Islamic Azad University

Journal of
Optoelectronical Nanostructures

Autumn 2018 / Vol. 3, No. 4

Simulation of RDX Decomposition Interacting with Shock Wave via Molecular Dynamics

Abbas Latifi[1], Seyyed Hamid Ahmadi[*, 1], Ali Khanlarkhani[2], Manochehr Fathollahi[3]

[1] Chemistry & Chemical Engineering Research Center of Iran (CCERCI), Pajohesh Blvd,17th km of Tehran-Karaj Highway, Tehran, Iran.
[2] Institute of Materials and Energy, Imam Khomeini Blvd, Meshkin Dasht, Karaj, Iran.
[3] Malek-Ashtar University of Technology, Shabanlou, Babaei Highway, Lavizan, Tehran, Iran.

(Received 16 Sep. 2018; Revised 17 Oct. 2018; Accepted 18 Nov. 2018; Published 15 Dec. 2018)

Abstract: Cylotrimethylenetrinitramine (RDX), with the chemical formula $C_3H_6N_6O_6$, is an energetic organic molecule used widely in military and industrial commodities of explosives. By stimulating RDX through exerting temperature or mechanical conditions such as impact or friction, decomposition reaction occurs at a very high rate. Molecular dynamics techniques and LAMMPS code with Reactive Force Field (ReaxFF) potential were employed to simulate initiation of RDX. Potential energy variations of the system were calculated over time for five different temperatures up to 100 ps. The products of decomposed system with respect to time were calculated at each stage of stimulation for different values of temperature and thermal initiation stimulation energy in NVT and NVE ensembles. The activation energy of decomposition was calculated 20.230 kcal.mol^{-1} through Arrhenius equation. The minimum required temperature to produce H_2 with temperature decomposition was about 2500 K and production times for several conditions were calculated. The amount of nitrogen and hydrogen production were increased with raising temperature and reached the maximum value at 3000 K. The minimum impetus energy required to form the light species H_2 is 66 kcal.mol^{-1}.`

Keywords: RDX, LAMMPS, Molecular Dynamics, Shock Wave, Simulation

1. INTRODUCTION

1,3,5-Trinitroperhydro-1,3,5-triazine also known as Cylotrimethylenetrinitramine or RDX, a secondary high explosive, is widely used in military and civil explosive devices that are able to safely release a significant amount of energy. The decomposition reaction can be initiated by increaseing applied heat and temperature to the extent more than its critical

---

[*] Corresponding Author E-mail: **ahmadi@ccerci.ac.ir**

value. The reaction is a spontaneous molecular decomposition reaction in solid state which releases energy about 335.5 kcal.mol^{-1}. Practically, shockwave is applied in order to initiate the reaction. Shockwave causes compression in this material leading to an increase in temperature of small areas of the charge. This compound in solid state belongs to the orthorhombic crystal system (space group Pbca), which consists of 8 molecules $C_3H_6N_6O_6$ per unit cell, equivalent to 168 atoms and the crystal parameters are as follows [1]:

$$a = 13.182,\ b = 11.574,\ c = 10.709\ \text{Å}, \qquad \alpha = \beta = \gamma = 90o$$

According to the calculations and the empirical evidences, the first step in decomposition of this molecule is the breakup of the weak bonds in $N\text{-}NO_2$ bond and release of NO_2.

Shockwave is of sudden change or disintegration in a series of thermodynamics quantities such as pressure, temperature and density of the system. This wave is generated mechanically or through explosion and propagates in the studied case. This wave is formed when the propagation speed of a disturbance is more than the longitudinal sound propagation speed in that environment. In order to describe a shockwave in an object, Hugoniot equation is used [2]:

$$U=C_o+Su \tag{1}$$

Where U, C_0, S and u show the shockwave speed, longitudinal sound propagation speed in the material, an empirical constant and the particles movement speed, respectively. The values of these quantities for different materials are measured empirically and are also determined from calculations. With the analytical relations, it is shown that increase in the internal energy of a system caused by the collision of a shockwave is proportional to the increase in the speed of particles caused by the applied shockwave.

$$E_{int}=\frac{1}{2}u^2 \tag{2}$$

Therefore molecular dynamics can be a useful tool for examining these changes. For reaction initiation, shockwave is applied in which pressure or velocity has to be higher than the critical value for matter. In lesser values, an instant decomposition would not happen in a desired reaction path. General approaches to generate an initiating shockwave is flyer impact with matter.

Flyer is a very thin and small plate which is accelerated by a plasma generator or laser towards the secondary high explosive plate. If the velocity of the flyer exceeds the critical value, decomposition and destruction will be accomplished in the secondary explosive [3,4].

In influenced area of shockwave with explosive material, the difference in temperature and pressure quantities are high and these variations in a very small time interval happen in atomic scale. The degree of the variations for a real system in longitudinal section less than 1 mm and in a time interval of less than a microsecond is about several GPa and temperature greater than 2000 K. In the real system, decomposition rate in a defects-free crystalline solid RDX, is about 8750 $m.s^{-1}$. With the assumption of linear decomposition speed along the system, time range variations must be in the scale of femtosecond.

Time-Resolved Spectroscopy technique is used to record events in molecular scale [5,6]. Methods based on Density Functional Theory (DFT) and quantum computing are exploited in variety of researches for single or dual molecular decomposition behavior [7-12]. DFT methods have been widely used to determine the structure and properties of different materials physics [13-17].

Molecular Dynamics (MD) techniques are used to investigate events in molecular scale, single cell and super cell [1, 15-20]. This technique is able to predict conducted events in molecular and atomic scales with respect to the introduced force field for RDX molecule with different precisions. In Molecular Dynamics techniques with use of Reactive Force Field (ReaxFF), the theory of bond degree is exploited in which bond degree between all atoms is calculated for a large structure for each simulation time step.

Therefore, formation or breakdown of a new bond can be investigated. From 2003, ReaxFF utilization for secondary explosives (C, N, O, H elements) has been reported [14, 23]. In the works of former researches, effect of shockwave on RDX molecule has been investigated initially as temperature surge in a region including a number of molecules. Effects related to crystal defects as well as crystal collision plate with the wave have been simulated using Molecular Dynamics techniques. Furthermore, the effect of shock wave collision with the system has been investigated as a collision of a number of RDX molecules with other molecules in different velocities [20-22]. Molecules collision velocity is assumed to be equal to shockwave velocity.

From 2003, use of Multiscale Shock Technique (MSST) on variety of materials (general and high-energy) in the US Lawrence Livermore National Laboratory (LLNL) has been started by Reed et al. in which for a relatively large system, different quantities of Hugoniot equation are simulated and determined with comparable accuracy in comparison with empirical values [23,`24].

In this study, the effect of thermal bath temperature and direct heat energy impetus on crystalline defect free RDX decomposition is investigated by reactive molecular dynamics.

2. SIMULATION DETAILS

2.1 Structure of system

To conduct the simulation, RDX cell structure was built first based on single cell structure (with the use of XRD crystallography results for RDX) [25]. This structure consists of 8 RDX molecules and 168 atoms. Simulation was conducted on 216RDX system with 4536 atoms. Nanoparticle of 216RDX is generated by reproduction of 3 units of 8RDX system in each dimension. Fig. 1 illustrates molecular structure of RDX molecule, its single cell and derived super cell. The physical dimensions of used system are as follows:

$$a = 39.546,\ \ b = 34.722,\ \ c = 32.127\ \text{Å} \qquad \alpha = \beta = \gamma = 90^{\circ}$$

2.2 Software

All the simulations in this research have been conducted using Large-scale Atomic/Molecular Massively Parallel Simulator (LAMMPS) which is a molecular dynamics software package. It is an open source software which is provided by Sandia International laboratories [26, 27]. Visual Molecular Dynamics (VMD) software is used to process the output information [28].

2.3 Potentials

In molecular dynamics a molecule is described as a series of charged points (atoms) linked by simple springs (bonds). The force field is a collection of equations and associated constants designed to reproduce molecular geometry and selected properties of tested structures. This nanoparticle density is based on the molecular weight of single RDX and the cell dimension that is equal to 1.806 g.ml-1. Boundary conditions were used for all simulations.

Reactive Force Field is the potential relating to chemical reactions in which bonds are formed or broken down and ultimately, a new chemical structure is achieved from the particles or system molecules. These force fields were developed by Van Duin et al. in The Industrial Institute of California. Their performance is also verified by several papers through the empirical experiments and approximate quantum computing [22].

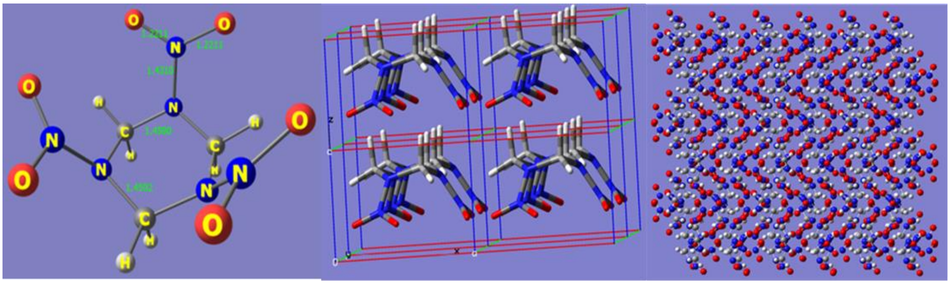

Fig. 1 Molecular structure of α-RDX (left), 8RDX single unit cell (Center) and 216RDX system (right)

Reactive Force Field is used in order to fill the gap between quantum mechanics and Empirical Force Field (EFF). Reactive Force Field relating to a molecular system contains charge equilibrium between atoms from which momentary bond degree is calculated in every time interval.

In simulation by using ReaxFF, the potential between atoms is altered and consequently other energies share will also alter. In Fig. 2, bending potential between two atoms is compared for reactive and non-reactive force field. Energy variations caused by bent bond is less in ReaxFF compared to the non-reactive force field and is closer to reality. Complexity of potential equation leads to increase in the computation time as well as increase in precision. The simulation with reactive force field potential is about a million times faster than DFT and 50 times slower than non-reactive force field [27, 30].

3. RESULTS

3.1 Energy transfer method

NVT and NVE ensembles are used in the calculations for shockwave exertion simulation on this structure. In NVT ensembles, the whole assembly was placed in a hypothetical thermal bath where temperature, volume and particles number are constant. Chosen temperatures are a criterion of the induced temperature due to the impact of shock wave on the RDX explosive.

In NVE ensembles, different quantities of thermal energy for a period of 500 fs were applied to the system. The time of 500 fs is selected based on the RDX explosion velocity and its cell dimension.

In NVT ensembles, the temperature range is set to be from 1500 to 3500 K. In fact, this temperature is a criterion for the shockwave strength which is supplied by a detonator. Temperature induction in the reaction initiation of RDX is provided by a detonator output, as shown in Fig. 3. Detonator is a device consisting of priming charge, a highly sensitive primary explosive and finally a secondary high explosive. Electrical detonator is excited through an electrical actuator and the output shockwave in the form of temperature induction and thermal energy flow causes the reaction initiation of RDX material. Energy of detonator released in very short time.

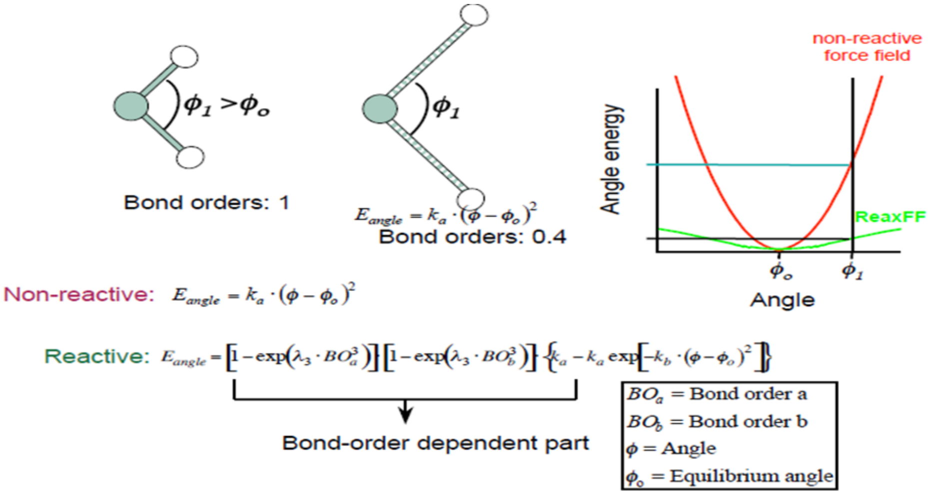

Fig. 2. Bending potential function comparison between atoms for non-reactive and Reactive Force Field as well as energy relative to their bond angles (With the permission of Van Duin [27])

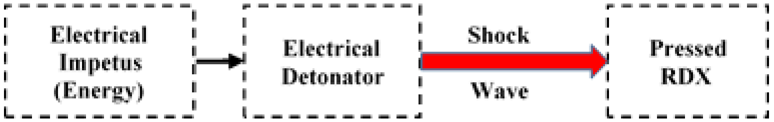

Fig. 3. A concept model for the reaction initiation of RDX explosive through shockwave induction using an electrical detonator.

3.2 Effect of temperature on the system's potential energy variations

RDX system was put in NVT ensemble with 5 different temperature conditions and variations in the potential energy were calculated using ReaxFF potential with 0.1 fs time step and the results are shown in Fig. 4 for 100 ps. The system's data are averaged and recorded in every 100 time steps (equivalent of 10 fs).

It is observed that variations have been made to the system with increasing bath temperature, which leads to its more stable than the initial state. More stable position of system means molecules resulting from decomposition are more stable. Changes in the potential energy of the system that are equivalent to rearrangement of atoms in molecules have begun with temperature induction.

The initial increase in potential energy is equivalent to breaking of the bonds. The decrease in potential energy is equivalent to the formation of new bonds and more stable molecules. The chemical stability of particles produced at 3000 K was higher than other temperatures.

3.3 Molecules from system decomposition at different temperatures

The bond order algorithm was used to calculate changes in chemical bonds (breaking or formation) from information that have stored for atomic moment intervals at each time steps. These calculations for molecular changes were done with post processing tools that released by LAMMPS site [27]. For RDX molecules decomposition, there are several possible species that their energy and stoichiometry is different.

Over time, intermediate species have converted to more stable molecules that are consequently a reduction in the system's potential energy.

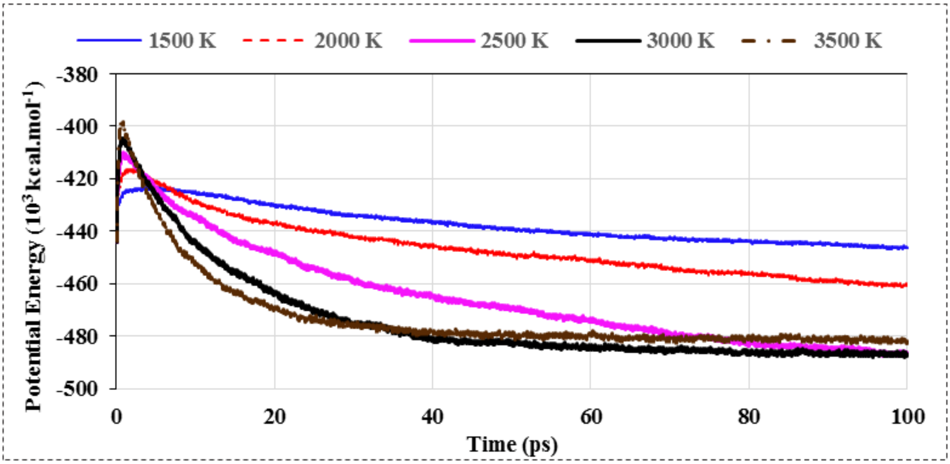

Fig. 4. Variations in potential energy of RDX system with NVT ensembles during time period of 100 ps with 0.1 fs time step using ReaxFF potential in different thermal baths

Chemical analysis of species resulting from RDX system decomposition is shown in Fig. 5 over simulation time for 5 different temperatures. Decomposition in RDX system has not happened in the temperature range of 1500-3500 K at times less than 130 ps. It is observed that with increasing temperature induction time for a constant temperature, the number of RDX molecules decreases. Water is the first stable produced molecule from decomposition of the system. The number of stable species such as H_2O, N_2, CO, CO_2 and H_2 are relatively increased with the increase in temperature and temperature induction time.

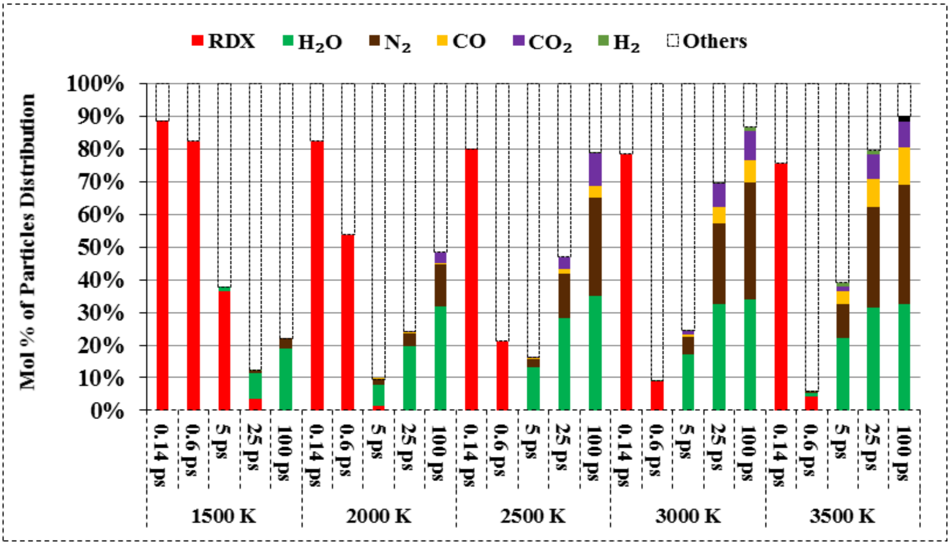

Fig. 5. RDX system particles distribution using ReaxFF potential during time period of 140 fs to 100 ps and 0.1 fs time step for several different temperatures.

Other species introduced are composed of less stable particles. The amounts of produced stable molecules have direct relation with the temperature level and induction time. At each selected temperature, the number of other species increases over time, but decreases with time development and conversion to more stable molecules. The time and temperature necessary to form hydrogen molecule is higher than other stable molecules. The total number of particles produced by the system decomposition has increased with increasing temperature and induction time of temperature. The variations of total species proportion with respect to temperature and time are shown in Fig. 6.

Diverse techniques are used for the anticipation of products resulting from explosion and they are compared with molecular dynamics outcomes with ReaxFF potential [28, 29]. The reported results in this research which are executed with the precise ReaxFF potential, have a very good conformity with the previous results.

The mean molecular mass of other constituent particles of RDX system (mid-range particles and molecules other than water, nitrogen, carbon monoxide, carbon dioxide and hydrogen under name of others) are shown in Fig. 7.

The mean weight of species is reduced with increasing the bath's temperature as well as time passes. In other words, the system is developed to equilibrium or forming stable particles and lesser molecular weight particles.

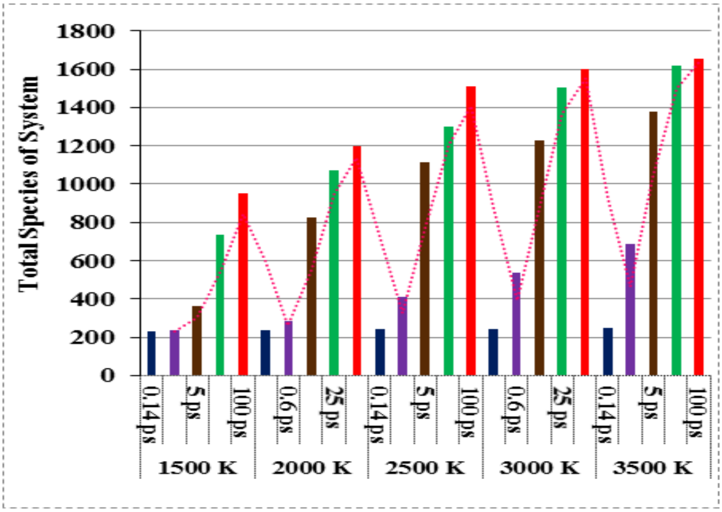

Fig. 6. The whole number of RDX system constituent particles during a time interval of 140 fs to 100 ps for several different temperatures with 0.1 fs time step using ReaxFF potential.

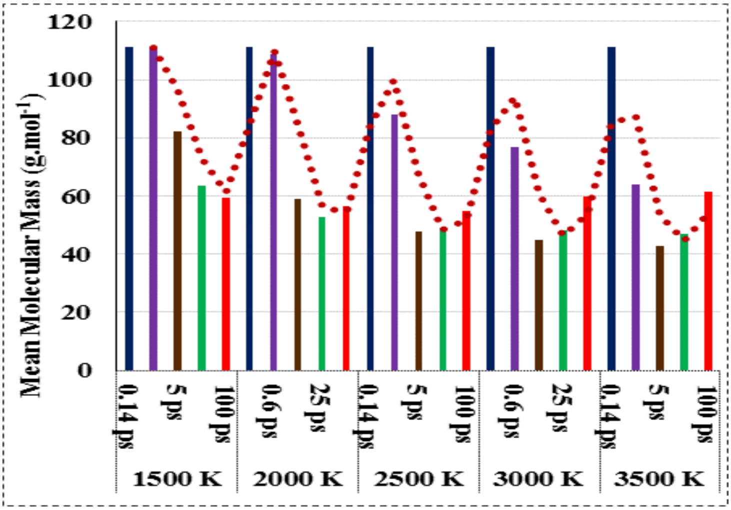

Fig. 7. Illustration of mean molecular mass of other RDX system constituent particles in time intervals of 140 fs to 100 ps for several different temperatures with 0.1 fs time step using ReaxFF potential.

The pressure of the system is related to its constituent particle numbers.

Increasing the temperature of the system leads to an increase in the number of high-energy particles. Particles with lower weight and with increasing pressure in the system have a vital role for the initiating steps of the reaction and its development.

The dependence of the system's complete decomposition time, in which all of the RDX molecules have been converted to other species, on its temperature is given in Table 1.

Table 1. Dependence of the system's complete decomposition time on its temperature

Temperature of system (K)	Decomposition time (ps)
1500	71.423
2000	15.403
2500	4.623
3000	2.414
3500	1.580

In order to determine the activation energy of RDX system decomposition reaction, the natural logarithm of the inverted decomposition time for total decomposed RDX molecules versus inverted temperature have been plotted using Arrhenius equation as shown in Fig. 8. The slope of this curve determines an activation energy of 20.230 kcal.mol^{-1}. Using molecular dynamics techniques and Arrhenius equation, the amount of activation energies for this substance at two different densities of 0.21 and 2.11 g.ml^{-1} are calculated respectively to be 26.6 and 23 kcal.mol^{-1}. Considering that the decomposition of this system leads to the release of energy and development of subsequent reactions, the use of the required time for degradation of the whole molecules for calculating the activation energy is more accurate than the method used by Stratchan [23]. The calculated activation energy in this research was for a defect-free crystalline nanoparticle.

3.4 Effect of thermal energy transfer to RDX system

From another perspective, applying shockwave to a system is in fact transferring of thermal energy to the constituent particles in a very short time interval.

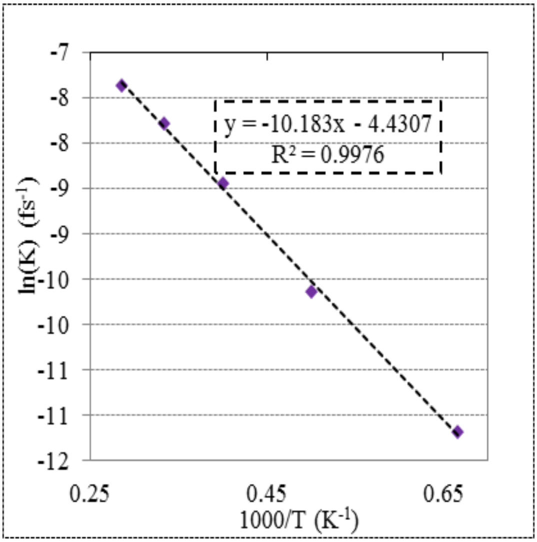

Fig. 8. Natural log illustration of inverted time, at which the whole RDX molecule is decomposed, in fs versus inverted temperature

According to the nanoscale dimensions used to simulate and detonation rate of crystalline RDX is 8750 m.s-1, the decomposition time of system will be about 500 fs. For this purpose, initially thermal energy is applied to the system for a period of 500 fs in each simulation time step and after this time, the energy source was removed. These calculations were carried out in the microcanonical ensemble (NVE conditions). Fig. 9 illustrates how direct heat is applied to the RDX system. In this model, it is assumed that RDX explosive is placed in an isolated container with a volume equal to the volume of the substance and walls with thermal insulations and the aforementioned energy is released symmetrically to the system in 500 fs.

This external energy is provided by the chemical bonds changes created in adjacent molecules. External transferred energy initially results in an increase in the potential energy of the system which is related to breaking of primary bonds and ultimately reduction in potential energy which related to formation of new chemical bonds. With the formation of new bonds and stable molecules, a reduction in the potential energy is observed.

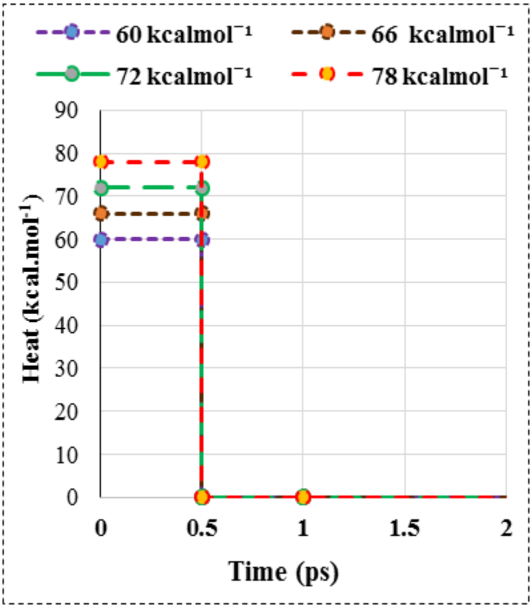

Fig. 9. Method of applying thermal energy to RDX system, giving energy for 500 fs and then energy cut-off until 150 ps.

Variations in the potential energy of the system versus time are shown in Fig. 10 for several different impetus energies that equal to different initiating conditions. Variations in the potential energy of the system were very finite for impetus energies of 54 kcal.mol^{-1} and less. This is related to very limited changes in the chemical bond of the system. In other words, for impetus energies of 54 kcal.mol^{-1} and less, the decomposition speed in the system is very slow to the extent that can be ignored in the simulation conventional time. Primary increase in potential energy of the RDX system is related to breakdown of the weakest N-NO_2 bond.

Applying thermal energy to the system leads to an increase in temperature. Variations in the induced temperature of the system is due to the forced thermal energy flux in 500 fs. The temperature of the system had progressed rapidly with increasing the stimulant energy as well as reached faster to an equilibrium.

The induced temperature in 500 fs for energy stimulus and the maximum temperature of the system after energy flux are shown in Fig. 11. Increasing the induced temperature was in accordance to the thermal energy flux to the system.

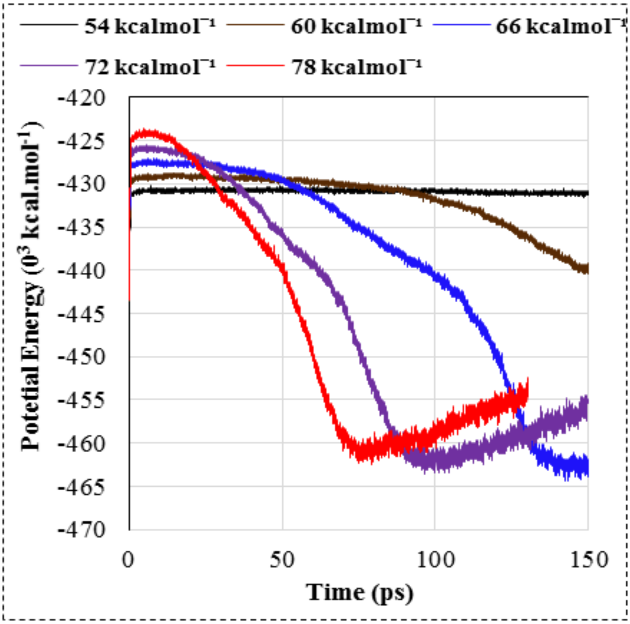

Fig. 10. A comparison in the variations of the potential energy of RDX system versus time which are excited with several different impetus energies for 500 fs.

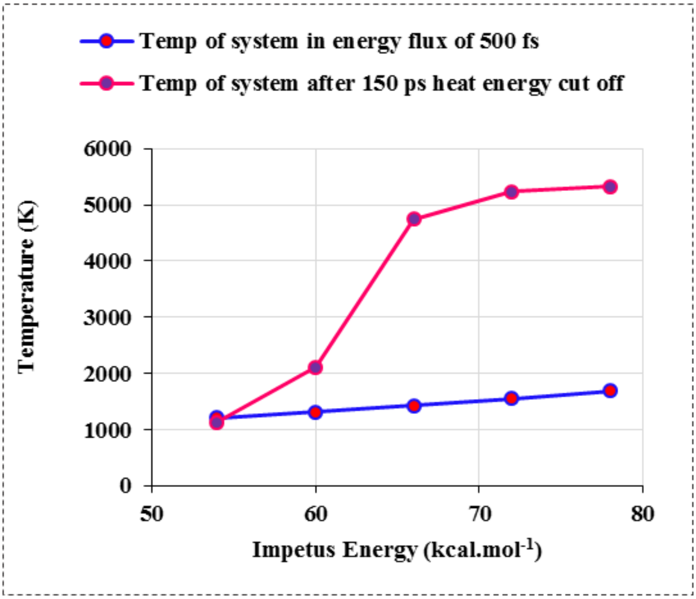

Fig. 11. Illustration of the induced temperature to RDX system due to forced thermal energy flux in 500 fs and the temperature in the system after 150 ps.

The temperature growth after energy cut-off was due to new chemical bonds formation and potential energy release that convert to the kinetic energy of the particles. This is related to very limited changes in the chemical bond of the system. In other words, for impetus energies of 54 kcal.mol^{-1} and less, the decomposition speed in the system is very slow to the extent that can be ignored in the simulation conventional time.

The produced species from the decomposition of heated RDX system with different values of impetus energy (thermal energy) are shown in Fig. 12. It is observed that in a period of 500 fs that induced thermal energy time, partial system decomposition is happened for each of the energy values. The time required for complete decomposition of system is proportional to the amount of impetus energy. Stable species like water is being found after 10 ps.

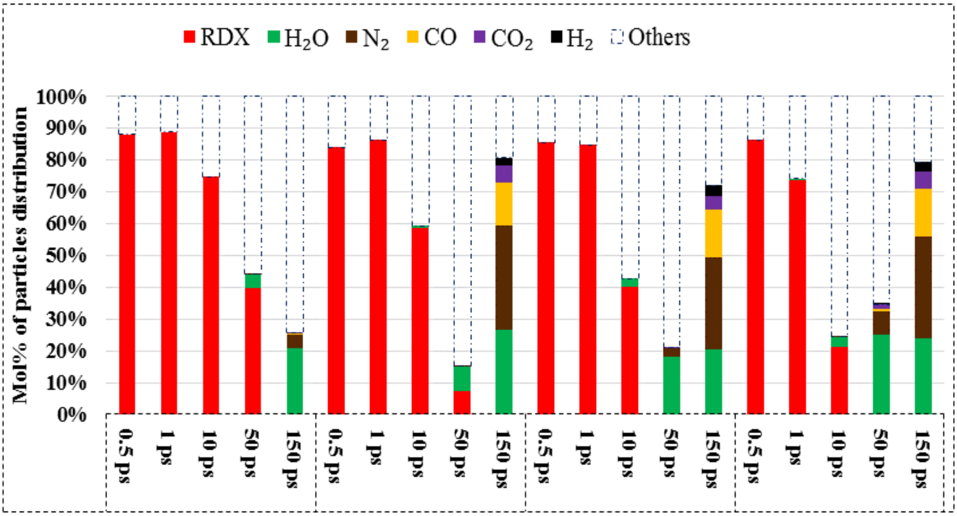

Fig. 12. Molecules resulting from decomposition of RDX system in several different time intervals which the thermal energy with different values are transferred for 500 fs and then removed.

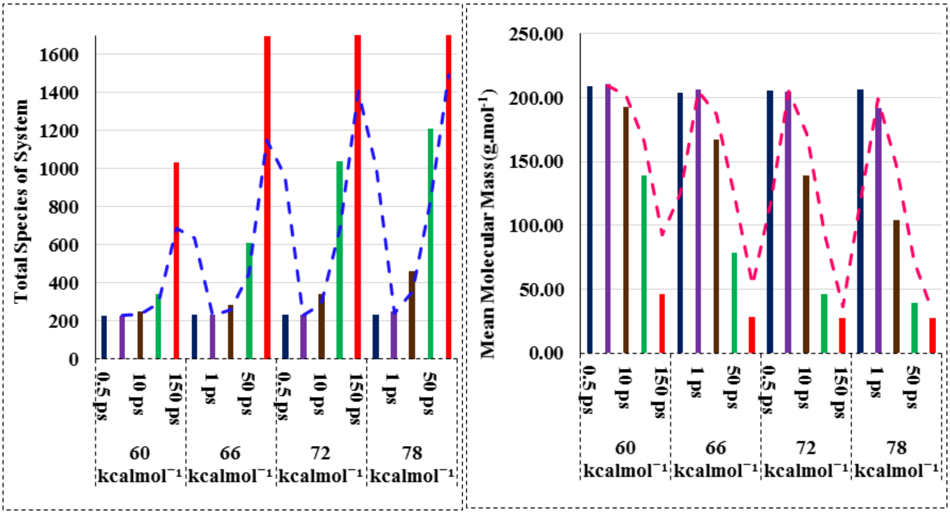

Fig. 13. Comparison of Total number of species resulting from RDX system decomposition (left) and mean molecular weight of particles (right) in several different time intervals and different thermal energy impetus that was transferred to them in 500 fs and then removed.

With the increase in primary impetus energy amount, the time required for the formation of stable species such as H_2O, N_2, CO and CO_2 has decreased. Impetus energy values at least 66 kcal.mol^{-1} and 113 ps time are needed for the formation of the light species such as H_2. With the existence of this species, due to its further reaction with the surrounding oxygen molecules and the oxidizing species, it has a great impact on the total output energy.

The dependence of the total number of particle resulting from the decomposition of the RDX system relative to the time and primary impetus energy is shown in Fig. 13. The average total number of species resulting from RDX system decomposition has increased with increasing initial impetus energy. It is expected that the generated pressure in the system is increased with increasing in the number of particles due to system decomposition.

The mean system's pressure is averaged in 1 ps and the results are shown in Fig. 14. The rate of increase in pressure and its equilibrium amount was proportional to the initiating power. When decomposition of the system leads to lighter molecules which proportional to a large number of them, the initiating power and also output power of the system will be increased.

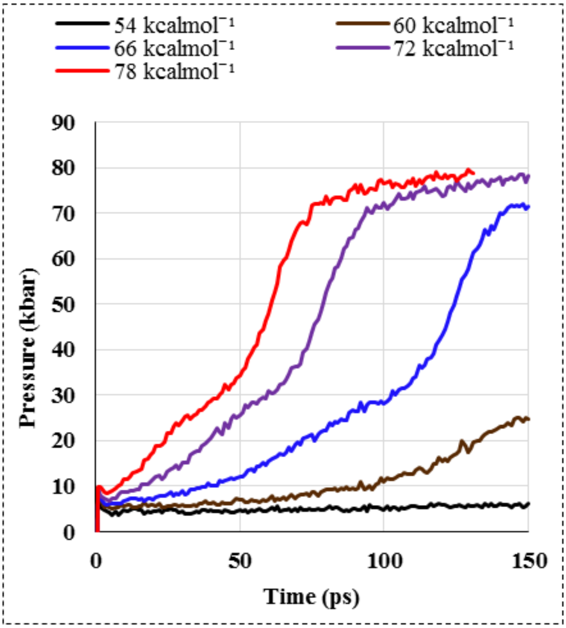

Fig. 14. Variations in the mean pressure of RDX system versus time which was exposed to different values of impetus thermal energy and then cut-off in 500 fs.

4. CONCLUSIONS

In this research, chemical reactions in molecular scale of a secondary High explosive like RDX was investigated in femtosecond time scale using molecular dynamics techniques and ReaxFF potential.

Considering very short time and high temperature and pressure, knowing these variations is not possible with the existing experimental techniques. The effect of shockwave on explosive substance was modelled in a form of constant temperature induction using NVT ensembles and thermal energy flux using NVE ensembles. It was shown that if a defect-free RDX disc is placed in a hypothetical thermal bath with different temperatures, the first broken down bond is the N-NO_2 bond which is in accordance with expectations and reported results with quantum methods. Variations in the potential energy, type and the number of molecules of the system due to decomposition are proportional to the bath's temperature.

The activation energy of the RDX system with NVT ensemble and the use of the Arrhenius equation was calculated to be 20.230 kcal.mol^{-1}.

It has been shown that if the hypothetical RDX particle with different thermal energy is only stimulated for 500 fs, the decomposition rate of the system will be proportional to the amount of heat transferred to the system. During 500 fs, the entire system has not been decomposed completely, but the energy produced from the formation of several new molecules can continue to complete decomposition. With the passage of time and increasing stimulation energy, the average molecular weight of the product decreases which leads to an increase in the number of products. Impetus energy values at least 66 kcal.mol^{-1} is needed for the formation of the light species H_2. Because of its low mass and high energy as well as its secondary reactivity with environment, hydrogen production path is very important in reaction growth.

Considering the fact that temperature and the pressure of the system are determinable in each time step, output power of the system can be determined with the assumption of isolated system during the simulation time.

REFERENCES

[1] Conroy, M. W.; Oleynik,I. I.; Zybin,S. V. C.; White,T., *Density functional theory calculations of anisotropic constitutive relationships in alpha-cyclotrimethylenetrinitramine*. J. Appl. Phys. 104 (2008, Dec) 113501-113505. Available: https://aip.scitation.org/doi/10.1063/1.3031216

[2] Boogerd, P.; Verbeek, J. H.; Stuivinga, M.; Van Der Steen, A. C.; Van Dar Put, P. J.; Schoon man, J., *General shock wave equation of state for solids*. J. Appl. Phys. 78 (1995, July) 5335-5344. Available: https://aip.scitation.org/doi/abs/10.1063/1.359712

[3] Nance, C. J., *Energetic material initiation device having integrated low-energy exploding foil initiator header*. (2009, Aug 11). US Patent 7,571,679 B2. Available: https://patents.google.com/patent/US20080148982A1/en

[4] Davies, H. R.; Chapman, D. J.; Vine, T. A.; and Proud, W. G., *Characterisation of an Exploding Foil Initiator (EFI) system*. 1195 (2009) 283-286. Available: https://aip.scitation.org/doi/abs/10.1063/1.3295125

[5] Patterson, J. E.; Dreger, Z. A.; Miao, M.; Gupta, Y. M., *Shock wave induced decomposition of RDX: Time-resolved spectroscopy*. J. Phys. Chem. A 112 (2008, Aug) 7374-7382. Available: https://pubs.acs.org/doi/abs/10.1021/jp800827b

[6] Dreger, Z. A.; Gupta, Y. M., *Shock wave induced decomposition of RDX: Quantum chemistry calculations*. J. Phys. Chem. A 116 (2012, April) 8713-8717. Available: https://pubs.acs.org/doi/abs/10.1021/jp8008282

[7] Schweigert, I. V., *Ab initio molecular dynamics of high-temperature unimolecular dissociation of gas-phase RDX and its dissociation products*. J. Phys. Chem. A 119 (2015, March) 2747-2759. Available: https://pubs.acs.org/doi/abs/10.1021/jp510034p

[8] Byrd, E. F. C.; Scuseria, G. E.; Chabalowski, C. F., *An ab initio study of solid nitromethane, HMX, RDX, and CL20: Successes and failures of DFT*. J. Phys. Chem. B 108 (2004, June) 13100-13106. Available: https://pubs.acs.org/doi/abs/10.1021/jp0486797

[9] Balu, R.; Byrd, E. F. C.; Rice, B. M., *Assessment of dispersion corrected atom centered pseudopotentials: Application to energetic molecular crystals*. J. Phys. Chem. B 115: 2011, P. 803-810. Available: https://pubs.acs.org/doi/abs/10.1021/jp107760k

[10] Wu, C.J., Fried, L.E., *First principles study of high explosive decomposition energetics*. Lawrence Livermore National Laboratory CA 94550 Eleventh International Detonation Symposium Snowmass, CO, (1998) 21 Aug. Available: https://www.osti.gov/biblio/8167

[11] Molt, R. W.; Watson, T.; Lotrich, V. F.; Bartlett, R. J., *RDX geometries, excited states, and revised energy ordering of conformers via MP2 and CCSD(T) methodologies: Insights into decomposition mechanism*. J. Phys. Chem. A 115 (2011, Jan) 884-890. Available: https://pubs.acs.org/doi/abs/10.1021/jp109695v

[12] Cawkwell, M. J.; Ramos, K. J.; Hooks, E.; Sewell, T. D., *Homogeneous dislocation nucleation in RDX under shock loading*. J. Appl. Phys. 107 (2010, Jan) 063512. Available: https://aip.scitation.org/doi/abs/10.1063/1.3305630

[13] H Salehi, P Amiri, R Zare Hasanabad., *Ab-initio Study of Electronic, Optical, Dynamic and Thermoelectric Properties of CuSbX2 (X=S, Se) Compounds.* jopn, 3 (2018, spring). Available: http://jopn.miau.ac.ir/article_2864.html

[14] S Ahmadi, M H Ramezani., *The structural and density state calculation of Boron and Nitrogen doped silicene nano flake*. jopn, 2 (2017, winter). Available: http://jopn.miau.ac.ir/article_2199.html

[15] S J. Mousavi., *First–Principle Calculation of the Electronic and Optical Properties of Nanolayered ZnO Polymorphs by PBE and mBJ Density Functionals*. jopn 2 (2017, Dec).

Available: http://jopn.miau.ac.ir/article_2570.html

[16] A. Moftakharzadeh, B. Afkhami aghdam., *Noise Equivalent Power Optimization of Graphene-Superconductor Optical Sensors in the Current Bias Mode*. jopn, 3 (2018, sep).

Available: http://jopn.miau.ac.ir/article_3040.html

[17] M. Jafary., *Electronic Transmission Wave Function of Disordered Graphene by Direct Method and Green's Function Method*. jopn, 1 (2016, sep). Available: http://jopn.miau.ac.ir/article_2049.html

[18] Strachan, A.; Van Duin, A. C. T. Chakraborty, D.; Dasgupta, S., *Shock Waves in High-Energy Materials: The Initial Chemical Events in Nitramine RDX*. Phys. Rew. Lett. 91 (2003, Aug) 895-898. Available: https://journals.aps.org/prl/abstract/10.1103/PhysRevLett.91.098301

[19] Sorescu, D. C.; Rice, B. M., *Thompson, D. L.; Intermolecular potential for the RDX crystal: A crystal packing, Monte Carlo, and molecular dynamics study*. J. Phys. Chem. B 101 (1997, Nov) 798-808. Available: https://pubs.acs.org/doi/abs/10.1021/jp9624865

[20] Warrier, M.; Pahari1, P. Chaturvedi, S., *Molecular dynamics analysis of the transient temperature increase at void locations in shocked materials: RDX and Cu*. J. Mol. Model. 21 (2015, July) 192 (1-10). Available: https://link.springer.com/article/10.1007/s00894-015-2737-7

[21] Zhang, L.; Zybin, S. V.; Van Duin, A. C. T.; Dasgupta, S.; Goddard, W. A., *Thermal decomposition of energetic materials by REAXFF reactive molecular dynamics*. AIP Conference Proceeding 845 (2006, Jan) 589-592. Available: https://aip.scitation.org/doi/abs/10.1063/1.2263391

[22] Strachan, A.; Kober, E. M.; Van Duin, A. C. T.; Oxgaard, J.; Goddard, W. A., *Thermal decomposition of RDX from reactive molecular dynamics*. J. Chem. Phys. 122 (2005, Jan) 054502. Available: https://aip.scitation.org/doi/abs/10.1063/1.1831277

[23] Reed, E. J.; Fried, L. E.; Joannopoulos, J. D., *A method for tractable dynamical studies of single and double shock compression*. Phys. Rew. Lett. 90 (2003, June) 235503-4. Available: https://journals.aps.org/prl/abstract/10.1103/PhysRevLett.90.235503

[24] Reed, E. J.; Maiti, A.; Fried, L. E., *Anomalous sound propagation and slow kinetics in dynamically compressed amorphous carbon*. Phys. Rew. E 81 (2010, Jan) 016607-9. Available: https://journals.aps.org/pre/abstract/10.1103/PhysRevE.81.016607

[25] Choi, C.S.; Prince, E., *The crystal structure of cyclotrimethylenetrinitramine.* Acta Crystallogr. Sect. B: Struct. Crystallogr. Cryst. Chem. B 28 (1972, May) 2857-2862. Available: https://onlinelibrary.wiley.com/doi/abs/10.1107/S0567740872007046

[26] LAMMPS is available at www.lammps.sandia.gov

[27] Plimpton, S., *Fast parallel algorithms for short–range molecular dynamics*. J. Comput. Phys. 117 (1995, March) 1-19. Available: https://www.sciencedirect.com/science/article/pii/S002199918571039X

[28] VMD is available at www.ks.uiuc.edu/Research/vmd

[29] Van Duin A C T, Dasgupta L, Siddharth D, Francois L, Goddard W A ReaxFF: *A reactive force field for hydrocarbons*. J. Phys. Chem. A 105 (2001, March) 9396-9409.

Available: https://pubs.acs.org/doi/abs/10.1021/jp004368u

[30] Van Duin , Reactive Force Fields: Concepts of ReaxFF. *Material and Process Simulation Center*, California Institute of Technology CH-121 lecture. (2008, Feb)

Available:
www.wag.caltech.edu/home/duin/Reax/ch121ReaxFF_introduction.pdf