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Fe/starch nanoparticle - *Pseudomonas aeruginosa*: Bio-physiochemical and MD studies

Soheil Rezazadeh Mofradnia [a], Zahra Tavakoli [b], Fatemeh Yazdian [b], Hamid Rashedi [c], Behnam Rasekh [d,*]

[a] Department of Chemical Engineering, Faculty of Engineering, Islamic Azad University North Tehran Branch, Tehran, Iran
[b] Department of Life Science Engineering, Faculty of New Science & Technology, University of Tehran, Tehran, Iran
[c] School of Chemical Engineering, College of Engineering, University of Tehran, Tehran, Iran
[d] Microbiology and Biotechnology Research Group, Research Institute of Petroleum Industry, Tehran, Iran

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ABSTRACT

In this research, we attempt to study biosurfactant production by *Pseudomonas aeruginosa* using Fe/starch nanoparticles. Fe/starch showed no bacterial toxicity at 1 mg/ml and increased the growth rate and biosurfactant production up to 23.91 and 20.62%, respectively. Surface tension, dry weight cell, and emulsification indexes (E24) were measured. Biosurfactant production was considered via computational techniques and molecular dynamic (MD) simulation through flexible and periodic conditions (by material studio software) as well. The results of software predictions demonstrate by radial distribution function (RDF), density, energy and temperature graphs. According to the present experimental results, increased 30% growth of the bacterium has been observed and the subsequent production of biosurfactant. The difference between the experimental results and simulation data were achieved up to 0.17 g/cm^3, which confirms the prediction of data by the software due to a difference of less than 14.5% (ideal error value is 20%).

1. Introduction

Due to enhancement of request for fossil fuels and the necessity of retrieving more of these reservoirs and the inability to completely exploitation of these reservoirs resulted in requirement for a new technology and biodegradable conditions [1–3].

Nowadays, environmental conservation and non-damage of the natural environment are one of the essential parameters of the process. The importance of microbial enhanced oil recovery processes has been attended as the new generation of studies and recovery techniques [2,3]. Microbial oil recovery (MEOR) is one of the enhanced oil recovery methods, in which bacteria and their byproducts are used to increase the oil stimulus in a reservoir [4,5]. Biosurfactant production is as a biodegradable and more advantageous element than artificial ones in EOR. Biosurfactants are secondary extracellular metabolites. These are produced at the initial of inertia phase by various species of microorganisms, including bacteria, fungi, and yeasts, which depending on the producer, has different chemical properties and molecular size [6,7].

To accelerate the biosurfactants production and to use nanotechnology and green engineering, metal nanoparticles application is a new study that has been welcomed and used by the adding various types of metal nanoparticles with microorganisms, intended to produce biosurfactants. Mono-metallic nanoparticles such as iron and gold nanoparticles effect on the biosurfactants production, an incorporation of two or more alloys or using different metals [8] have greater effects besides microorganisms. A study on the interaction of nanoparticles with bacteria is of increasing interest. Different reports also have shown that nanoparticles can improve the growth of bacteria and biosurfactant production [9]. Zero-valent iron nanoparticles tend to condense rapidly that leads to loss of their reactivity. Hence, dispersion of Fe^0 nanoparticles is an essential step to improving the efficiency of their reaction. Numerous particle-stabilizing agents have been used including carboxymethyl- cellulose, starch and resin. Starch is a nontoxic, inexpensive and substance biodegradable that can be used as an effective dispersant for iron nanoparticles [10,11]. Certainly, it should be noted that about microorganisms' difference can be seen in the results because the study of this product is conducted by microorganisms such as *Bacillus*, *Bacillus subtilis*, *E. coli* [12] and *Nocardiopsis* sp. [10] which each of them alone has shown different production results and quality of it.

The difference is also evident in alloy type and how to use, and it affects the production system. Bioinformatics surveys and molecular dynamics simulation have led to many improvements in the molecular domain targeting two different subjects and significant issues. Accurate use of thermodynamic and physical parameters achieved the prominent analysis.

* Corresponding author.
E-mail address: rasekhb@ripi.ir (B. Rasekh).

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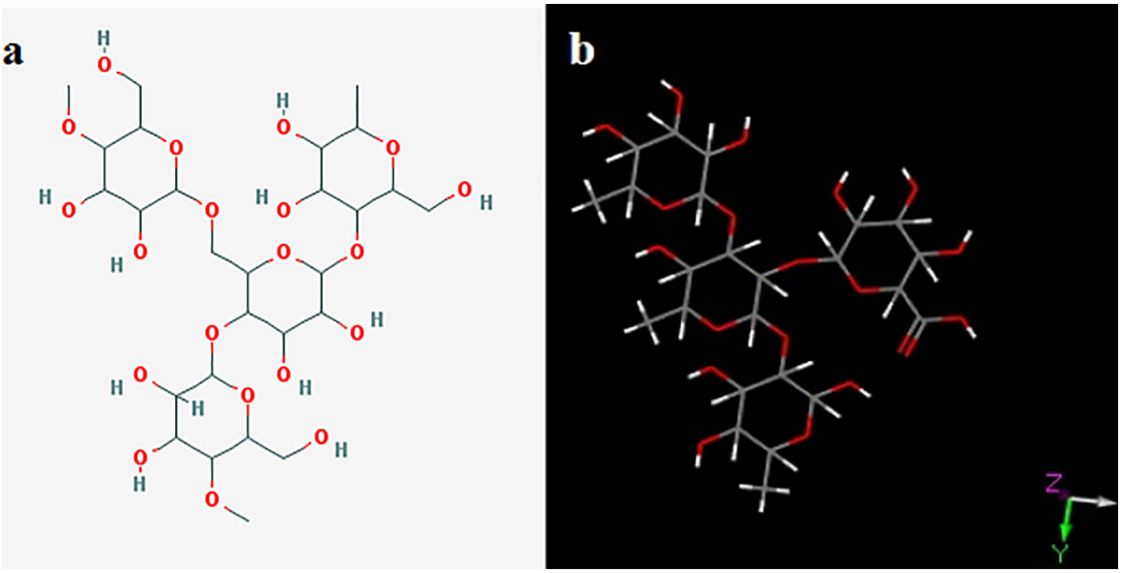

Fig. 1. a. Chemical structure of Starch. b. Spatial structure of Starch in software.

Molecular dynamics simulation predicts the structure and main properties of the material such as stability, intermolecular penetration, and interactions between phases [13]. In targeted drugstore field, molecular dynamics software allows us to study the properties of the drug molecule and interactions between them by disbursing the minimum cost for experimental methods [14,15]. Furthermore, molecular dynamic simulation can be employed to study the behavior of complex materials in molecular-scale of various science branches, especially nanotechnology and biology [16]. This kind of simulations has noticed in many sub-disciplines because of predictability of drug effect. The most crucial studies in the field of medicine are biologic treatments for prevalent cancers, using structures such as mycelium and liposome [17,18]. Meanwhile, the study of drug components influence, manufacture of pharmaceutical structures, and extraction of the best formulation is one of the molecular simulations strengths [17,19–21].

Application of this software has become so popular and progressed that in numerous industrial infrastructure sciences and conductivities [22,23]. In many morphological structures [24], the effect of material size on reactivity and on thermodynamic parameters [25], investigation of effects of temperature and some elements that could influence on conductivity [26], solid state recrystallization during the thermal and mechanical annealing of nano-particles and other structure [27,28] were investigated by MD studies. The survey of dynamic properties and heat exchange effects [29,30], direct targeting by nanoparticle [31] were moreover studied via molecular dynamics simulation.

In this paper, we try to make a prominent study in Nano-based manufacturing fields on the biosurfactant production, using metallic zero-capacity nanoparticles through engineering analyzes and fundamental principles of chemical engineering and nanotechnology. Biomass, surface tension and Emulsification activity (E24) were evaluated, too. Therefore, we studied the interactions between the zero-valent iron nanoparticles and *Pseudomonas aeruginosa*, as a production model, to investigate the effects of nanoparticles on biosurfactant production and microorganism growth. Activity, stability and structure of *Pseudomonas aeruginosa* were analyzed while nanoparticles were added to the medium. The mechanism of interactions between the nanoparticles and *Pseudomonas aeruginosa* was considered by molecular dynamics simulation. The thermodynamic interaction process between the zero-valent iron nanoparticles and *Pseudomonas aeruginosa* were considered as well.

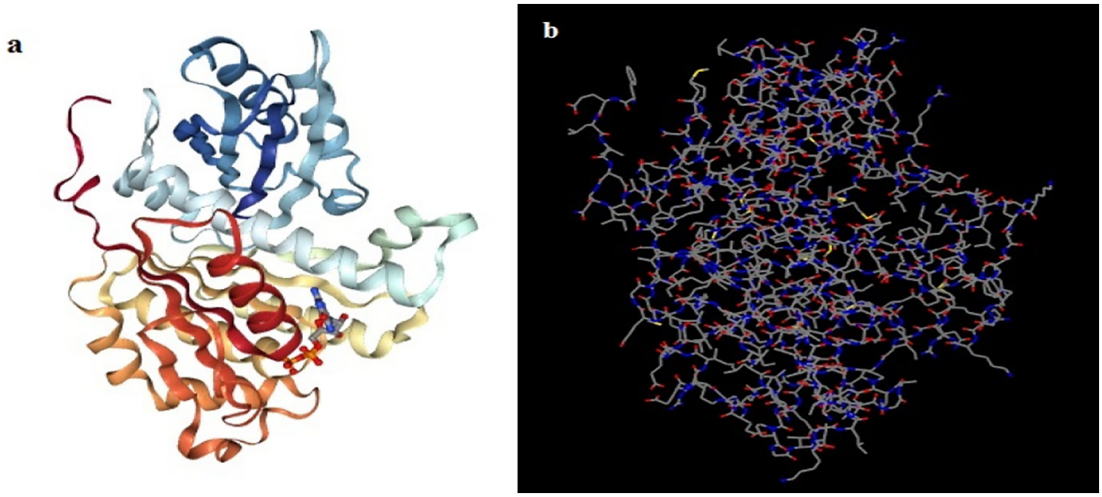

Fig. 2. a. Spatial structure of *Pseudomonas aeruginosa* in RCSB. b. Structure of microorganism after loading in software.