohesive energy density (CeD) was obtained from the simulation and used to calculate the surface tension. The molecular dynamics simulation ran in this study has found that the presence of silica nanoparticle did not improve the mobility of the surfactant. This is because the comparison between a system that does not have the presence of silica nanoparticles shows that its diffusivity value was higher and has lower surface tension than a system contain silica nanoparticles.

Keywords— **Enhanced Oil Recovery, Surfactant Flooding, Silica Nanoparticles, Alpha Olefin Sulfonate, Molecular Dynamics.**

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CHAPTER ONE

INTRODUCTION

1.1 RESEARCH BACKGROUND

Crude oil from reservoirs that left after primary and secondary oil recovery contain about two-third of the original oil in place. Much of the original oil is trapped by the high capillary pressure from water in the reservoir's pores. Enhanced Oil Recovery (EOR) or tertiary recovery is introduced to extract more oil remain in the reservoir up to 80% of the unrecoverable oil reserves (Envirofluid, 2014). The importance of EOR is emerging now because of the recent global rise in energy demand which is expected to be met by the oil and gas industry (Ogolo et al, 2012). Surfactant flooding is one of the current chemical EOR methods used where mixture of water and surfactant is flooded in the oil reservoir to form an oil bank. This method can creates advantageous conditions in order to mobilize trapped oil (Sandersen, S. B., n.d.).

In EOR using chemical method, surfactant flooding bring enhancement due to its ability to interact with water and oil. Surfactants consist of a polar which is a head section that attract with water and a non-polar which is a tail section that attract with oil. These characteristics play a key role in EOR as it will help in the process of oil detachment from rocks or pores in the reservoir and form emulsions that can ease the sweep efficiency. The wetting agents have in surfactant makes the interfacial tension between oil and water to decrease, allow it to overcome the high capillary pressure required to move oil out of very small pores (Emegwalu, 2009). Among the many types of surfactants, alpha olefin sulfonate (AOS) surfactant was figured out as a good candidate in this surfactant flooding in EOR due to its high compatibility in hard water, high detergency capability and good wetting and foaming properties. The drawback applying this method is that the foam is not stable which may led to easily to break due to extreme reservoir conditions and high loss-rate of surfactant during the process (Khezrnejad et al, 2014). It is challenging as high salinity and high temperature may not provide the conducive condition for the foam to work at best (Kokal, 2010).