Damghan University Press

Journal of Nano Simulation
journal homepage: jons.du.ac.ir

Volume 2, Issue2, Spring 2026, 1-9
DOI: 10.22128/jons.2026.3170.1015

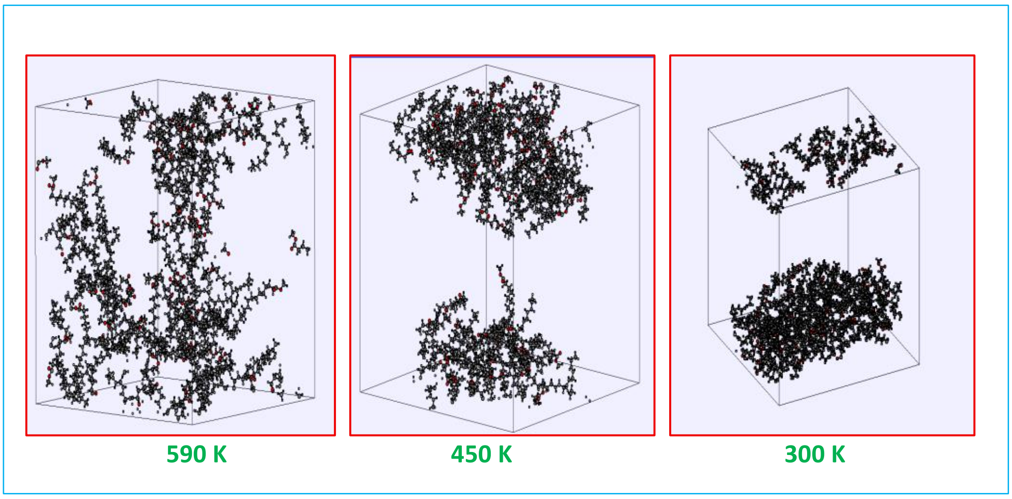
Evaluation of structural and bulk properties of α -Linoleate methyl ester biodiesel using Molecular Dynamics simulations

Mahvash Yarahmadi*, Jaber Jahanbin Sardroodi
Molecular Simulation Lab., Azarbaijan Shahid Madani University, Tabriz, Iran.

HIGHLIGHTS

- Structural and bulk properties of α-linoleate methyl ester biodiesel were evaluated using DFT, Monte Carlo, and Molecular Dynamics simulations.
- DFT was used to obtain the lowest-energy optimized structure of α-linoleate methyl ester in vacuum.
- Monte Carlo configurations were employed as input for Molecular Dynamics at 298 K and 1 atm to model the liquid phase.
- An annealing cycle from 600 K to 300 K with NPT MD was applied to explore equilibrium properties at ambient conditions.
- Molecular Dynamics showed the best agreement with experimental data, highlighting its suitability for predicting biodiesel behavior.

GRAPHICALABSTRACT



ARTICLE INFO

Article history:
Received: 2025-11-29
Received in revised form: 2026-02-10
Accepted: 2026-05-29

Available online

Keywords:
α-Linoleate Methyl ester
DFT
Monte Carlo
Molecular Dynamics
Biodiesel

ABSTRACT

Today, replacing fossil fuels with biofuels is essential due to their pollution and non-renewability. Biodiesel, a biofuel, has unique environmental properties and similar performance to diesel fuel. The strategic component of biodiesel is the α-linoleate methyl ester molecule, in which the acidic properties of fatty acid chains, hydrogen bond formation strength, and other thermodynamic parameters that determine the quality of biodiesel have not been well studied. In this study the bulk properties of α -linoleate methyl ester has been investigated using molecular dynamics computations. At first step, the optimization structural with the least energy for a α- Linoleate methyl ester molecule in the vacuum state was determinate by the density functional theory (DFT). In the second step, the state and equilibrium phase of a set of α- Linoleate methyl ester molecules were simulated using two methods: Monte Carlo and Molecular Dynamics. At this step, the Monte Carlo simulation output was used as the Molecular Dynamics input, and the Molecular Dynamics simulation was run at a temperature of 298K and a pressure of 1 atm. In the third step, the system was converted to a gaseous state at 600K and brought to 300K using the annealing technique. At 300K, Molecular Dynamics was performed in the NPT ensemble. The results of these simulations were compared with together and with experimental data to gain a better understanding of the structure and behavior of this compound under different conditions and it was observed that Molecular Dynamics provided the best results.

Aurhor corresponding mahvashyarahmadi832@gmail.com

1- Introduction

Clean fuels operate cleaner than gasoline due to their inherent physical and chemical properties [1-3]. Combustion of clean fuels produces fewer unburned compounds and environmentally harmless products with less chemical activity for ozone formation [4,5]. Clean fuels also reduce the intensity of the increase and accumulation of atmospheric CO2, thus helping to better control global warming [6,7]. Biodiesel is one of the best clean fuels, produced from mono alkyl esters of long-chain fatty acids from renewable natural resources such as vegetable oils or animal fats [8]. The edible and non-edible vegetable oils used to produce biodiesel including rice bran, jatropha, coconut, castor, soybean, cottonseed, sunflower, peanut, safflower, palm oil, and any other non-edible waste, can be used to make biodiesel [9-11]. Biodiesel molecules are simple hydrocarbon chains that do not contain aromatic and sulfur substances, they use a large amount of O2, which makes complete combustion more reliable [12]. The most important advantages of biodiesel fuel include: similarity to diesel fuel in many physical and chemical properties[13], sustainable development, non-toxicity and recyclability up to 100 times [14], Biodiesel is carbon neutral (all CO2 released during consumption is absorbed from the atmosphere for the growth of the oil plant) [15], increased efficiency and engine lifetime with good lubricating properties[16], unlimited miscibility with diesel fuel in any ratio without changing the structure of diesel engines[17].

The general process for producing biodiesel, after refining the oil-free gum extract and drying it, is a two-step process: first, esterification of the fatty acid with an acidic catalyst, and then transesterification of the triglyceride with an alkaline catalyst [18]. Figure 1 shows the overall reaction for producing biodiesel.

In this reaction, biodiesel is produced through the transesterification of vegetable oils or animal fats with short-chain alcohols, typically methanol or ethanol, in the presence of a catalyst. This process yields fatty acid methyl esters (FAMEs), which are the primary components of biodiesel, and glycerol as a byproduct [19].

Among these FAMEs, α-linoleate methyl ester is an important component derived from linoleic acid, a polyunsaturated fatty acid found in various vegetable oils. The α-linoleate methyl ester is an essential component for improving biodiesel properties, such as viscosity and combustion characteristics, and contributes to its quality and performance [20]. This compound provides oxidative stability to biodiesel for storage and uses in diesel engines [21]. Standards such as EN 14214 specify an acceptable range of α-linoleate methyl ester content in biodiesel fuel to ensure optimal performance and stability, typically between 1% and 15% by mass [22].

Given the hundreds of times increase in oil prices over the past half century, the increasing energy consumption due to the growth of the world's population, and the non-renewable nature of fossil resources, extensive research has been conducted on alternative fuels, especially biodiesel fuels. In a research work to improve the performance of biodiesel at low temperatures and reduce production costs, the pyrolysis process has been used to produce low molecular weight compounds with high energy density. In this research, the pyrolysis pathway has been investigated at the atomic scale using ab initio calculations and suitable reactants have been engineered to maximize the energy of the molecules created. The

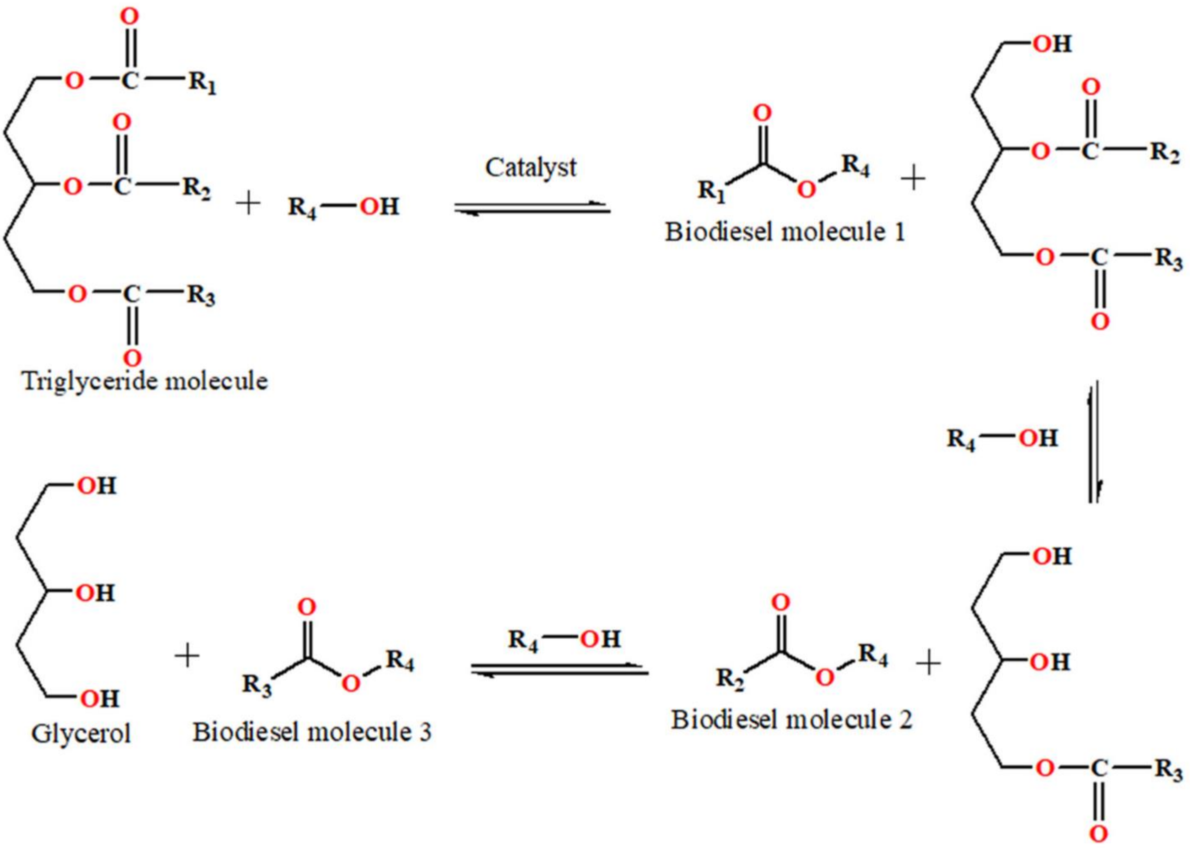


Figure 1. Three-step transesterification process of biodiesel producing.

thermodynamic properties of these molecules have been determined using molecular dynamics calculations [23]. Poonam Syal and et al. have developed a method to replace acidic or alkaline catalysts with enzymatic catalysis to producing clean biodiesel with greener grade. In this method, targeted motions and MD simulations of a methanol-stable lipase YLIP9 from Yarrowia lipolytica MSR80 were studied to develop a biodiesel enzyme. This enzyme increased the transesterification rate of palm oil in the presence of methanol by 8-fold [24]. The engineered thermal cracking mechanisms at the atomic level of methyl linoleate and methyl oleate have been studied using B3LYP, M06-2X, and B97D density functional theory methods in order to produce thermally stable biodiesel [25]. The liquid-vapor equilibrium as a function of temperature and surface tension of three pure long-chain fatty acids (linoleic, oleic, and palmitic acids) and the extrapolation of critical point properties were performed using molecular dynamics simulation and the direct determination of phase coexistence method [26]. Felipe A. Perdomo and et al. have developed a clever way to predict the thermophysical properties of biodiesels by evaluating the structure and composition of fatty acids using the SAFT-γ method. The global optimization is performed by implementing a simulated thermal annealing algorithm to determine the SAFT-γ parameters of groups that are fully representative of biodiesel compounds. These parameters are consistent with existing experimental data for similar chemical families such as secondary alkanols and short-chain esters. This method improves the quality and energy profile of biodiesel by modifying its structure and components [27]. Achieving coupled cluster theory using Kohn–Sham density functional theory (DFT) to accurately calculate the thermochemical properties of large biodiesel molecules; with this method, the bond dissociation enthalpies (BDEs) of seven molecules of methyl linolenate, propene, methyl formate, cis-3-hexene, 1,4-pentadiene, methyl butane, 1-pentadiene, 1-4-pentadiene, methyl butane, and 1-pentate were accurately obtained [28]. Investigations of the combustion dynamics of biodiesel produced by supercritical methanol transesterification show that increasing the number of C=C double bonds increase the combustion temperature, resulting in delayed combustion in the engine, such that the combustion temperature of biodiesel is lower than that of crude vegetable oil, but higher than that of petroleum diesel [29].

2. Computational Details

The geometries of the LAx molecule were optimized using different levels of quantum-chemical calculations. Pre-optimizations were performed by applying the molecular mechanics (MM) method using MM1 force field. The high computational speed of MM makes it easier to perform a better optimization using a higher level of computational methods. This optimized structure was taken and the semi-empirical self-consistent-field molecular-orbital (SCF-MO) method at PM3 level within the restricted Hartree–Fock (RHF) formalism was applied to fully optimize the structures and calculate the vibrational spectra. At the final stage, the geometry taken from PM3 was used to perform single-point calculations with the DFT. The DFT calculations were realized using the 6-31G basis set and hybrid functional B3LYP. The calculations MM and PM3 were carried out with the Gussian-09 program package [18].

Harmonic frequency analysis indicated that all stationary points were found to be true minima (there was no imaginary frequency). force constants using matrix Hessian is calculated and it is fully optimized and vibrational frequencies computed makes no negative force constant (k). Not existence the imaginary frequency means that the structure is the most stable state of the surface potential. Molecule α- Linoleate methyl ester with pack formulation ($C_{19}H_{32}O_2$) And the IUPAC name of cis, cis, cis – 9,12,15 – octadecatri enoulate methyl ester of esterified compounds derived from fatty acids plant oils.

3. Results and discussion

The naturally occurring cis configuration was always considered in the structure optimization. This constraint is also justified by the fact that the reaction rates of singlet oxygen with a double bond are optimized structure of the molecule α- Linoleate methyl ester along with the number of atoms and the diagram the convergence of the structure energy of the molecule (Figure 2) during the structural optimization using DFT calculations with B3LYP hybrid function with the basic set 6-31G show. As shown in the figure 3 the molecular shape curved (folded) by the calculation, it forms one of the best stats for energy minimum structure for stability and structural studies of molecules using AM1.

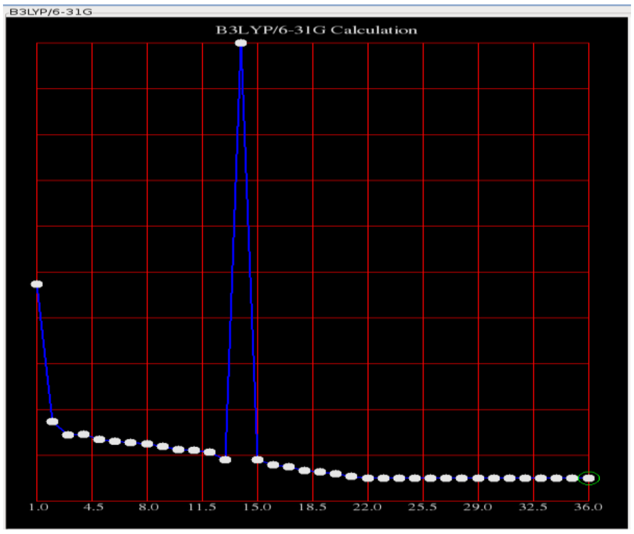


Figure 2. the optimized structure of the molecule α- Linoleate methyl ester using DFT calculations

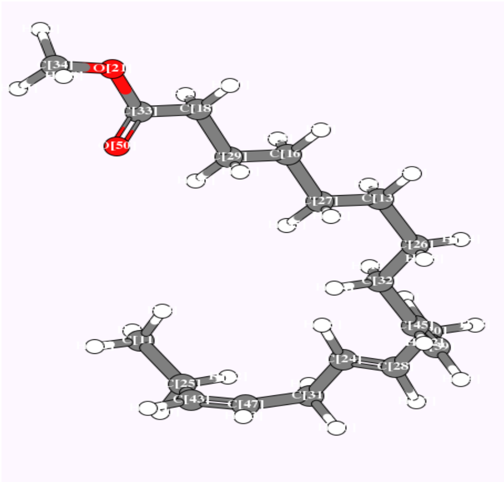


Figure 3. the convergence of the structure energy of the molecule α- Linoleate methyl ester during the structural optimization using DFT calculations

The electronic properties of molecules with computation methods B3LYP/6-31G obtained. The properties of dipole moment and molecular orbital is included. Figure 4 shows the highest occupied molecular orbitals (HOMO) as well as the dipole moment of the molecule is shown. HOMO orbitals in the molecule α- Linoleate methyl ester over carbon atoms with number 11 and 14 located where between double bonds C_{15}-C_{16}, C_{12}-C_{13}, C_9-C_{10}. As you can see in figure 5 the LUMO orbitals in the molecule α- Linoleate methyl ester is on the carbonyl group.

The electron parameters obtained with the same method have been shown in the Table 1.

Table 1. value of electron parameters obtained with single-point method

structure	E_g (eV)	LUMO (Hartree)	HOMO (Hartree)	Dipole moment (μ) (Debye)	Optimization energy (Hartree)
α-Linoleate methyl ester	-0.22203	-0.00860	-0.23063	+1.8337	-893.47

3.1. Calculation of Monte Carlo (MC) simulation

For MC calculation we need initial optimized structure. This structure obtained by DFT calculation were explained in the previous part.

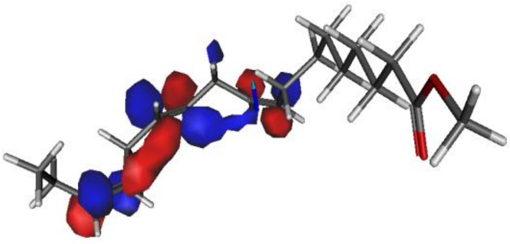


Figure 4. HOMO orbitals in the molecule α- Linoleate methyl ester.

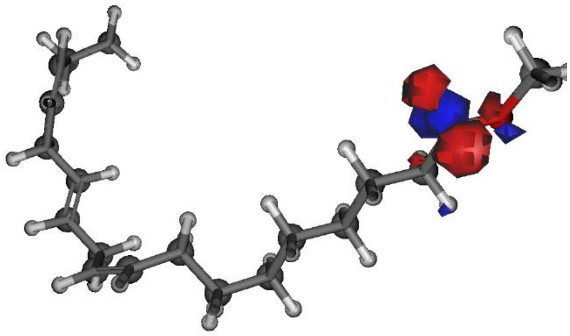


Figure 5. LUMO orbitals in the molecule α- Linoleate methyl ester.

Initial optimized structure has itself optimize energy and other structure parameters for creating input file of MC simulation. MC Simulation have been done in isothermal- isobaric ensemble, because of the pressure, temperature and number of moles is constant. To control path of the simulation density of the molecules have been calculated from the final volume. The MC simulation have been done to obtain the input files for molecular dynamics simulations. Because the molecular motions, configure stigmatized and more accurate structural parameters for molecular dynamics simulation input files provides by this way.

3.1.1. Computational details

Monte Carlo simulation studied by MCCCS Towhee7.0.2. software with Lennard-Jones potential. Simulations were implemented in conditions constant temperature of 298 K and constant pressure 1 bar. Force field used in the input file Dreiding. The number of 64 molecules were placed in the box. The calculating of Coulomb forces and periodic boundary conditions were applied in all directions. The used Coulomb forces cut off radius was 16 Å. Total number of Monte Carlo steps simulation was selected 1750000.

3.1.2. Monte Carlo analysis

To verification implementation of a true simulation at the end of the simulation, it must converge some thermodynamic parameters such as temperature, pressure and energy. For analysis of the Monte Carlo results evaluation of the energy fluctuations in the chart to ensure a proper simulator and radial distribution function in order to determine the phase diagram of the of molecules at ambient temperature are need.

3.1.2.1. Energy diagram

The total energy is the sum of kinetic and potential energy, so it must be a conserved quantity. For fluctuations of energy investigation, the energy change for each step can be evaluated by Monte Carlo simulation. Whatever in every step for more precise simulation and properties are calculated closer to reality. Figure 5 shows the energy fluctuations for molecule α- Linoleate methyl ester.

Whatever obvious in the Figure 6 is intensive decrease of energy. System stablished with decrease energy. After system being equilibrium, energy changes be very low and constant. Fluctuation value of energy was decreased about 0.763%.

3.1.2.2. The radial distribution functions

Considering the fact that the radial distribution function is a valuable measure to describe the structure of the system. It is important that we have a correct interpretation of the radial distribution function graphs. Figure 7 shows the radial distribution function of the molecule α- Linoleate methyl ester that obtained in the Monte Carlo calculations. The peak in distance 1 to 1.5 Å is related on bonding interactions. There is a link to this interaction that related to the double bonds.

The peak appeared in the region of 1.5 to 5 Å related to hydrogen bonding and van der Waals interactions and the peak in the range 5 to 6 related to coulomb interactions. The hydrogen and Coulomb interactions did not study in this system. Intensively and number of picks shows system in investigated conditions is liquid.

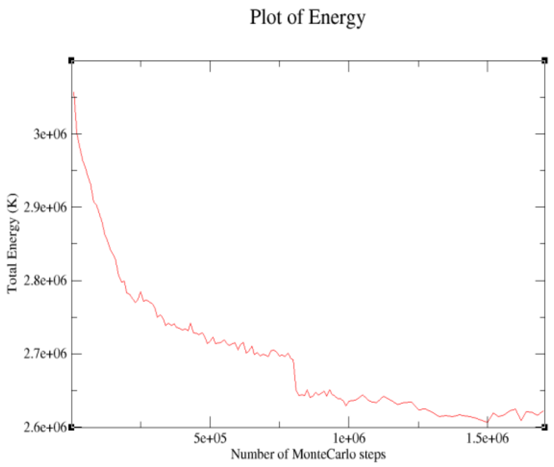


Figure 6. the energy fluctuations for molecule α- Linoleate methyl ester in MC simulation

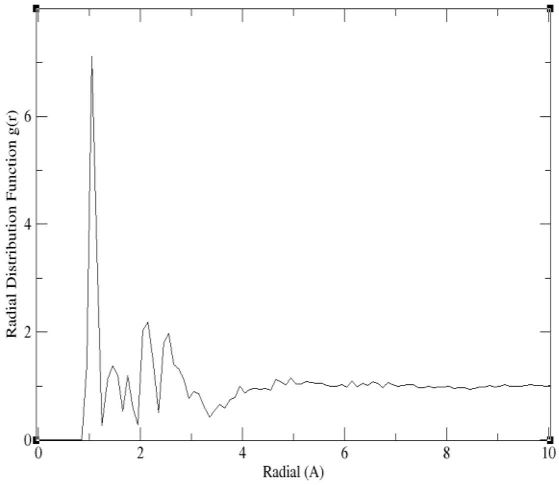


Figure 7 . The radial distribution function shows that the molecule α-Linoleate methyl ester was obtained in the Monte Carlo calculations.

3.2. Molecular dynamics simulations (constant pressure and temperature NPT)

Aimed of Biodiesel study in molecular dynamics simulations to obtain the thermodynamically stable at surrounding conditions is, therefore we can with molecular dynamics simulation molecule α- Linoleate methyl ester at constant pressure and temperature in the bulk state calculate these parameters. for calculations we need to appropriate input files. Due to the structural parameters were optimized with the DFT calculations couldn't create appropriate input files for software DL-POLY 1.9 classic, therefor the Monte Carlo calculations to create two FIELD and CONFIG files. Monte Carlo calculations appropriate structural parameters and random configurations for set of molecules in the system to calculation of MD provides.

3.2.1. Computational details

Molecular Dynamic simulation run with software DL-POLY classic 1.9. Motion equation is differentialized with jumping Verlet algorithm and periodic boundary conditions were applied in all directions and Lennard-Jones potential is performed with cut off 8Å. We used berendsen thermostat and barostate. Simulations were implemented in conditions constant temperature of 298 K and constant pressure 1 bar. Dreiding Force field was used in the input file. The number of 64 molecules placed in the box. The coulomb forces cut off radius was 16 Å. Total number of steps simulation 3000000 was selected where run in time 3ns. Molecular Dynamic simulation analysis the evaluation of the energy fluctuations in the chart to ensure a proper simulator, compared density obtained from MD calculations to the experimental values and also, analysis the radial distribution function in order to determine the phase diagram of the of molecules at ambient temperature and pressure.

3.2.2. Energy diagram analysis

Energy diagram calculations based on MD simulation run time, and this chart is drawn from the total energies Conformational, Coulomb and van der Waals is achieved. Conformational energies of structures related molecular energy (vibrational energy, rotational, bending, etc.) and Coulomb energy have information related to part of interactions between charges and Van der Waals energy interactions between the molecules. Figure 8 shows fluctuation molecule α-Linoleate methyl ester at zero Celsius degrees. Value of fluctuation energy is of degree 10^{-4} and the error percentage value is: $\frac{(2.975-2.946)}{(2.960)} \times 100 = 0.97$, as well as you can see in figure 8 to 1000ps equilibrium created in the system then begins MD simulation.

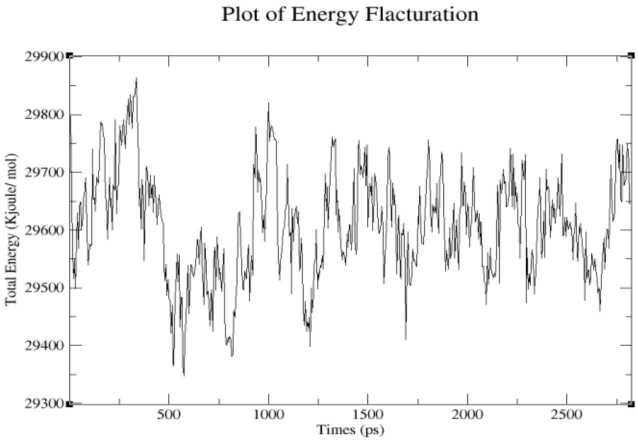


Figure 8. fluctuation molecule α- Linoleate methyl ester in MD simulation NPT

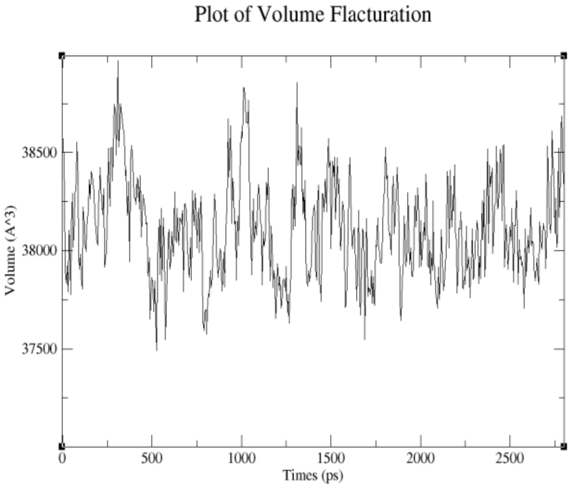


Figure 9 changes volume in the NPT set at 273 K and 1atm.

During the simulation of the physical properties are important. To ensure the correct implementation of the simulation, the density of the molecules employed according to the type of set (NPT). As can be seen in table (2), the calculated density has 9.47% percentage error. And you can see changes volume in the figure 9, too. Also, the Figure 10 shows RDF manner in NPT conditions.

Table 2. Density obtained from MD calculations and the experimental value.

calculated density	empirical density
0.8097 gr/ml	0.895 gr/ml

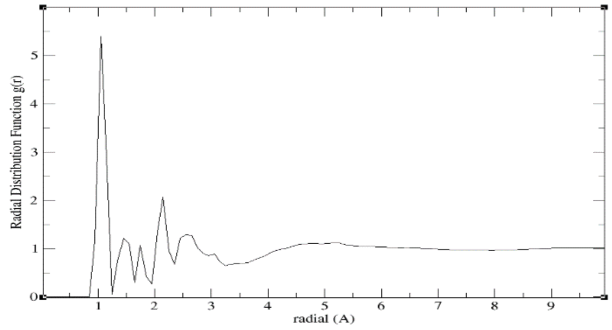


Figure 10. The radial distribution function Molecular Dynamics simulation in NPT ensemble

3.2.3. Annealing constant temperature and volume with molecular dynamics simulations

In this section, we investigate the phase changes along with temperature changes. We started simulation at high temperature step by step to lower the temperature; the process is called temperature annealing. The temperature annealing is a procedure that the temperature of a system to gradually and the set time interval reduce to reach the desired temperature. During the annealing process, the molecules of the gaseous state to the liquid and their true form in nature reach. Annealing in set of NVT from temperature 600 K to 300 K begin with temperature interval 10 degrees to reach the final temperature. After the system processes, we simulated environmental conditions (pressure 1 atm and temperature 300 K) to determine the equilibrium state. The results of the annealing molecular dynamics simulations divide two parts.

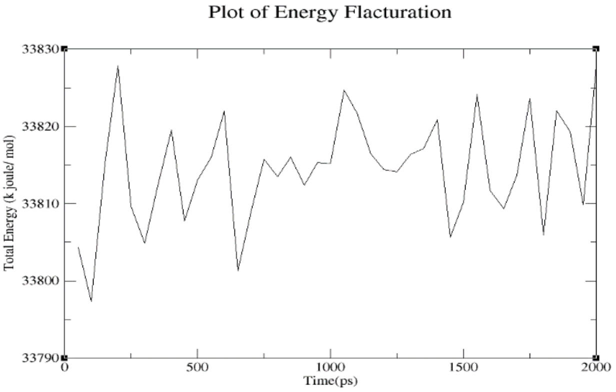


Figure 11 Energy fluctuation at temperature 300K in NVT set

3.2.3.1. Energy diagram analysis

At the all examined temperatures, fluctuations of energy were studied to sure how balance the system. Simulation system equalized at the lower temperature. The purpose of the annealing temperature is to achieve last temperature range therefore we examined only fluctuations in the temperature of the latest range 300 K. Figure 11 shows the fluctuation energy at temperature 300K in NVT set. As you can see the value of energy fluctuation is of degree 10^{-4} and the error percentage value is:

$$\frac{33828-33798}{33810}\times 100 = 0.0887$$

3.2.3.2. The radial distribution function curves

In this part, the radial distribution function of the atom to atom was used to detect phase changes; After a radial distribution function curves obtained for all atoms; it was found that the corresponding RDF O_3-C_2 best represent the phase changes in the RDF graph to have a single episode. As the figure 12 shows, the system is a gas at high temperatures because curves peak are lacks the soft.

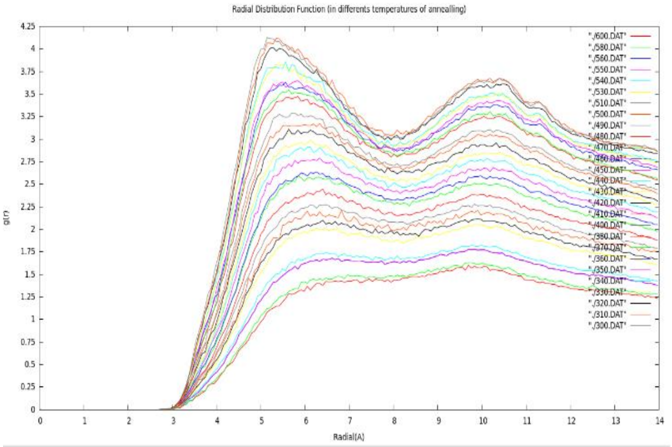


Figure 12 . RDFs related O_3-C_2 in different temperatures annealing.

at lower temperatures shoulder curves are found and become two separate peaks. In the liquid phase molecules are closer together, thus increasing the intensity peaks, the first peak between 5Å shows in the liquid phase the maximum molecular density at this distance then the curve drops distance, between 10.5Å again increases are shown the second layer of molecules. As it evidenced in figure 12, by reducing the temperature the density of molecules was increased. Molecules are gaseous at the 590K and by reducing the temperature gradually the molecules go to be liquid.

We noticed accurately figure 13 a lot of empty space. there is in the simulation box, for to create final balance in system and to reach the system maximum density at the end of annealing the molecules in the set NPT with 1500000 stages were simulated. The good results were obtained. Whatever we referred previously we required perform system in the end of annealing and in the final temperature 300K and pressure 1atm. This work led to final equilibrium created in the system and thermodynamic parameters calculated better form.

3.2.4. Results of Molecular Dynamics simulation in NPT ensemble after annealing

Energy diagram analysis and the radial distribution function curve were studied for this system. For this study the energy fluctuation has been shown in the figure 14. After 2ns with energy reduce created thermodynamically equilibrium in the system and MD simulation begin. Figure 15 Shows the radial distribution function Molecular Dynamics simulation in NPT ensemble after annealing.

During the simulation of the physical properties are important. To ensure the correct implementation of the simulation, the density of the molecules employed according to the type of set (NPT). The calculated density has 9.47% percentage error. And you can see changes volume in the Figure 16, too.

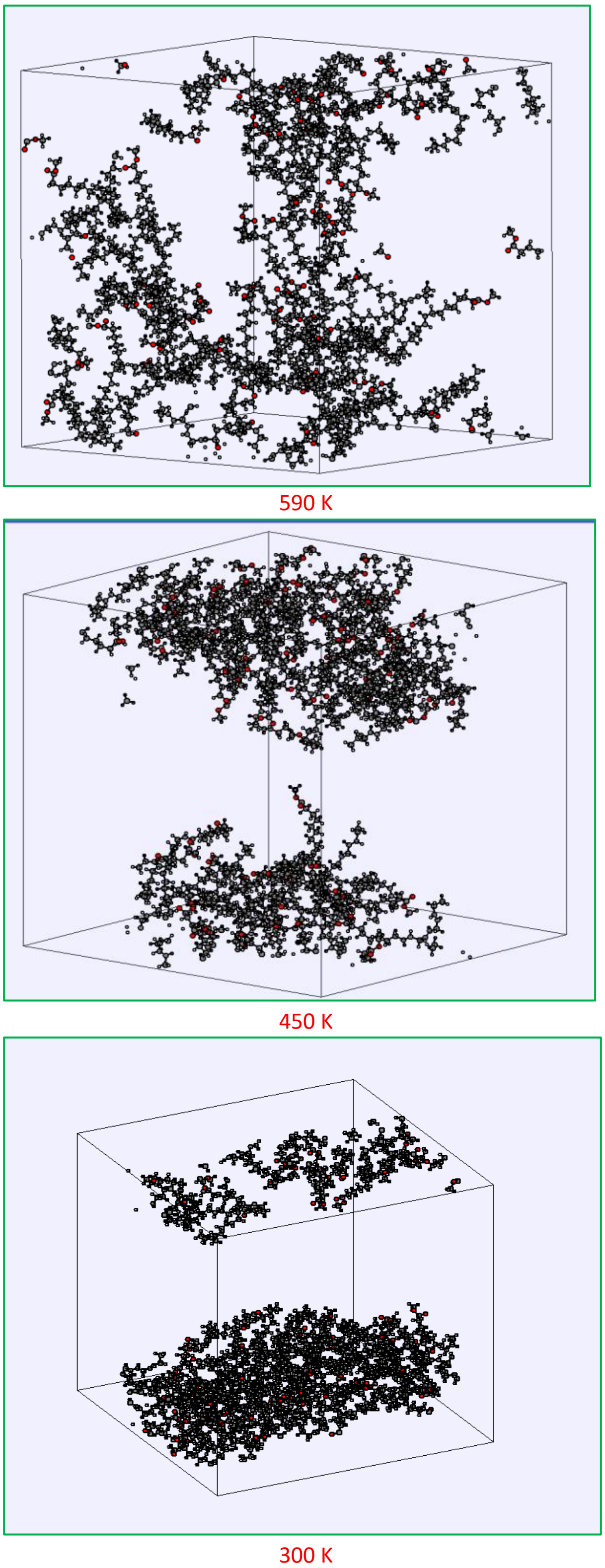


Figure 13. Molecules of α-linoleate methyl ester in different temperatures annealing

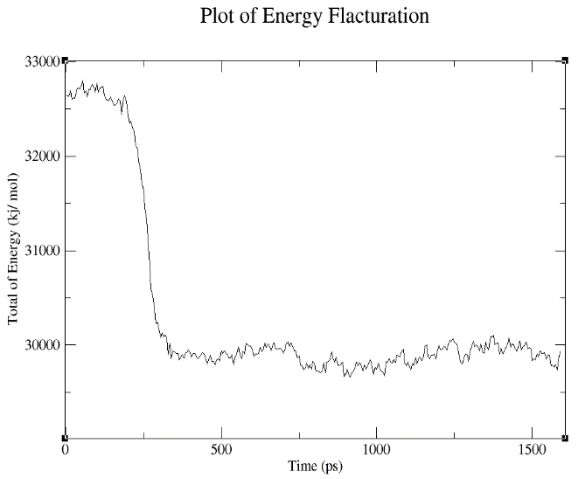


Figure 14. Energy fluctuation in Molecular Dynamics simulation in NPT ensemble after annealing.

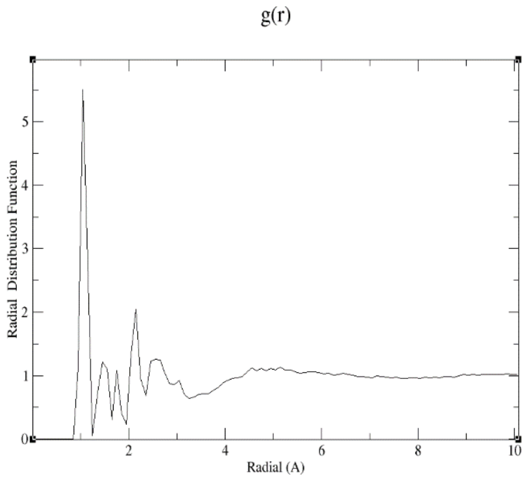


Figure 15. The radial distribution function Molecular Dynamics simulation in NPT ensemble after annealing.

3.3. Comparison of Monte Carlo and Molecular Dynamics

The aim of this simulation study was reaching to the conditions that molecules thermodynamically have the maximum stability. Initial Monte Carlo simulation to generate inputs for the MD calculations, in the second phase MD simulations were performed in NPT. In the third step the system was in gaseous state at the temperature of 600K with annealing technique reached liquid state in temperature at 300K and in the NPT ensemble. The results of these calculations done numerical and of the graphical analysis were performed to just make sure the simulation. For that to get the best out of calculations we need to compare the results of various calculations. Therefore, first, we compare the results of molecular dynamics and Monte Carlo simulations in NPT and we propose the best method, then the results of molecular dynamics simulations in NPT was carried out at the end of annealing were compared with the results of the two methods.

3.3.1. Comparison RDFs of each three method

In the Figure 17 RDFs of each three-method compared together. As the diagram shows the investigated phase is liquid.

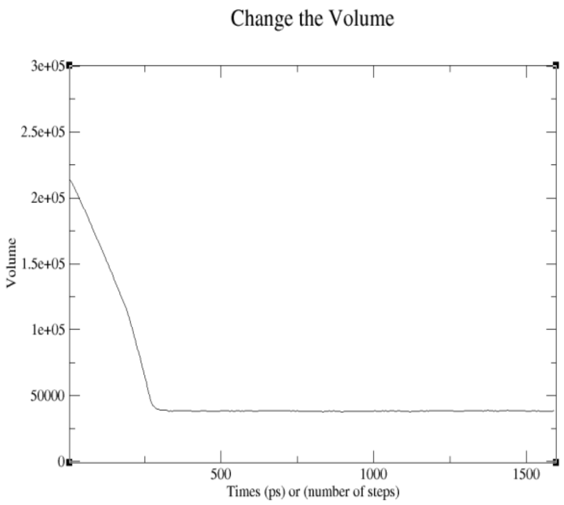


Figure 16 Changes of volume in the NPT set at 300 K and 1 atm.

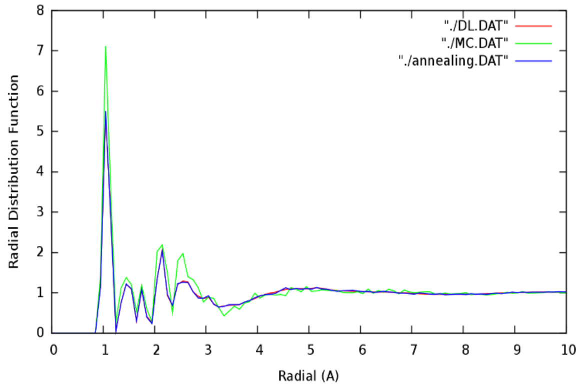


Figure 17 RDF's of each three-method compared together

3.3.2. comparison energies of MD in NPT ensemble and MD after annealing

The fluctuation range of MD and MC simulation in NPT ensemble compared together in the previous. The value of calculated fluctuation for MC is 0.763 and for MD is 0.97. Therefore, we can say in the both way value of fluctuation is constant. You can see in figure 18 energy of annealing calculation 200 kJ/mol is higher, because annealing calculation at temperature 300K and MD calculation at temperature 298K. Two-degree temperature increase to mean have bigger two degree of freedom, therefore kinetic energy NPT simulation in the end of annealing is higher. In figure 19 variations of volume NPT, and NPT in the end of annealing compared together.

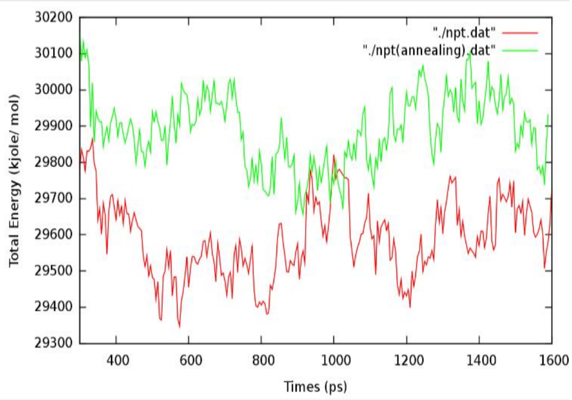


Figure 18. comparison energies of MD in NPT ensemble and MD after annealing

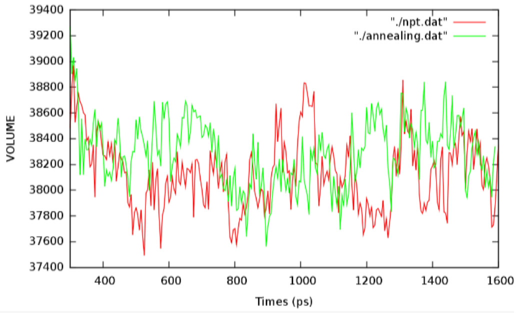


Figure 19. Variations of volume NPT and NPT in the end of annealing compared together.

4. Conclusions

MC and MD simulations include set of the molecules in order to simulate the state and the phase equilibrium of the considered molecule. The MD simulations were performed in two ways. The sequential that in the first method output of MC simulation was used as input in MD and at temperature of 298K and a pressure of 1 bar the MD simulations were performed. In the second sequential the gaseous state at a temperature of 600K system temperature with annealing technique has reduced 300K. So, at 300K temperature the MD simulations with system when N, P and T are constant, was performed. Then the graphical and numerical simulation results are analyzed and the results of MC and MD simulations have been compared with together and also MD simulations and the results have been compared with together. It was observed that the MD give the best results. In addition, some equilibrium parameters of α-Linoleate methyl ester was calculated using the results the above three modalities. Larger for the “cis” than for the “trans” configuration.

References

[1] Song, C. An overview of new approaches to deep desulfurization for ultra-clean gasoline, diesel fuel and jet fuel. *Catalysis Today*. 2003, 86(1–4), 211–263.

[2] Bizzo, W.A., Calan, B., et al. Safety issues for clean liquid and gaseous fuels for cooking in the scope of sustainable development. *Journal of Energy for Sustainable Development*. 2004, 8(3), 60–67.

[3] Arslan, O., Özdalyan, B. Influence of fuel types and combustion environment on emissions. *MSU Journal of Science*. 2020, 8(1), 747–756.

[4] Ameer, S., et al. Air pollutants all are chemical compounds hazardous to ecosystem. *World Journal of Pharmaceutical Sciences*. 2014, 2(8), 729–744.

[5] Burkholder, J.B., Cox, R.A., Ravishankara, A.R. Atmospheric degradation of ozone depleting substances, their substitutes, and related species. *Chemical Reviews*. 2015, 115(10), 3704–3759.

[6] González, K.R.A., et al. Determination of liquid–vapor equilibrium and critical properties of fatty acids for biodiesel production through molecular dynamics. *Journal of Physics: Condensed Matter*. 2022, 34(21), 214002.

[7] Ogunkunle, O., Ahmed, N.A. Overview of biodiesel combustion in mitigating the adverse impacts of engine emissions on the sustainable human–environment scenario. *Sustainability*. 2021, 13(10), 5465.

[8] Demirbas, A. Importance of biodiesel as transportation fuel. *Energy Policy*. 2007, 35(9), 4661–4670.

[9] Patil, P.D., Deng, S. Optimization of biodiesel production from edible and non-edible vegetable oil. *Fuel*. 2009, 88(7), 1302–1306.

[10] Atabani, A.E., Silitonga, A.S., Ong, H.C., Mahlia, T.M., Masjuki, H.H., Badruddin, I.A., Fayaz, H. Non-edible vegetable oils: a critical evaluation of oil extraction, fatty acid compositions, biodiesel production, characteristics, engine performance and emissions production. *Renewable and Sustainable Energy Reviews*. 2013, 18, 211–245.

[11] Yang, C.Y., Fang, Z., Li, B., Long, Y.F. Review and prospects of Jatropha biodiesel industry in China. *Renewable and Sustainable Energy Reviews*. 2012, 16(4), 2178–2190.

[12] Westbrook, C.K. Biofuel combustion. *Annual Review of Physical Chemistry*. 2013, 64, 201–219.

[13] Mishra, V.K., Goswami, R. A review of production, properties and advantages of biodiesel. *Biofuels*. 2017, 9(2), 273–289.

[14] Esmaeili, H. A critical review on the economic aspects and life cycle assessment of biodiesel production using heterogeneous nanocatalysts. *Journal of Fuel Processing Technology*. 2022, 230, 107224.

[15] Mondal, M., Goswami, S., Ghosh, A., et al. Production of biodiesel from microalgae through biological carbon capture: a review. *3 Biotech*. 2017, 7(2), 99.

[16] Pereira, F.M., et al. Impact of pure biodiesel fuel on the service life of engine-lubricant: a case study. *Fuel*. 2020, 261, 116418.

[17] Makareviciene, V., et al. Solubility of multi-component biodiesel fuel systems. *Bioresource Technology*. 2005, 96(5), 611–616.

[18] Van Gerpen, J. Biodiesel processing and production. *Fuel Processing Technology*. 2005, 86(10), 1097–1107.

[19] Ma, F., Hanna, M.A. Biodiesel production: a review. *Bioresource Technology*. 1999, 70(1), 1–15.

[20] Mohan, B., Yang, W., Yu, W. Effect of internal nozzle flow and thermo-physical properties on spray characteristics of methyl esters. *Applied Energy*. 2014, 129, 123–134.

[21] Christensen, E., McCormick, R.L. Long-term storage stability of biodiesel and biodiesel blends. *Fuel Processing Technology*. 2014, 128, 339–348.

[22] Arbeitsgemeinschaft Qualitätsmanagement Biodiesel e.V. (AGQM). *Quality Management of Biodiesel*. Berlin, Germany, 2014.

[23] Wan, S., Coveney, P.V. On the calculation of equilibrium thermodynamic properties from molecular dynamics. *Physical Chemistry Chemical Physics*. 2016, 18(44), 30236–30256.

[24] Syal, P., et al. Targeted mutations and MD simulations of a methanol-stable lipase YLIP9 from *Yarrowia lipolytica* MSR80 to develop a biodiesel enzyme. *International Journal of Biological Macromolecules*. 2017, 104, 78–88.

[25] Bakker, M. Improving biodiesel through pyrolysis: direct dynamics investigations into thermal decomposition of methyl linoleate. *University of Nebraska – Lincoln*. 2015. Thesis/Dissertation.

[26] González, K.R.A., et al. Predicting the physical–chemical properties of biodiesel fuels assessing the molecular structure with the SAFT-γ group contribution approach. *Journal of Physics: Condensed Matter*. 2022, 34(21), 214002.

[27] Perdomo, F.A., Millan, B.M., et al. Estimation of pure-component physical properties of biodiesel. *Energy*. 2014, 72, 274–290.

[28] Li, X., Xu, X., You, X., Truhlar, D.G. Benchmark calculations for bond dissociation enthalpies of unsaturated methyl esters and the bond dissociation enthalpies of methyl linolenate. *Journal of Physical Chemistry A*. 2016, 120(23), 4025–4036.

[29] Cheng, J., Li, T. Combustion dynamics of biodiesel produced by supercritical methanol transesterification. *Fuel Processing Technology*. 2015, 131, 409–413.