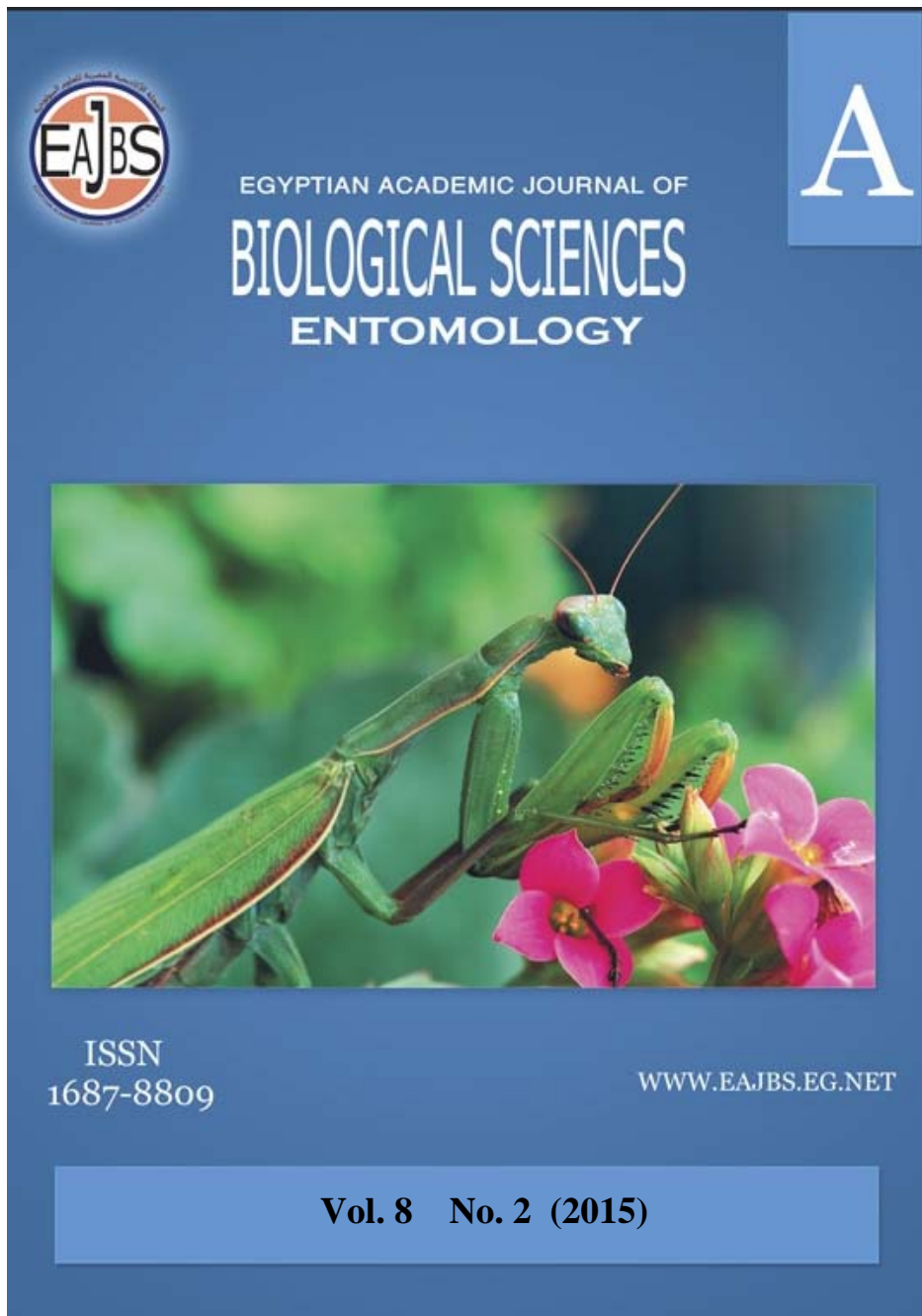


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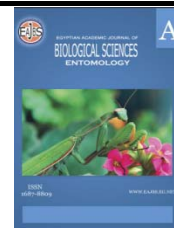


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The Theoretical Study of Molecular Dynamics To Design An Ultra-nano-Filtration For Diazinon Removal In Water Median

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ABSTRACT

Accumulation of pesticides in particular organophosphorus in water achieved a global warning. Therefore, acquiring technical knowledge on ultrafiltration is necessary in environmental purification. Theoretical designs are the first step in construction of a successful commercial product. In this research, three models of single-wall-carbon-nanotube (SWCNTs) were simulated by NAMD software to assess potential application as an adsorbent. Diazinon entrapping in SWCNTs is the desirable result. Three SWCNT models include: CNT 5,20 (diameter 5 nm, length 20 nm), CNT 10,20 (diameter 10 nm, length 20 nm) and CNT 10,20-SEM (diameter 10 nm, length 20 nm by flowing water and external electrical filed). The CNT 10,20-SEM demonstrated suitable entrapping process and potential ability to apply in industrial filtration.

INTRODUCTION

Accumulation of toxins in food, water, soil and air is one of the important concerns of human and the environmental health. Based on statistical reports from around the world, over 1 billion pounds of pesticides are used in the United State (US) each year and approximately 5.6 billion pounds are used worldwide (Alavanja 2009). Since dangerous effects of pesticides are accumulated in body during long time, people mostly ignore the mentioned risk. In many studies, the effect of organic chemicals is examined in soil, aquatic environment and the resulting toxicity on plants and animals. Accumulation of toxic compounds high half-life such as synthetic chemicals, pesticides, salts, heavy metals and radioactive substances in soil and water have adverse effects on growing of plants, animals and human health. The final destination of major part of pesticides, especially in developing countries, is surface water and groundwater sources, soil, and eventually human body. According to the report published by the World Health Organization, pesticide poisonings doubled in developing countries during the past decade (Shah and Iqbal 2010). The organophosphates, common insecticides were used, known generally as one of the most dangerous components among pesticides. Residual of organophosphate pesticides are common pollutants in ecosystem, and food (Baireddy *et al.* 2011).The

acetyl cholinesterase (AChE) enzyme as primary objective inhibited by organophosphates, which results in accumulation of acetylcholine (Colovic *et al.* 2010; Baireddy *et al.* 2011). Toxicity effects of organophosphates disrupt wide range of organs, vital systems of the body (Shah and Iqbal 2010), and produce free radicals (Hariri *et al.* 2010). Diazinon and Chlorpyrifos are commonly used thionophosphorous organophosphate pesticides (Colovic *et al.* 2010; Morgan *et al.* 2011) which can be penetrated through the digestive system, the skin, and respiratory tract (Shah and Iqbal 2010). Updated documentation of pesticide removal by CNTs introduced following. The water contaminated by Diuron and Dichlobenil (herbicides) was refined by MWCNTs (Chen *et al.* 2011). The potential of modified MWCNTs to Diuron adsorption were documented by Deng *et al.* (2012a). The capacity of SWCNTs tested for adsorption of a phenoxy acid herbicide (4-chloro-2-methylphenoxyacetic acid). Over-ally, the use of CNTs for pesticide removal appears to be less studied than other organic contaminants. Considering the wide-spread use of pesticides, more effect, should be directed to investigate the removal of pesticide residues from drinking water and wastewater (Yu *et al.* 2014). It is hard to study the CNT–pesticide interface by experimental methods, thus many researchers use the molecular simulation (MD) as the Computational Molecular Microscope (Reza Kalani and Tajkhorshid 2014). For example, interaction between SWCNTs and polymers was studied by molecular dynamics simulation (Zaminpayma and Mirabbaszadeh 2012). In this research, three models of single-wall-carbon-nanotube (SWCNTs) were simulated by NAMD software to assess potential application as an adsorbent. Three SWCNT models include: CNT 5,20 (diameter 5 nm, length 20 nm), CNT 10,20 (diameter 10 nm, length 20 nm) and CNT 10,20-SEM (diameter 10 nm, length 20 nm by flowing water and external electrical filed).

MATERIALS AND METHODS

Molecular dynamics simulation:

MD simulations were done with molecular dynamics software called NAMD (Phillips *et al.* 2005). The CHARMM and CHARMM General Force Field (CGFF) were used for parameterization of absorbent and pesticides (Mayne *et al.* 2013). The molecular models and structure file of CNTs were built with Tcl-Tk console of VMD software. The absorbent complex were composited with one nanotube that both ends covered by two water boxes. The pesticides were placed in water box. Periodic boundary conditions were applied on a 19, 19, 52 Å box with the long-range electrostatics calculated using the particle-mesh Ewald method (PMEGridSpacing 1.0 Å). Simulation spaces partitioning were configured by switchdist 9 Å, cutoff 10 Å and pairlistdist 12 Å. The complex was neutralized with sodium chloride. All the simulations were performed in the constant temperature and constant volume canonical ensemble (NVT). To accelerate simulation, all-atoms of nanotubes were fixed. The Verlet algorithm with time step of 2 fs was used for calculating the motions. Constant temperature controlled by Langevin dynamics with damping coefficient (γ) of 1/ps. The equilibration stage was 100 ps. After this stage, the total simulations were conducted for 10 ns. The main idea of this section was filtration of pesticides by nanomaterial in industrial process. To simulate a flow in pipe purifier, a constant force of 0.2 Kcal/mol/Å along the -z direction was applied to a 5.7 Å -thick water layer. External electric force field applied in household water filtration systems was simulated by 0.15 kcal/mol/ Å /e in -y direction.

RESULTS AND DISSECTION

Simulation of Diazinon Entrapment into SWCNTs

In the all simulation models, the dynamic process of entrapping Diazinon has been simulated with SWCNTs. Three models of SWCNT were constructed including armchair (5,20) with water permeation force, (10,20) with water permeation force and (10,20) with water flow force (0.2 Kcal/mol/Å) in external electrical force field. The entrapping process is shown in Figure 1. In the same configurations, Diazinon was aligned along one side of channel nanotube. In armchair (5,20) SWCNT, the insertion stage (As one of the most important steps in trapping) into SWCNT was failed at all simulation time. The same phoneme was occurred in armchair (10,20) SWCNT with a little difference. Initially permeation force endeavored to insert Diazinon but pyrimidine residues prevented (Fig. 1).

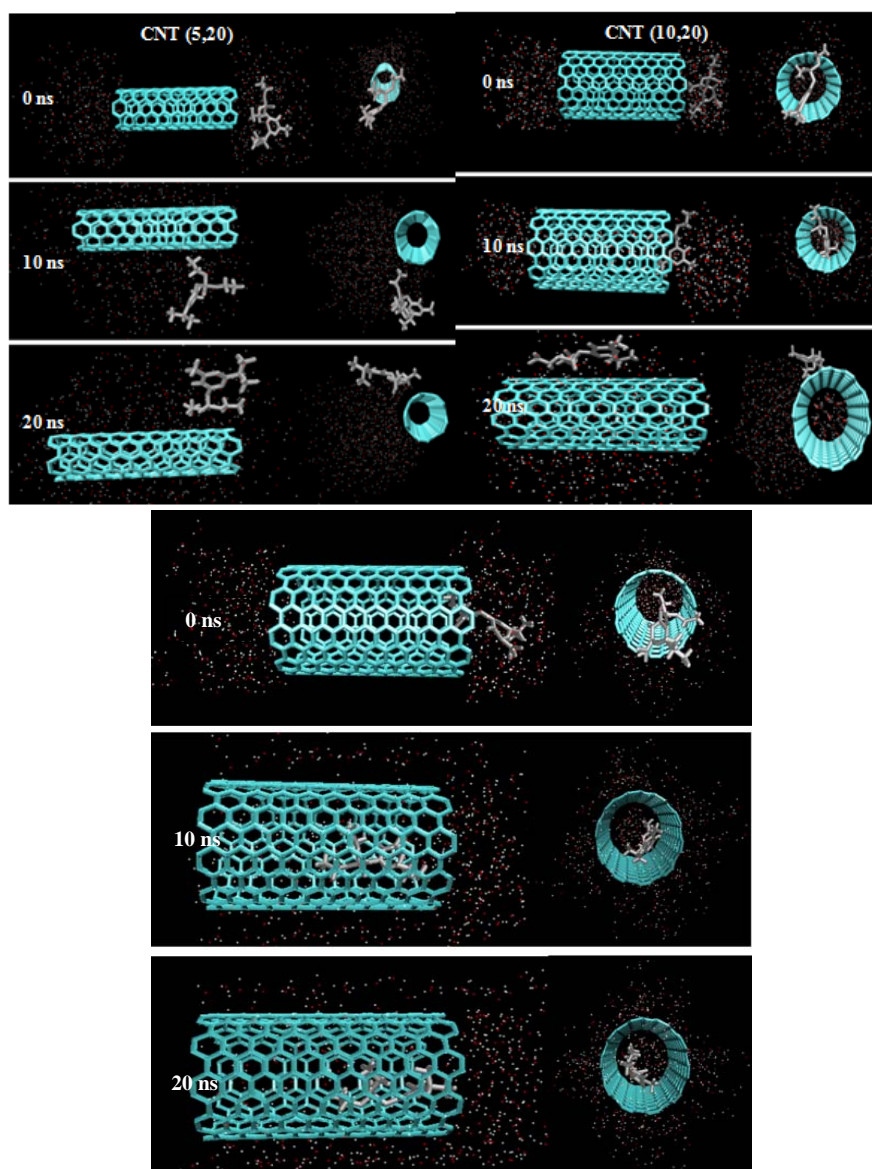


Fig. 1: Entrapping process of Diazinon into three nano-adsorbent in three-episode times of MD (0 ns, 10 ns and 20 ns)

Continuous movement of water molecules ejected aliphatic residues out. Failing in insertion process caused Diazinon immersion on the outside the nanotube which means the failure in entrapping process (Fig. 1). The full entrapping of Diazinon into SWCNT (1020-SEM) was completed at around $t=1$ ps. To monitor and confirm entrapment, root mean square deviations (RMSD), fluctuations (RMSF) and the distance (d) between centre of Diazinon and SWCNT were utilized. RMSD values of Diazinon were used to monitor the conformational stability of absorbent. In fact, the null hypothesis was analyte that was absorbed inner channel of CNTs with the least movement and fluctuations. The focus of RMSD values shows Diazinon entrapping and stabilizing occurred only in SWCNT (1020-SEM) (Fig. 2). RMSD plot of SWCNT (1020-V) confirmed the insertion of aliphatic residue at 0-14 ns and then the ejection of Diazinon.

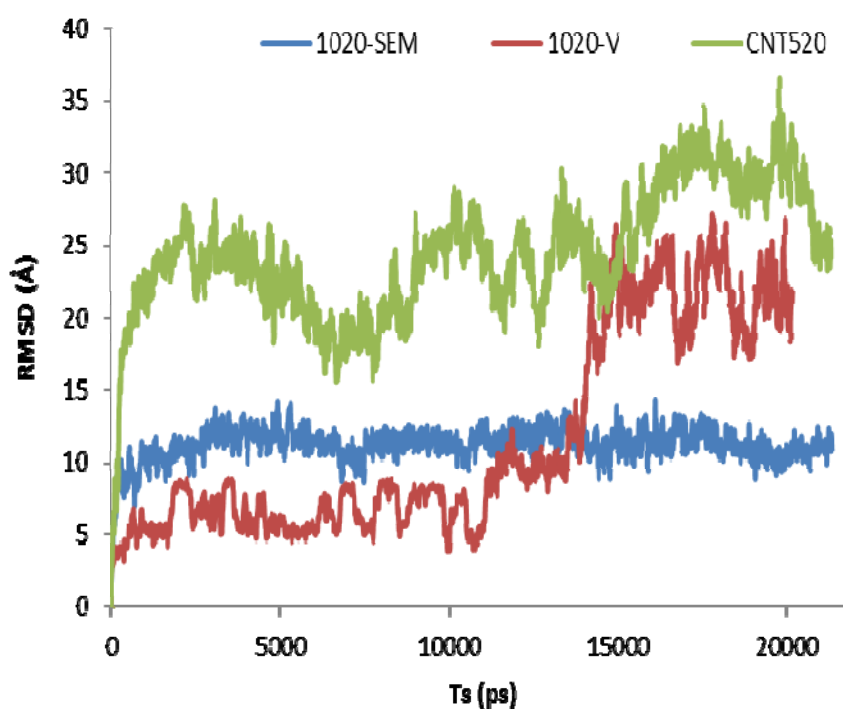


Fig. 2: RMSD fluctuation of Diazinon showed conformation stability in molecular dynamics

This ejection caused Diazinon instability and untrapping phoneme. RMSF values measured residue flexibility over the whole simulation time. RMSF plot of SWCNT (10,20-V) displayed insertion failure at 14 ns and consequently increasing in Diazinon fluctuations (Fig. 3c). RMSF data were not efficient in demonstrating the entrapping process while clearly described the entry and ejector process of Diazinon (Fig. 3). Assessing the distance fluctuations play an important role in the evaluation of Diazinon encapsulation.

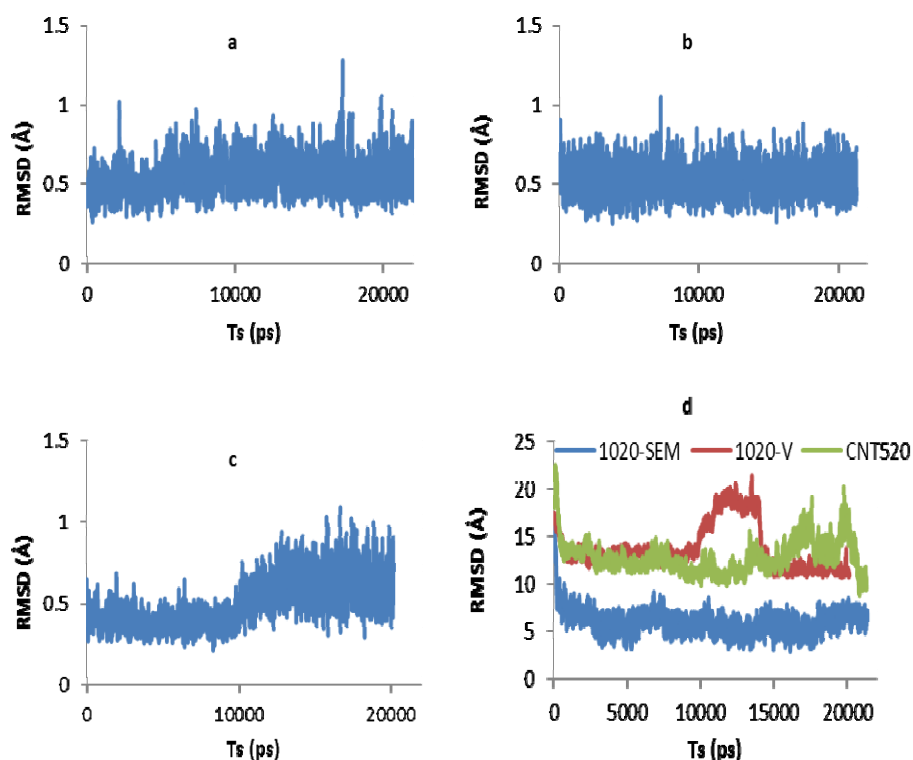


Fig. 3: RMSF fluctuation of Diazinon showed conformation flexibility in molecular dynamics (a) RMSF CNT(5,20), (b) RMSF CNT(10,20-V) and (c) RMSF CNT(10,20-SEM); (d) distance plot between center of Diazinon and SWCNTs

The distance (d) between Diazinon and SWCNTs as a function of simulation time showed in Figure 3d. The distance curve of SWCNT (1020-SEM) decreases rapidly at the first 1 ps (confirm very fast spontaneous insertion) and plateaued at all timescale of MD (confirm Diazinon fixed appropriated opposition inner SWCNT). The distance results in the SWCNT (1020-V) are consistent with the RMSD and RMSF results. In order to assess the potential effects of the SWCNT diameter and external electrical force field on the entrapping of Diazinon, the dynamic simulations of one Diazinon molecule into three models of SWCNTs were used.

The present results indicated that Diazinon cannot spontaneously entrap into the SWCNT (5,20) and (10,20-V). Because of the electron flow in y axis in (10,20-SEM) SWCNT, Diazinon was rotated in suitable direction to enter the nanotube channel. The external diameter and length of CNTs on the pesticides recovery was documented by (El-Sheikh *et al.* 2007). The mentioned researcher reported that the highest recovery was correlated with external diameters of CNTs and kind of pesticides. The sorption rate followed the appropriate surface/volume ratio of CNTs, which is in well agreement with the current simulation results. The electrocoagulation process is developed treatment for filtrated water and wastewater. This technique is invasive method because it uses electrodes and transferring electron without adding any materials. The simulation trajectory analysis of SWCNT (1020-SEM) was consistent with the experimental electrocoagulation results which were performed by (Bazrafshan *et al.* 2007). Bazrafshan (*et al.* 2007) were reported that electrocoagulation process (iron electrodes) was suitable technique for Diazinon removal from aqueous solution (optimal condition pH=3 and voltage=40 V DC). the current simulation results have good agreement with Bazrafshan (*et al.* 2007) report.

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