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Molecular Dynamics Studies of Polymer Systems

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Abstract

The goal of this work was to determine if molecular dynamics as represented by the United-Atom method employed by the DL_POLY2 software package could explain polymer phenomena such as melting point temperature, glass transition temperature, crystallization, and density, and assess the effect of side group length, branching, chemical structure, length of polymer, and temperature. The verified model will then serve as a confident tool in the prediction of the properties of polymeric systems. The aim was to apply molecular dynamics simulations to polymers relevant to the running shoe industry.

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Introduction

Motivation: Running Shoes

Running shoes provide cushioning to the foot upon impact with the ground. The most common material used in the midsole of the shoe (the part of the shoe that provides the cushioning) is ethylene vinyl acetate or EVA foam. (Shorten, 2000, p. 4) This foam has air or other gasses trapped inside the cells of the foam that upon compression, exit the cell. (Shorten, 2000, p. 12) After the shoe has left the ground, and the EVA foam is not under compression, air is drawn back into the cells. This occurs because of the elastic properties of the EVA. This cycle repeats with every step taken. The rebound time of EVA foam ranges from minutes to hours. (Wilson, 2007, p. 1372) Eventually the cells start to become permanently deformed. (Wilson, 2007, p. 1371) The foam cells draw in less air at a slower rate, hindering the full expansion to their original position. Running shoes become 'worn out' when the foam cells no longer provide a satisfactory amount of cushion.

The degradation of polymers has yet to be fully understood due to their complex chemical nature. Degradation can occur from environmental interactions such as light radiation, heat, swelling, dissolution, scission, and chemical reactions with atmospheric oxygen for instance. (Callister, Jr., 2007, pp. 655-657) During the active lifetime of a running shoe the interest would be in modeling the deformation rather than the degradation of the polymer network. As waste is becoming an increasingly important topic, efforts to use to environmentally friendly polymers in running shoes have been on the rise. Modeling polymers to assess their properties is an important task towards understanding how running shoes perform and degrade with time.

Project Goals

The aim of the current work is to assess simple polymer systems that will lay the groundwork for eventually modeling complex EVA foam and its eventual deformation and degradation. Key areas for future studies include the modeling of various types of crosslinking and polymer orientations. The goal is to provide a foundation for running shoe companies to build upon. The ability to assess newly proposed polymers and their improved characteristics before experimentation will save time and reduce waste.

Background

Polymers

Polymers are large molecules of high molecular weight composed of repeating units called monomers. Most contain a high percentage of carbon and hydrogen. (Callister, Jr., 2007, p. 492)

Properties

The properties of polymers are affected by their different chemical and structural characteristics. Their composition (types of atoms, length of chains, degree of branching, etc.) determines these characteristics. For example, the degree of crystallization affects density, stiffness, strength, and ductility. The degree of crosslinking (described below) affects the stiffness, and the chemical makeup of the polymer affects the melting and glass transition temperatures. (Callister, Jr., 2007, p. 489)

Polymerization, or Growth of Polymers

Addition Polymerization

Addition polymerization usually occurs through radical addition, where an initiator molecule, usually peroxide, is degraded to produce two radicals. These radicals attack the double bonds of short molecules, in the case of polyethylene, an ethylene molecule, forcing an electron from the double bond to become an unpaired on the opposite side of where the peroxide attacked. This unpaired electron (radical) can now attack an ethylene molecule on its own, and continue the polymer growth. The unpaired electron on the carbon atom attacks the double bond of the neighboring ethylene molecule, creating a carbon-carbon single bond. This forces the other electron previously participating in the double bond to the other side of the molecule, opposite of the attack. This in turn creates another unpaired radical electron which continues to propagate the chain. (Wade Jr., 2009)

Condensation polymerization

Condensation polymerization forms polymers through the elimination of a small molecular weight byproduct when two reactant species come together. The reactant species can be the same or different molecules. The number of reactive sites each building block molecule has determines the type of polymer that can result from polymerization. Building block molecules with two reactive sites, termed bi-functional, form linear chains. A molecule with only one reactive site terminates the chain, whereas molecules with three or more reactive sites, tri-functional or higher functional monomers have the ability to form branching, crosslinks, and polymer networks. Typically condensation polymerization reactions are slower than those of addition polymerization. This type of polymerization also tends to produce lower molecular weight polymers. (Callister, Jr., 2007, p. 593)

Ring opening polymerization

Ring opening polymerization is a process that involves breaking open a cyclic ring to grow the polymer. This progression of chain growth can employ techniques from both types of polymerization described above (Davis, 2004, p. 44).

Basic Structures of Polymers Examined

Polyethylene

Polyethylene is the most basic of olefinic polymers, consisting of the repeating unit $-(C_2H_4)-$. This polyolefin is a homopolymer, consisting of only one type of repeating unit. (Callister, Jr., 2007, p. 496) Figure 1 below, shows the basic structure of polyethylene. Carbon atoms make up the backbone of the chain and are colored grey. Hydrogen atoms are colored white.

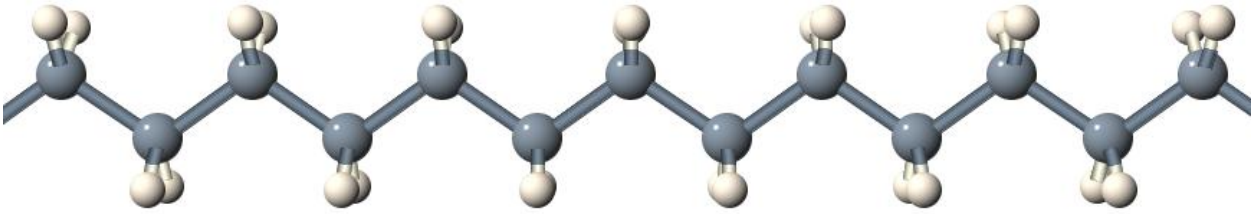

Figure 1: High Density Polyethylene (HDPE) Structure

Branched Polyethylene, or Low Density Polyethylene (LDPE)

Low density polyethylene is a branched version of polyethylene, where side chains extend out from the main chain. Figure 2 below is an image of LDPE where only the carbon atoms are shown.

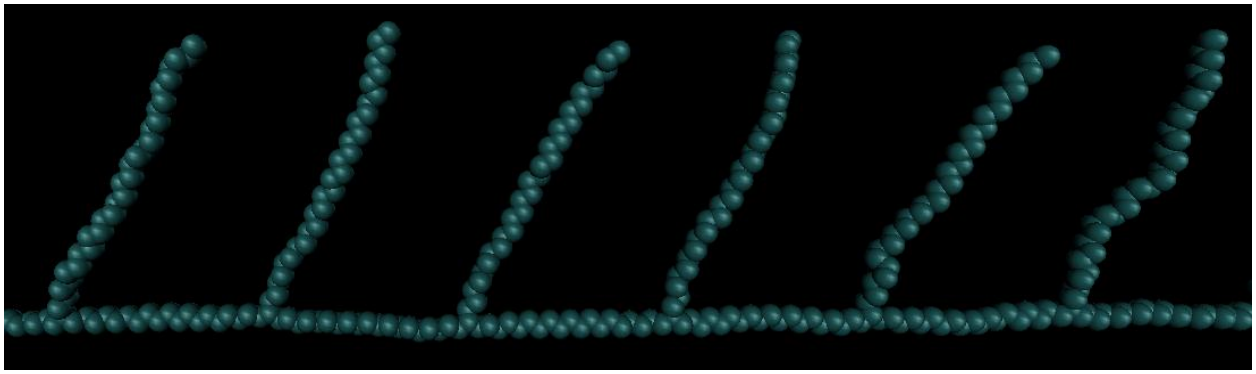

Figure 2: Low Density Polyethylene (LDPE) Structure

Polypropylene

Polypropylene is another olefinic polymer. From the basic polyethylene structure, one of the substituent hydrogen molecules is replaced with a methyl group. The repeating unit is $-(C_2H_3CH_3)-$. This polyolefin is a homopolymer as polyethylene is, consisting of only one type of repeating unit. (Callister, Jr., 2007, p. 496) Figure 3 below shows the basic structure of polypropylene. The carbon atoms are colored grey and the hydrogen atoms are colored white.

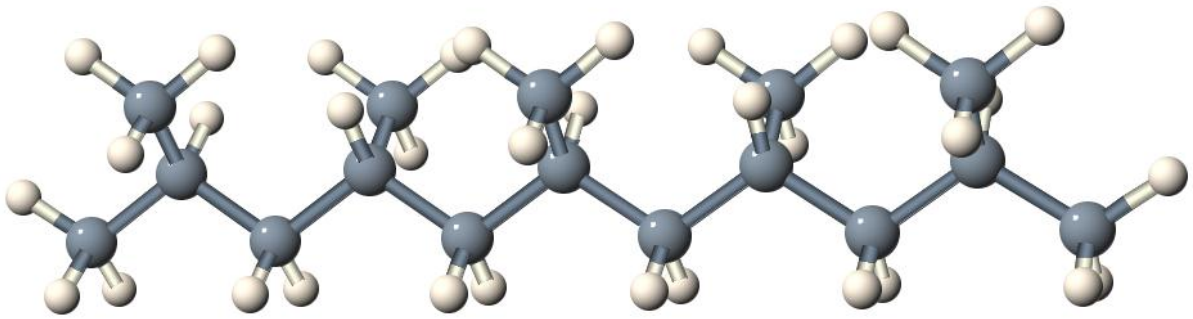

Figure 3: Polypropylene Structure

Ethylene Vinyl Acetate

Ethylene vinyl acetate is a copolymer. This term refers to a polymer chain with different repeating units (Callister, Jr., 2007, p. 495). The two repeating units are ethylene $–(C_2H_4)–$ and acetate $–(C_2O_2H_3)–$. Running shoes typically have 18 percent by weight vinyl acetate, with the remainder being ethylene. (Verdejo & Mills, 2002, p. 582) Figure 4 below shows the basic structure of ethylene vinyl acetate with one acetate group. The carbon atoms are colored grey, the hydrogen atoms are colored white, and the oxygen atoms are colored red.

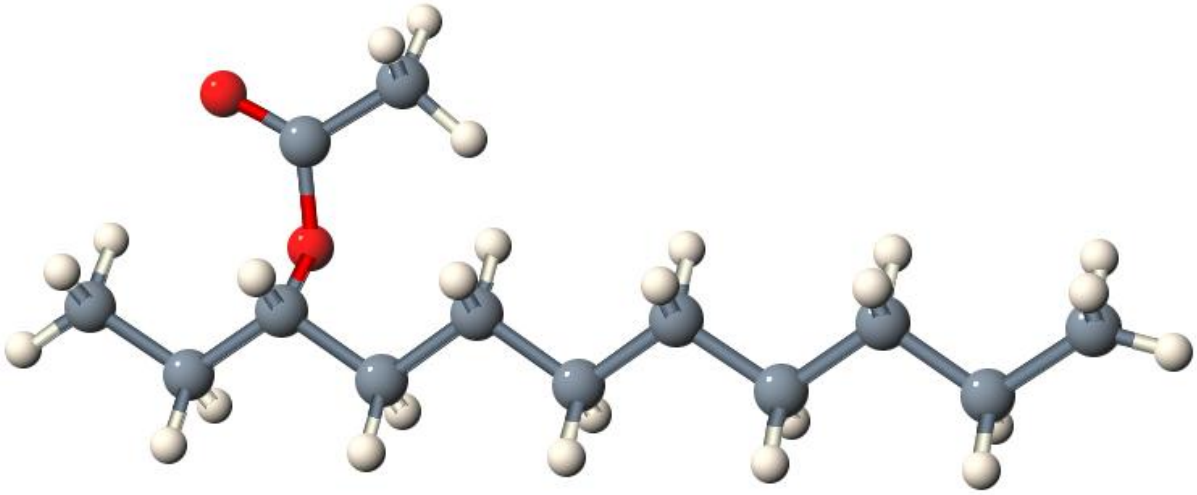

Figure 4: Ethylene Vinyl Acetate (EVA) Structure

Degree of Polymerization

The degree of polymerization, DP, describes the number of repeat units or monomers that have joined together to form a polymer chain. The degree of polymerization for a polymer is given by the equation $DP = M_n/m$, where M_n is the number average molecular weight of the given sample and m is the

molecular weight of the monomer. The number average molecular weight is a weighted average representing the molecular weight of the most abundant chains. For a given polymer sample, the degree of polymerization is the average number of monomers per polymer chain. (Callister, Jr., 2007, p. 498)

Critical Molecular weights

The critical molecular weight of a polymer is the minimum molecular weight that a polymer needs to have to exhibit its steady state bulk properties. At this molecular weight the chain dynamics cross over from free (or Rouse) to entangled (or reptation). Free chain dynamics explain the unattached nature of the polymers. They are free to move and slide over other chains without much hindrance. Entangled dynamics explain chains that are of a certain length where interactions with other neighboring chains greatly affect their movement. The chains are considered intertwined, as they are not able to freely move. (Drzewinski & van Leeuwen, 2006) Polymer chains with less than the critical molecular weight have transient properties. (Kausik, Mattea, Fatkullin, & Kimmich, 2006) Just as ethane, butane, and octane are essentially short chains of polyethylene and have different properties, polymer chains of different lengths have different properties as well. Only once the chains exceed the threshold length (or mass) known as the critical molecular weight, do they start to exhibit consistent properties. At this length the tangled nature of the chains allows the van der Waals forces to act steadily as the chains are hindered from moving freely over each other. Van der Waals forces are the long range attractive forces that act on neighboring molecules. Critical molecular weights are different for each polymer. Polymers exhibiting more flexible behaviors and minimal branching have much higher critical values than those with rigid backbones and high degrees of branching which promote tangling.

Branching

Branching is the term used for polymers that are not linear. Branched polymers are those that have multiple secondary chains that extend out from the main chain. (Callister, Jr., 2007, p. 502) Polymer branching occurs when monomers have more than two reactive sites, or are tri-functional or multifunctional. (Callister, Jr., 2007, p. 593) When the monomers have these unique properties, side reactions can occur at multiple points during polymer formation resulting in branching. The higher the degree of branching, the more the packing efficiency is reduced, effectively lowering the polymer density. (Callister, Jr., 2007, p. 502)

Crosslinking

Crosslinked polymers are created when adjacent chains are fused together by covalent bonds. The more places that neighboring chains are linked together, the higher the degree of crosslinking the polymer has. When polymers become highly crosslinked, they assume a three-dimensional structure and are termed network polymers. (Callister, Jr., 2007, p. 503)

Vulcanization was the first form of synthetic crosslinking. Natural and synthetic rubber when heated with sulfur form sulfur bridges or links between the long polymers. Vulcanization treats unsaturated polymers where the double bond in the backbone of the chain is broken and bonds to the sulfur crosslinking chain. (Encyclopedia Britanica, 2012, p. 1) These links are covalently bonded and effectively rebound the shape of the material after an induced stress, giving it elastic properties. (Encyclopedia Britannica, 2012, p. 1) (Odian, 2004, p. 740)

Unfortunately this basic method of vulcanization crosslinking does not work for saturated polymers like EVA or polyethylene. Organic peroxides are used to crosslink such macromolecules without double bonds. Peroxides when heated form radicals that are able to attack the backbone of saturated polymers and create sites for crosslinking. A common organic peroxide crosslinking agent for EVA is dicumyl peroxide shown in Figure 5 below. (Arkema, 2009, p. 5)

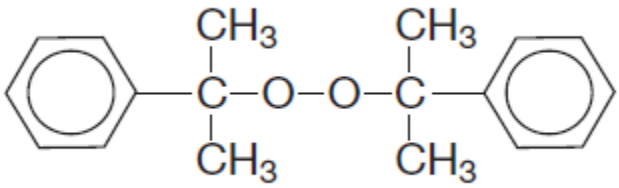

Figure 5: Crosslinking agent Dicumyl Peroxide Structure

Foams

Foams are expanded plastics that are more rigid than dense polymers at any given weight. Foams collapse under impact or compressive stresses, but are able to absorb much of the energy transferred to them, a basis reasoning for their use as cushioning agents in running shoes. Foams can be produced by injecting gasses into a quantity of polymers in the liquid state. Upon cooling, the plastic traps the gasses within the network forming a foam. (Encyclopedia Britannica, 2012)

Computational Chemistry and Molecular Dynamics

Simulations are important in the chemical industry as precursors to industrial change. Simulations of proposed processes are needed to assess changes in current processes or for the initialization of new ones. Computational chemistry and molecular dynamic simulations are used to examine the physical properties of molecular systems to determine the possibility of manufacture or implementation. Using these methods the individual atoms or molecules are simulated. (The NSF Blue Ribbon Panel on Simulation-Based Engineering Science, 2006)

Basic Theory

Computational chemistry, sometimes called theoretical chemistry or molecular modeling, combines quantum mechanics theory with the simplifying approximations of a model to solve practical problems. (Cramer, 2002, p. 2) The observable chemical properties of a system are fundamentally described by the theorems of quantum mechanics. (Cramer, 2002, p. 4)

The minimum input needed to model an isolated molecule is the types of component atoms and their relative positions. (Cramer, 2002, p. 5) Molecules are constantly in motion (bond stretching, bond rotation) and rarely at any given point have the same exact geometry as other molecules of the same type within the system. (Callister, Jr., 2007, p. 501) For the model to more closely represent actuality therefore, all molecular geometries are captured by molecular dynamics into what is known as a complete potential energy surface (PES). (Cramer, 2002, p. 6) Molecular dynamics simulations attempt

to ‘map’ the PES for given molecules to find local energy minima, or the most stable geometric configurations. (Cramer, 2002, p. 5)

Molecular dynamics simulation involves step-by-step solutions of Newton’s equations of motion. It uses atomic coordinates, or the relative positions of the atoms, comprised of inter-atomic distances, bend angles, and torsion angles, to calculate the potential energy of the molecule. (Allen, 2004, p. 2) The simulation runs through a range of each of these parameters to find the optimum geometry of the molecule, in which it has the lowest potential energy. This range of each of the parameters is defined by the force field potential used in the simulation. There are different force fields to choose from, each working best for different types of molecular systems. Some of them are described below.

Inaccurate properties of the bulk system result from simulations of small numbers of molecules, as a large part of them comprise the surfaces. To address this, periodic boundary conditions are introduced that surround the sample simulation box with replicas on all sides. The system becomes much larger and properties are able to be measured with the entirety of the system encapsulated with mirror images.

The current work utilizes molecular modeling as defined by Cramer (p4). The aim is “to focus on a target system having a particular chemical relevance (e.g., for economic reasons) and to be willing to sacrifice a certain amount of theoretical rigor in favor of getting the right answer in an efficient manner.” (Cramer, 2002, p. 4) Many simulations are based around simplifying approximations that decrease the time it takes for the computer to work through the calculations. For example, harmonic potentials are used to describe bonds and angles, but are commonly replaced by fixed values to save computational time. One simplification used in the current work, as well as in a many polymer modeling papers, is the United-Atom method. This method groups together multiple atoms into a pseudo atom. The number of parameters mentioned earlier, such as bond lengths and angles, therefore, decreases significantly as the number of ‘atoms’ in the system is reduced.

In molecular dynamics simulations, force field denotes the parameters of the potential used to calculate the forces acting on the atoms of the system being modeled. Different atom types are described with various defining parameters such as bonds, angles, dihedrals, and long-range interactions based on the particular surrounding environment of each atom. One such force field developed by William L. Jorgensen is known as OPLS (Optimized Potential for Liquid Simulations) force field, shown below in Equation 1. This force field describes the velocities of the atoms within the system through summations of the bonds, angles, torsions, and Lennard-Jones potentials. (Marcon, Vehoff, & Ghiringhelli, 2007) In Equation 1, b is the bond length, θ is the bond angle, b_0 and θ_0 are the equilibrium values, K_b and K_θ are the force constants, ω is the dihedral angle and V_n the corresponding force constant, and γ is the phase angle. The parameters r_{ij}, ε_{ij}, σ_{ij}, q_i, and q_j are the ‘atom’ separation, Lennard-Jones well depth, Lennard-Jones size, and partial charges, respectively, for the pair of interaction sites i and j. (Duan, et al., 2003)

$$V(\{\overrightarrow{r_N}\}) = \sum_{bonds} \frac{1}{2} k_b (r - r_0)^2 + \sum_{angles} k_\theta (\theta - \theta_0)^2 + \sum_{torsions} \frac{1}{2} V_n [1 + cos(n\omega - \gamma)] + \sum_{i=1}^{N-1} \sum_{j=i+1}^{N} \left\{ 4\varepsilon_{ij} \left[\left(\frac{\sigma_{ij}}{r_{ij}} \right)^{12} + \left(\frac{\sigma_{ij}}{r_{ij}} \right)^{6} \right] + \frac{q_i q_j}{4\pi\varepsilon_0 r_{ij}} \right\}$$

Equation 1: Functional Form of OPLS

Lennard-Jones potentials are used to approximate the interactions between two neutral molecules. These potentials take into account the short range Pauli Repulsion forces as well as the long range van der Waals attractive forces from dipole-dipole interactions. Lennard-Jones potentials are able to be transferred from molecule to molecule as they define a single functional group and their non-bonded interactions. They are therefore able to be incorporated into larger more complex molecules that have substituent groups corresponding to those previously defined by the potentials. In the United-Atom force field the transferability of these potentials is known as “transferable potentials for phase equilibria” (TraPPE-UA). (Kamath, Robinson, & Potoff, 2005, p. 46)

Previous Molecular Dynamics Simulations of Polymers

Polymer Collapse

Zhan and Mattice examined simulations of Poly (1, 4-trans-butadiene). Simulations were run to calculate the volumes and densities of this polymer in a vacuum with no periodic boundary conditions and also with periodic boundary conditions in two planes, leaving the third dimension at a large value to represent infinite space. In their findings the polymer exhibited a globular structure when left to equilibrate in a vacuum for 1500 picoseconds. Simulations with periodic boundary conditions in two dimensions forced the polymer into a coil or thin film. They concluded that this was a result of secondary bonding interactions with mirror images of the polymer in adjacent cells. (Zhan & Mattice, 1994)

Temperature Effects on Density in Dense Polymer Systems

The structures and equilibrium properties of dense polyethylene polymer systems through the use of Monte Carlo simulations have been simulated. Employed was a new technique using rigid bonds and bond angles. The range of chain lengths studied were 10-60 carbon atoms long with systems ranging from 3-20 chains. Through simultaneous simulation of a constant volume configurational simulation and an isobaric-isothermal simulation, the most accurate densities of dense polymeric systems were obtained. Lower densities were reported compared to literature when simulating a single chain of polyethylene 60 segments long. Simulations of three polyethylene chains of 60 segments long provided more accurate density data. The simulations of density values ranging from 0-200 degrees centigrade (273-473K) produced a trend that matched the experimental data. The simulations followed the experimental data trend of decreasing density with increasing temperature. (de Pablo, Laso, & Suter, 1992)

The condensed –phase optimized molecular potentials for atomistic simulation studies (COMPASS) force field was used for the molecular systems of myo- and neo-inositol. The study examined the heat of sublimation, density, melting point, and glass transition temperature. The melting point and glass transition temperature plots were defined by cell volume as a function of temperature. Melting point determination utilized system models in the crystalline state, while glass transition temperature determination made use of system models in the amorphous state. Using the plots, the values for these properties were determined by sudden shifts in slope. Values obtained for these properties matched well to experimental data found in literature. (Watt, Chisholm, Jones, & Motherwell, 2004)

Chain dynamics of polymer melts confined to micrometer thick layers were studied. Properties of the polymer melts restricted to the film layer were different than those of the bulk polymer melt. Polymers of molecular weights below the critical value in the confined space were shown to change over from Rouse to reptation dynamics. (Kausik, Mattea, Fatkullin, & Kimmich, 2006) An explicit study of the cross over from Rouse to reptation dynamics in polymers developed a simple model for a one-dimensional chain. The model focused on hernia annihilation and creation which allowed the links of the chain to change between slack and taut. The new model allowed the interchange rate to increase significantly from previous models making the study of the cross-over behavior possible. (Drzewinski & van Leeuwen, 2006)

Branching Effects on Bulk Properties

Rheological properties of polymer melts were studied for polyethylene chains of varying molecular architecture. Linear, star, H-shaped, and comb-shaped structures were used to examine the bulk properties. Branched molecules were found to differ in properties from linear chains of the same molecular weight in the area of viscosity. The study concluded however, that despite the property changes with shape variance, the rheological properties will be most affected by the chain length and degree of branching. (Jabbarzadeh, Atkinson, & Tanner, 2003)

Transferable Potentials for Phase Equilibria United-Atom (TraPPE-UA)

The TraPPE-UA force field was used to model branched alkanes. Lennard-Jones interaction parameters for methine and quaternary carbon groups were added to the model. Critical temperatures and saturated liquid densities were used to optimize these parameters to fit the force field model. The vapor-liquid coexistence curves (VLCC) were then determined for small alkane isomers. Densities were studied using the isobaric-isothermal ensemble. The TraPPE-UA force field was concluded to under predict second virial coefficients, and show small deviations from experimental data of saturated vapor pressures and densities for normal alkanes. The force field also slightly over predicted the critical temperatures of the larger branched alkanes. (Martin & Siepmann, 1999)

The TraPPE-UA force field was extended to include parameters for the functional groups ether, glycol, ketone, and aldehyde. The parameters were optimized using vapor-liquid coexistence curves. Small molecules with the functional groups were simulated for determination of a variety of properties. The simulations resulted in very close fits to experimental data for critical temperatures and normal boiling temperatures. (Stubbs, Potoff, & Siepmann, 2004)

The TraPPE-UA force field was assessed through simulations of carboxylate esters. Partial charges were taken from the optimized potentials for liquid simulations (OPLS) force field. The model was used to determine vapor-liquid coexistence curves, vapor pressures, and critical temperatures, saturated liquid densities, and critical densities of four esters studied. The critical densities and azeotrope of methyl acetate and methanol were both in very close agreement with experimental data. Pure component vapor pressures were over predicted which resulted in the offset of pressure-composition diagrams. The diagrams did show good qualitative trends. (Kamath, Robinson, & Potoff, 2005)

Methodology

Programs

DL_POLY

"DL_POLY is a parallel molecular dynamics simulation package developed at Daresbury Laboratory." (DL_Poly2 user manual)

Input Files

Several input files are needed for the simulations and are described below.

The FIELD file

The FIELD file defines the nature of the molecular forces governing the molecules being modeled. This file contains force field information partitioned into three categories; general information, molecular descriptions, and non-bonded interaction descriptions.

The CONFIG file

The CONFIG file contains the initial coordinates of the molecule. The atom entries of this file with specified coordinates correspond to the FIELD file atom entries, so that together, they construct all the parameters needed to run the DL_POLY simulation.

The CONTROL file

The CONTROL file is responsible for defining the design system parameters and variables. This file specifies the temperature, pressure, timestep, time duration desired for geometry optimization/equilibration, the job time length, etc.

Output Files

The DL_POLY program produces output files from completed simulations described below.

The HISTORY file

"The HISTORY file is the dump file of atomic coordinates, velocities, and forces." (DL_Poly2 user manual) This file contains the coordinates, velocities, and forces at each timestep interval specified in the CONTROL file.

The REVCON file

The REVCON file produces the final atomic coordinates, velocities, and forces. It can be used to restart or continue a simulation. In the current work, the REVCON file is used to assess final geometric configurations along with occupying volume and box volume used in density calculations.

The STATIS file

The STATIS file is a collection of energy data from the simulation recorded for each timestep interval specified in the CONTROL file.

The REVIVE file

The REVIVE file is an accumulation of statistical results and is to be renamed as REVOLD and used as an input if a continuation of a simulation is desired.

The OUTPUT file

The OUTPUT file includes specifications on force fields and simulation control gathered from the CONTROL and FIELD file inputs. This file relays simulation progress, a summary of statistical data which includes the diffusion coefficients, a sample of the final geometric configuration, and radial distribution functions.

DL_FIELD

DL_FIELD is a program designed by Daresbury Laboratory intended to assist in the use of DL_POLY programs. The program creates CONFIG, CONTROL, and FIELD input files for DL_POLY from the user's simple atomic configuration in xyz form. DL_FIELD is able to utilize CHARMm and AMBER force field files in the creation of the input files needed for DL_POLY.

McVol

McVol is a program used in the determination of the volume occupied by a molecule. The program is used in the evaluation of configurational volume to assess changes in volume resulting from shape changes during simulation. The program uses radii of a given distance specified by the user around each atom. In polymer simulations the chains fold in on one another. As this occurs, the radius around each atom becomes slightly overlapped, thus decreasing the calculated volume. A straight chained polymer therefore would have the highest calculated volume.

Visual Molecular Dynamics (VMD)

VMD is a program used to view the simulations. The program converts the data of the HISTORY file of DL_POLY2 into a motion picture of the molecular system.

United Atom Force Field

The united atom method was employed as the program DL_POLY2 could not handle large polymer systems. The computational time required to calculate all required bond energies etc. for each methylene/methyl/methionine group increases as the hydrogen atoms in these groups add to the number of bond angles and dihedrals. These extra attributes dramatically increase the amount of calculations that DL_POLY2 needs to perform and therefore increase computational time excessively to the point where computational chemistry for molecular dynamics purposes becomes senseless. The united atom method groups the carbon hydrogen groups commonly found in the main chain backbone of vinyl polymers. Methyl, methylene, and methionine groups or singular carbon atoms without hydrogen are lumped into one pseudo-atom with a set of its own potentials and parameters. Bond lengths are fixed. Atom mass and charge, angles, dihedrals, Lennard-Jones potentials, and atomic coordinates are still specified. Dihedrals are specified using optimized potentials for liquid simulations (OPLS force) force field data. (Kamath, Robinson, & Potoff, 2005, p. 47)

Force field data known as TraPPE-UA was used for this work. (Kamath, Robinson, & Potoff, 2005, p. 47) (Martin & Siepmann, 1999) (Stubbs, Potoff, & Siepmann, 2004)

Bond	Bond Length, r_0 (A)
CH_x-CH_Y	1.54
CH_2=CH	1.33
C-CH_x	1.52
O-H	0.945
C-O	1.344
O-CH_x	1.41
CH=O	1.217
C=O	1.229

Table 1: United-atom transferable potentials for bond lengths

United-atom transferable potentials for bond lengths are shown in Table 1 above. Bond lengths are specified for various types of connected atoms. Values are reported in angstroms.

Bond Angle	θ_0 (degrees)	k_θ/k_b (kcal/mol)
< CH_x-CH_2-CH_Y	114	124.20
< CH_x-CH-CH_Y	112	124.20
< CH_x-C-CH_Y	109.47	124.20
< C-O-CH_3	115	124.20
< O-C=O	125	124.20
< O-C-CH_3	110	140.30
< O=C-CH_3	125	124.20
< CH_3-O-H	108.5	110.09
< CH_x-CH_Y-O	112	99.96
< CH_x-O-CH_Y	112	120.03
< CH_x-C(=O)-CH_Y	117.2	124.20
< CH_x-CH=O	121.4	124.20

Table 2: United-atom transferable potentials for bond angles

United-atom transferable potentials for bond angles are shown in Table 2 above. Bond lengths are specified for various types of connected atoms. Values are reported in degrees.

Torsional Interactions	c_0/k_b (kcal/mol)	c_1/k_b (kcal/mol)	c_2/k_b (kcal/mol)	c_3/k_b (kcal/mol)
CH_x-O-C=O	9.3717	4.3599	4.0917	-0.3048
CH_x-O-C-CH_Y	0.0000	4.2884	4.1692	0.3921
CH_2=CH-O-C	0.0000	3.3743	3.1080	0.1719
CH-O-C-CH_x	-0.0288	1.9735	1.0347	-0.2752
CH_Y-CH_x-C=O	4.0451	-1.4644	0.1149	-0.5827
CH_Y-CH_x-O-C	0.0000	1.4414	0.3254	1.1093
CH_x-CH_2-CH_2-CH_Y	0.0000	0.6658	-0.1355	1.5725
CH_x-CH_Y-O-CH_z	0.0000	1.4414	-0.3254	1.1093
CH_x-CH_2-CH_2-O	0.0000	0.3510	-0.1060	1.5300
O-CH_2-CH_2-O	1.0000	0.0000	-0.5000	2.0001
CH_x-CH_Y-C=O	4.0451	-1.4644	0.1149	-0.5827
CH_x-CH_2-CH-CH_Y	-0.4989	0.8520	-0.2223	0.8769
CH_x-CH_2-C-CH_Y	0.0000	0.0000	0.0000	0.9167
CH_x-CH-CH-CH_Y	-0.4989	0.8520	-0.2223	0.8769

Table 3: United-atom transferable potentials for torsional interactions

United-atom transferable potentials for torsional interactions are shown in Table 3 above. Torsional interactions are specified for various types of connected atoms. Values are reported in kcal/mol.

Non-Bonded Interactions	Molecule Type	σ Length (A)	ε/k_B (kcal/mol)	q (e)
$CH_3(sp^3)$	ether/alcohol/aldehyde	3.75	0.1947	0.25[a]/0.265[b]/-0.043[c]
$CH_2(sp^3)$	ether/alcohol/aldehyde	3.95	0.0914	0.25[a]/0.265[b]/-0.043[c]
$CH(sp^3)$	ether/alcohol	4.33	0.0199	0.25[a]/0.265[b]
$C(sp^3)$	ether/alcohol	5.8	0.0010	0.25[a]/0.265[b]
$CH_3(sp^3)$	all other	3.75	0.1947	0
$CH_2(sp^3)$	all other	3.95	0.0914	0
$CH(sp^3)$	all other/aldehyde	4.68	0.0199	0/-0.043[c]
$C(sp^3)$	all other/aldehyde	6.4	0.0010	0/-0.043[c]
O	ether	2.8	0.1093	-0.5
O	alcohol	3.02	0.1848	-0.7
H	alcohol		0.0000	0.435
$CH(sp^2)$	aldehyde	3.52	0.1073	0.525
$O(sp^2)$	aldehyde	3.05	0.1570	-0.482
$C(sp^2)$	ketone	3.82	0.0795	0.424
$O(sp^2)$	ketone	3.05	0.1570	-0.424

Table 4: United-atom transferable potentials for non-bonded interactions

United-atom transferable potentials for non-bonded interactions are shown in Table 4 above. Lennard-Jones potentials and atomic charges for various atoms are specified for non-bonded interactions. Values for Lennard-Jones size (σ) are in angstroms, Lennard-Jones well depth (ε) is in kcal/mol, and partial charges (q) are in units of electron volts. ([a] For sites adjacent to the ether oxygen. [b] For sites adjacent to the alcohol oxygen. [c] For sites adjacent to the aldehyde carbon.)

Non-bonded interactions are described by Equation 2 below, where r_{ij}, ε_{ij}, σ_{ij}, q_i, and q_j are the 'atom' separation, Lennard-Jones well depth, Lennard-Jones size, and partial charges, respectively, for the pair of interaction sites i and j.

$$U(r_{ij}) = 4\varepsilon_{ij}\left[\left(\frac{\sigma_{ij}}{r_{ij}}\right)^{12} - \left(\frac{\sigma_{ij}}{r_{ij}}\right)^{6}\right] + \frac{q_i q_j}{4\pi\varepsilon_0 r_{ij}}$$

Equation 2: Non-bonded Interaction Potential

Lonentz-Berthelot rules were used as shown below in Equation 3 and Equation 4 to calculate van der Waals interactions for other combinations of atoms not specified in Table 4 above. (Kamath, Robinson, & Potoff, 2005, p. 47)

$$\sigma_{ij} = \frac{\sigma_{ii} + \sigma_{jj}}{2}$$

Equation 3: Combining rules for different sizes of Lennard-Jones parameters

$$\varepsilon_{ij} = \sqrt{\varepsilon_{ii} * \varepsilon_{jj}}$$

Equation 4: Combining rules for different well depths of Lennard-Jones parameters

Bond angle bending is controlled by a harmonic potential shown in Equation 5 below. θ is the measured bond angle, θ_0 is the equilibrium bond angle and k_0 is the force constant.

$$U_{angle} = \frac{k_\theta}{2}(\theta - \theta_0)^2$$

Equation 5: Harmonic Potential

Torsional interactions separated by three bonds are described by Equation 6. ϕ is the dihedral angle and c_i are the Fourier constants listed in Table 3.

$$U_{torsion} = c_0 + c_1[1 + cos(\varphi)] + c_2[1 - cos(2\varphi)] + c_3[1 + cos(3\varphi)]$$

Equation 6: Torsional Interaction Potential

(Kamath, Robinson, & Potoff, 2005, p. 48)

Simulations

Parameters

A simulation time for the polymer chains of 1500 seconds was chosen as the minimum run time based on the 1994 paper Molecular Dynamics Simulation of the collapse of Poly(1,4-trans-butadiene) to a globule and to a thin film by Zhan and Mattice. This time duration provides a sufficient time for the system to reach steady state. (Zhan & Mattice, 1994)

The time step of the simulation controls the time value jump between each stepwise calculation. The larger the time step, the faster the simulations are able to reach the desired job end time, but the larger the resulting error in data extracted from the simulation. Larger time steps of 5 fs have been shown to result in dramatic energy drifts. (Izaguirre, Reich, & Skeel, 1999, p. 9853) The time step used for all simulations in the current work was 1 fs.

Various temperatures were used in the simulations of the current work. To assess temperature related trends, simulations of system temperatures ranging from 100K to 800K were used. The extremes were simulated to extrapolate more accurate mid-range temperature data to more clearly show the trends, and not used in explicit value retrieval. Molecular dynamics simulation temperatures have been shown to deviate from actual temperature, (Jobic, Smirnov, & Bougeard, 2001), which is a compounding reason for the broad range of temperatures used in the current work. A far-reaching series of temperatures was used to encompass the entirety of each of the trends examined.

A NVT simulation, known as a canonical ensemble, is based on the temperature and volume of the system having specified average values. A NPT simulation, known as an isothermal-isobaric ensemble, is based on the pressure and temperature of the system having a specified average values, while the volume is able to fluctuate. (Hunenberger, 2005, p. 111)

Polymers

Four polymer types were simulated, straight chained polyethylene or high density polyethylene (HDPE), branched polyethylene or low density polyethylene (LDPE), polypropylene (PP), and ethylene vinyl acetate (EVA). Geometries, coordinates, and force field data (CONFIG and FIELD files) were developed for various lengths of the main chain ranging from 10 pseudo atoms long (a degree of polymerization of 5 – DP of 5) to 5000 pseudo atoms long (a degree of polymerization of 2500 – DP of 2500).

Polymer Chain Length

To assess how chain length affects polymer structure, NVT simulations of each chain length for a given polymer type were run. To isolate the singular molecular chain, the simulations were performed with no periodic boundaries as a single polymer alone in space. This eliminated the possibility of mirror chain interactions between adjacent cells as well as decreased the simulation time. The simulations were run at 300K for 3000 picoseconds to fully reach steady state equilibrium.

Pressure

To determine whether a pressure difference of 1atm changed the density of polymer, two simulations were run for polyethylene with chain lengths of 2000 pseudo atoms. The precursor NVT simulation

equilibrated the 1 chain polymer system for 3000 picoseconds at 300K and 0atm. Following this, the first NPT simulation was run at 0atm for 1500 picoseconds, and the second NPT simulation at 1atm for the same length of time.

Density

To examine the density difference between single and multiple polymers chain systems, a single polymer with a chain length of 2000 pseudo atoms, and four chains of the same length were each run for high density polyethylene and polypropylene. NVT simulations were run for 3000 picoseconds with no periodic boundary conditions to equilibrate the system. NPT simulations were then run for 1500 picoseconds using thermostat and barostat relaxation times of 0.5fs for both. Simulations were run at 300K and 0atm.

Crystallization

Polymer systems of HDPE were simulated at various low temperatures to assess the degree of ordering among the chains. Four chains of 2000 pseudo atoms were examined at temperatures as low as 100K. Systems of 20 chains 500 pseudo atoms in length, 25 chains 200 pseudo atoms in length, and 50 chains 100 pseudo atoms in length were also studied. The chains were initially linear and adjacent with the low temperatures held constant from the beginning of the simulations. Another series of simulations was run where the system of 50 chains 100 pseudo atoms in length was initially equilibrated at 1000K to imitate a liquid polymer melt. The temperature was slowly decreased in each subsequent simulation which was a continuation of the last.

Melting Point

To evaluate the melting point of high density polyethylene and polypropylene, NVT simulations of four chains each of 2000 pseudo atoms in main chain length were run for various temperatures surrounding their respective experimental melting points found in literature. These simulations were run for 3000 picoseconds with no periodic boundary conditions to equilibrate the system. The final geometries retrieved from the REVCON files were then used to start new NPT simulations. These simulations were run for 1500 picoseconds at each respective temperature and at 0atm. The temperatures ranged from 100K to 800k and clustered around the polymer type's experimental melting point.

High density polyethylene polymer systems of a larger number of macromolecules were simulated. Systems of 50 chains 100 pseudo atoms in length, 25 chains 200 pseudo atoms in length, and 20 chains 500 pseudo atoms in length were simulated.

Results

Polymer Structure - Chain Length Effects

HDPE, LDPE, and PP molecules with main chain lengths ranging from 10 to 5000 pseudo atoms long were simulated each for 3000 picoseconds with time steps of 0.01 picoseconds. Each polymer simulation started with a straight chain molecule. Using no periodic boundary conditions, the polymers collapsed in on themselves forming globules.

Globule Formation

Globule formation times were qualitatively extracted through visual methods by viewing the HISTORY output files of DL_POLY using the program VMD. Globule formation was determined to be the initial point of the chain coming together.

A range of HDPE, PP, and LDPE polymer lengths were simulated for 3000 picoseconds at 300K and 0 atm. Figure 6, Figure 7, and Figure 8 below, display globule formation times for various lengths of polymer chains. The plots show a general trend that as the length of the polymer increases, the time to form a globule also increases.

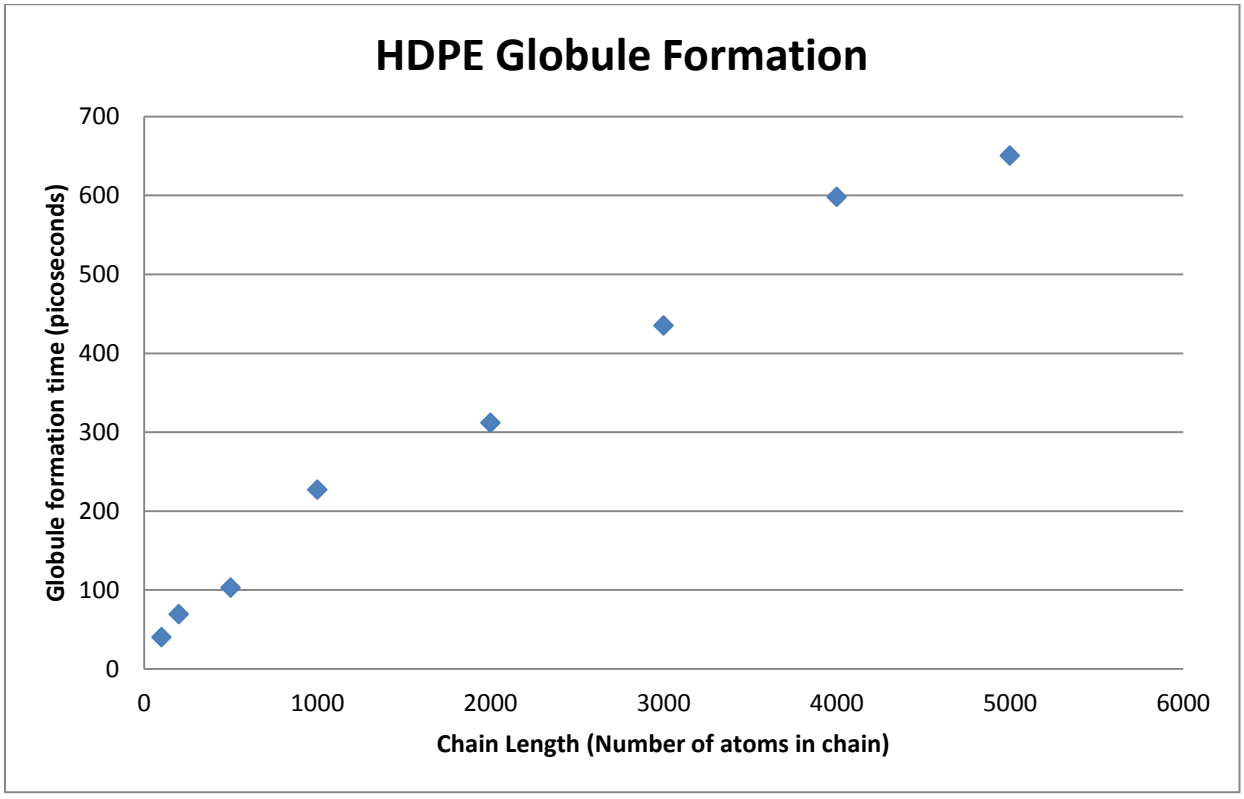

Figure 6: Globule Formation Time of High Density Polyethylene (HDPE) for various chain lengths

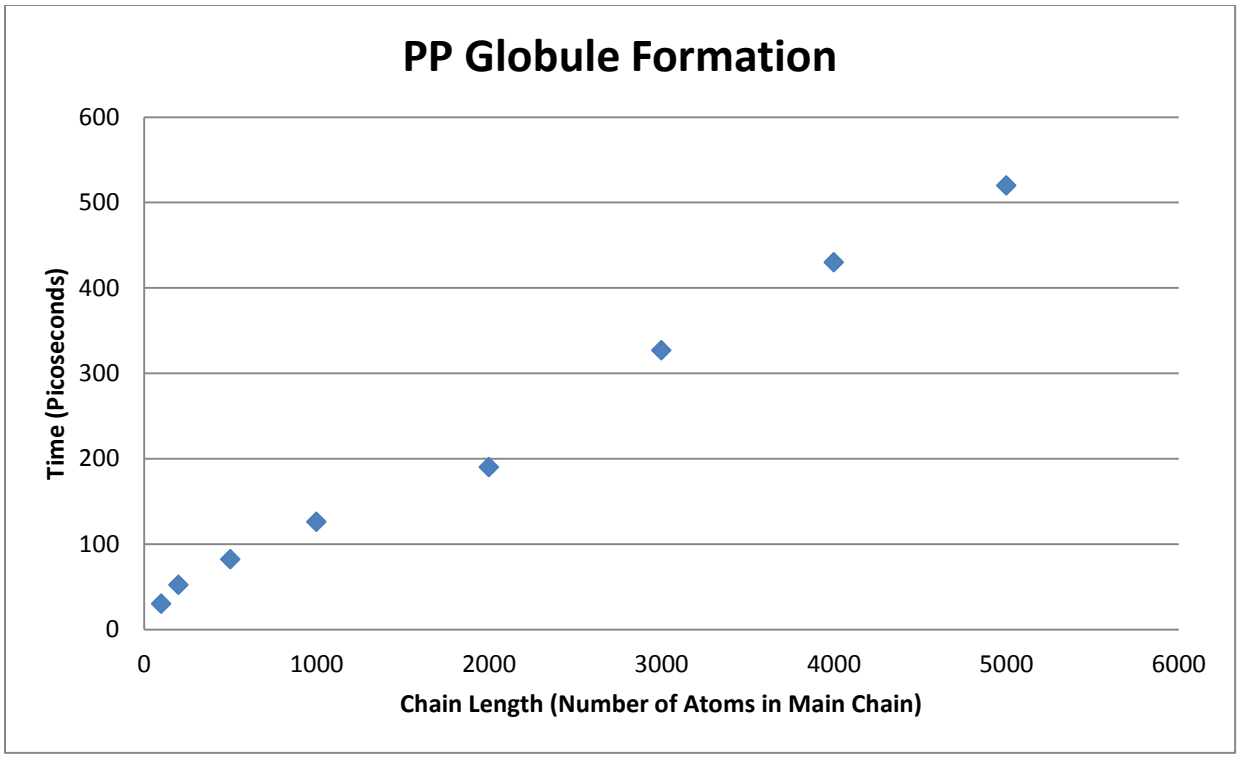

Figure 7: Globule Formation Time of Polypropylene (PP) for various Chain Lengths

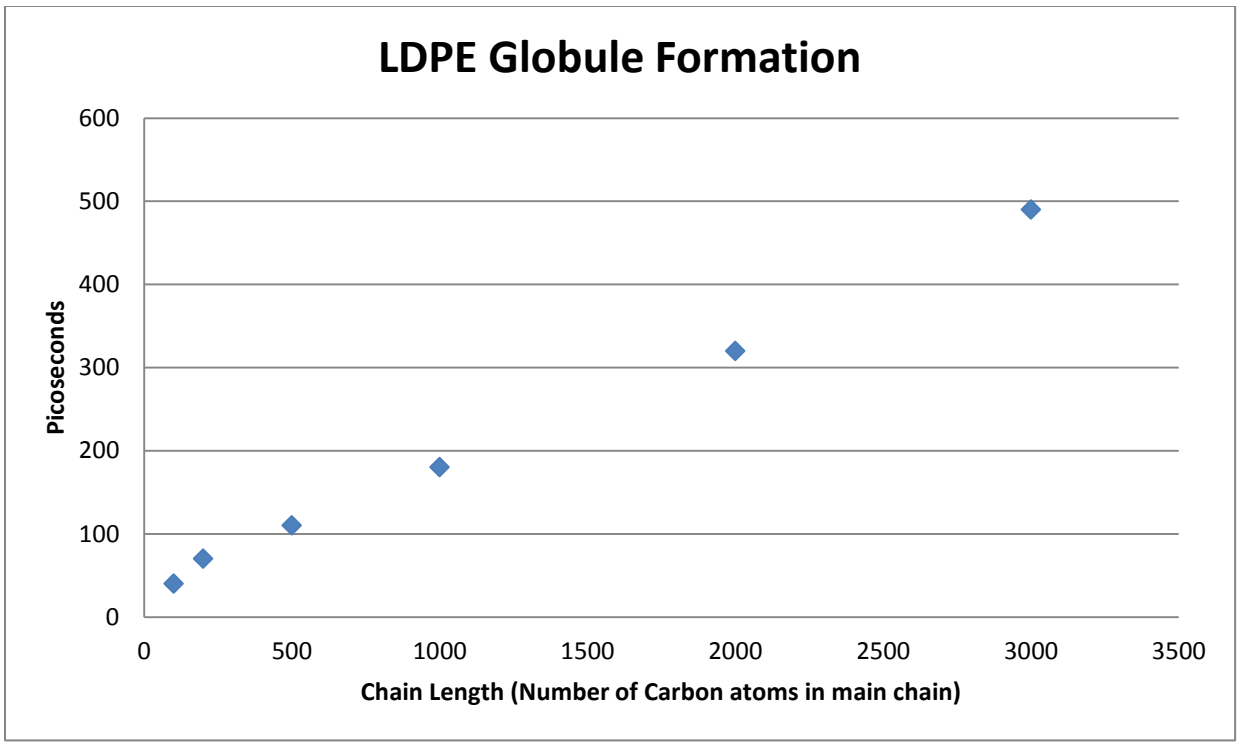

Figure 8: Globule Formation Time of Low Density Polyethylene (LDPE) for various Chain Lengths

Figure 9, Figure 10, and Figure 11 are a different interpretation of the data shown above. The following plots display the globule formation time of HDPE, PP, and LDPE on a per atom basis. The simulations were run at 300K and 0atm for 3000 picoseconds. Each plot levels off and reaches a steady state value. This shows that as the chain length increases over a certain point, the globule formation time on a per atom basis becomes constant.

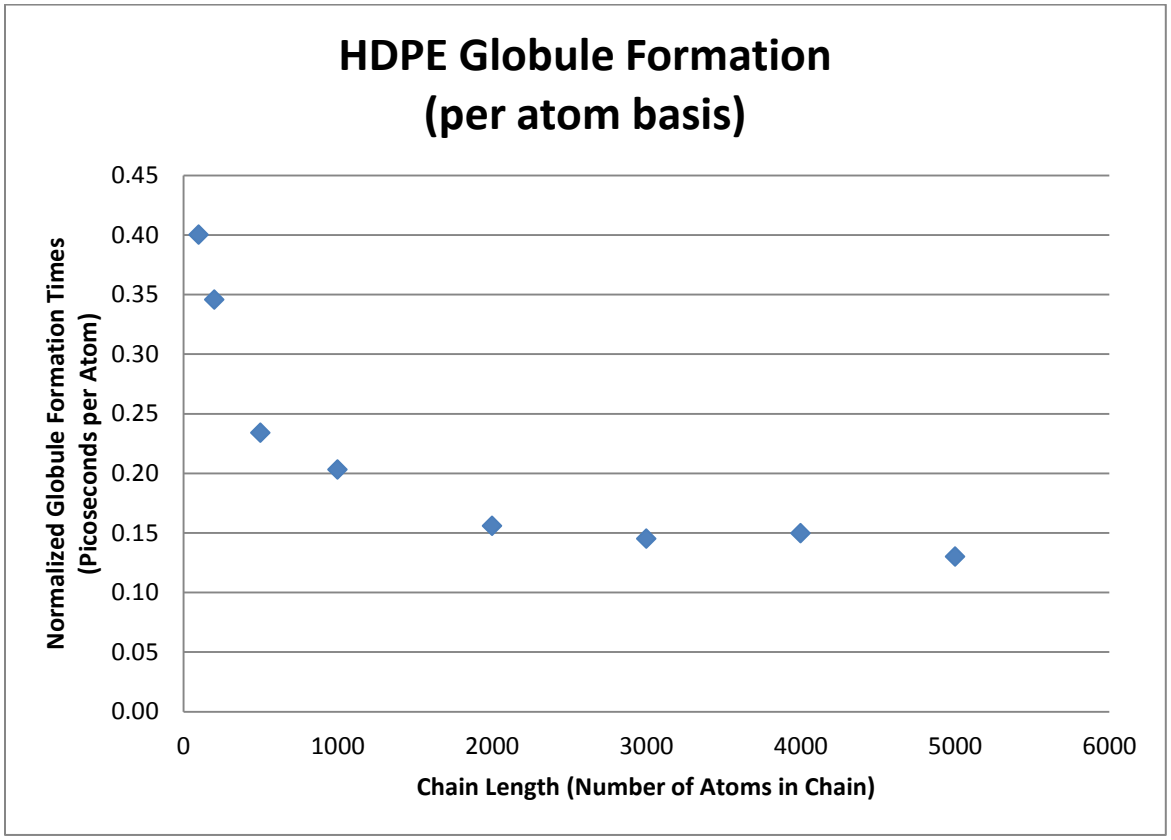

Figure 9: Normalized Globule Formation Time of High Density Polyethylene at various Chain Lengths

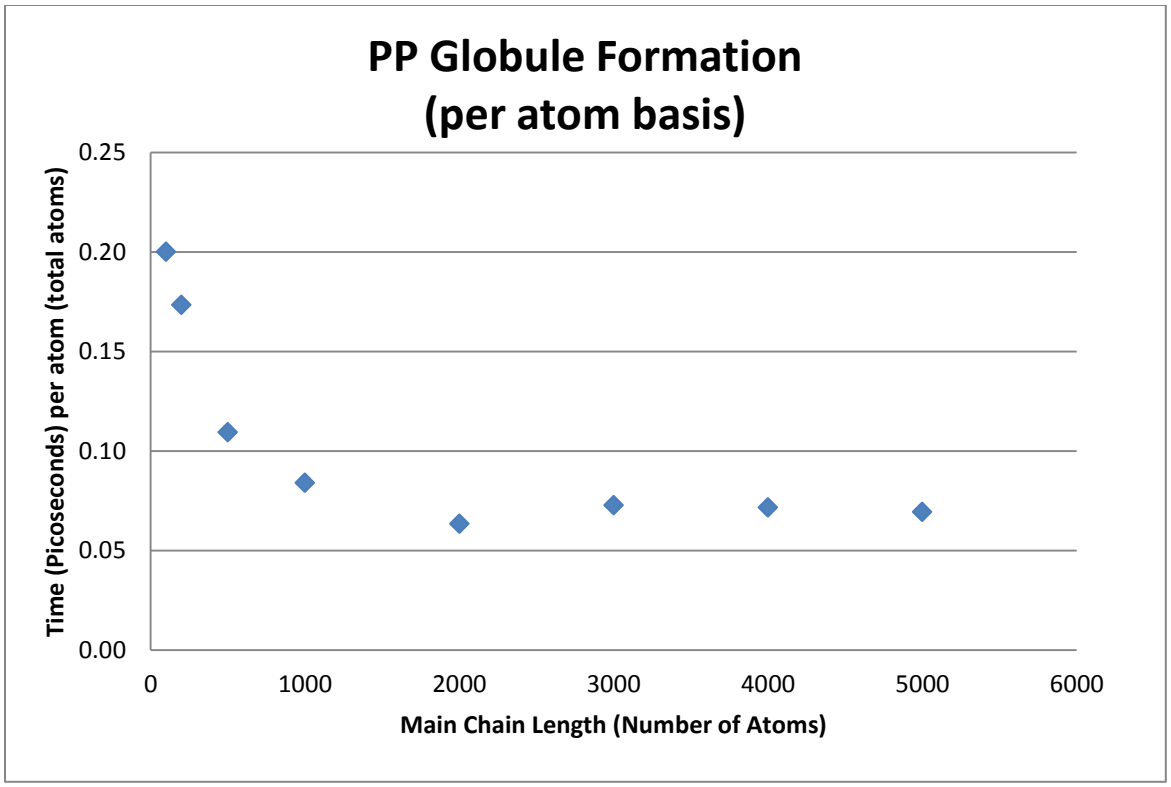

Figure 10: Normalized Globule Formation Time of Polypropylene at various Chain Lengths

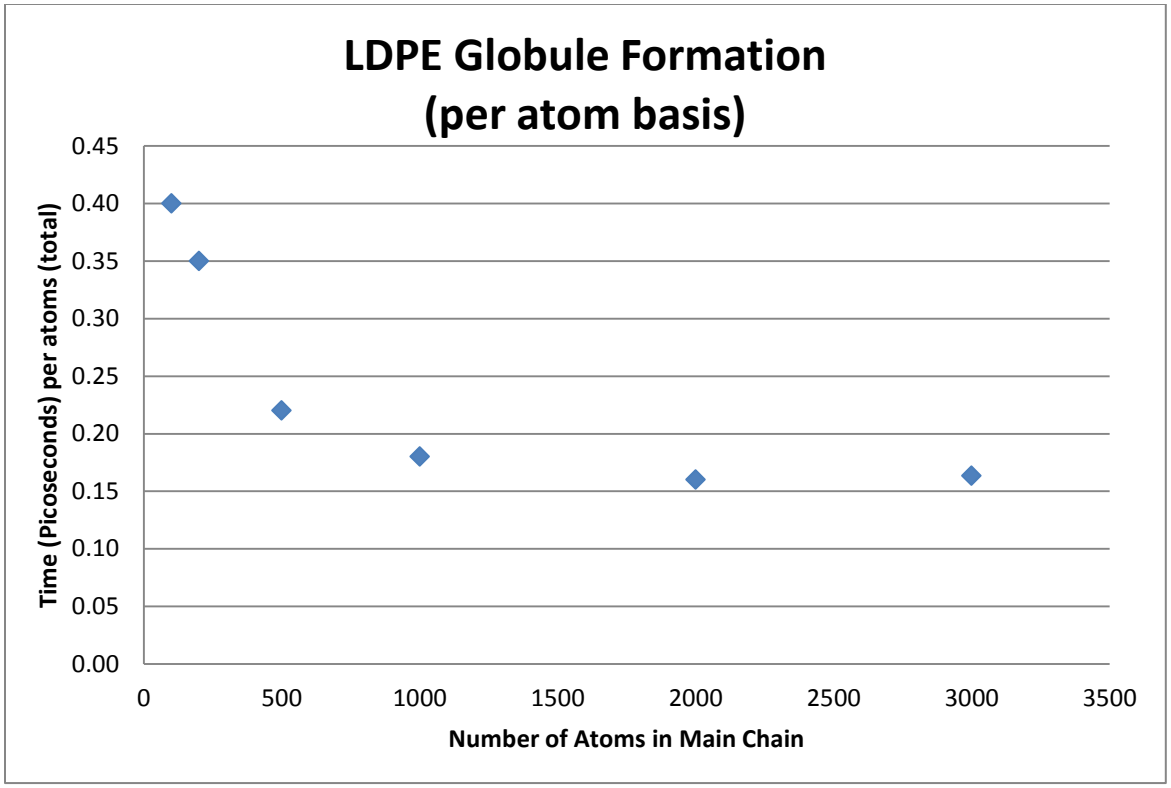

Figure 11: Normalized Globule Formation Time of Low Density Polyethylene at various Chain Lengths

Volume Calculations

The volume occupied by the polymer using a 1.9 angstrom radius around each united atom was calculated using the McVol program. Figure 12 below shows high density polyethylene chains of various lengths simulated with no periodic boundary conditions at 300K and 0atm for 1500 picoseconds. These simulations produced globule-type structures. As the chain length increases, the van der Waals volume increases.

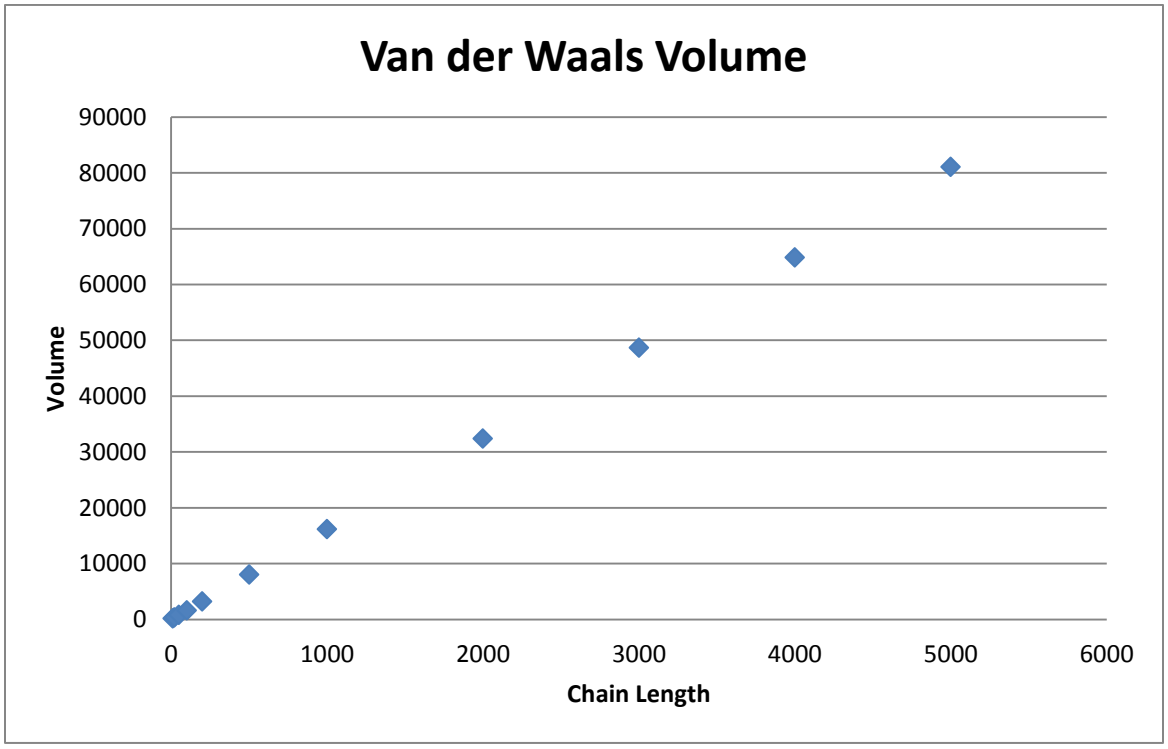

Figure 12: Van der Waals Volume as a function of Chain Length

Figure 13 below, shows the van der Waals volume data for the same set of simulations on a per atom basis. The volume per atom drops significantly as the chain length increases. When the polymer chain becomes a certain length, the volume per atom reaches a constant value.

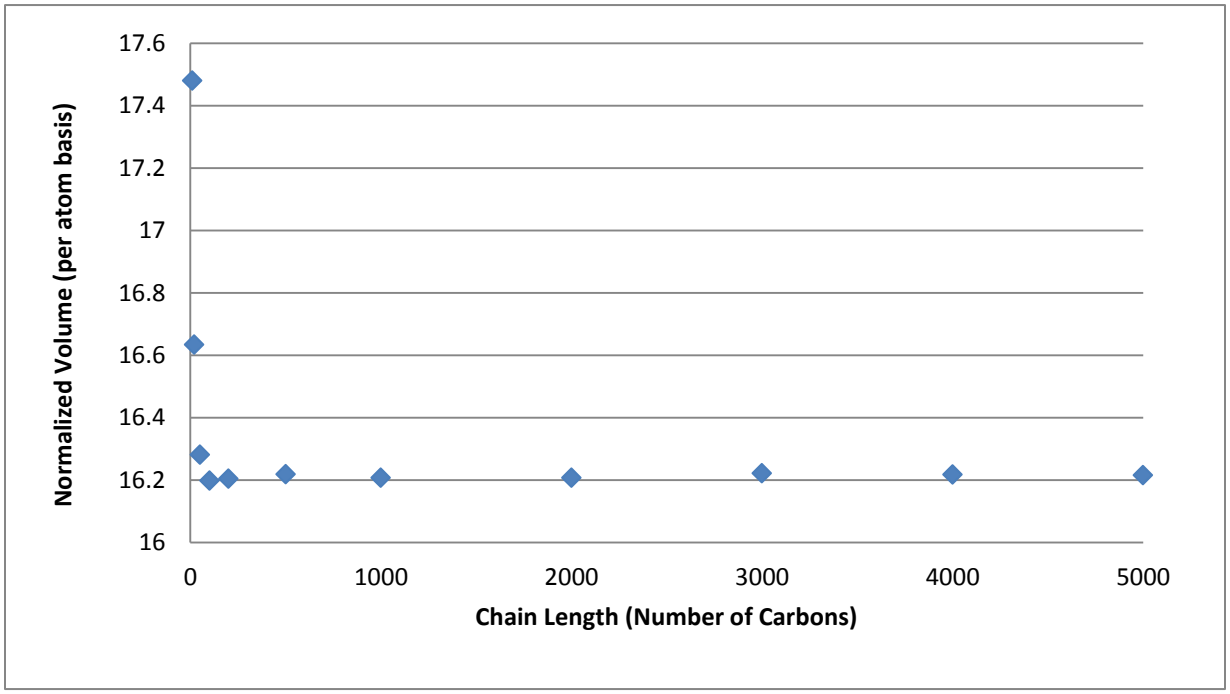

Figure 13: Normalized VDW Volume (per atom basis)

Polymer System Energy

The total system energy of high density polyethylene chains was simulated under no periodic boundary conditions at 300K and 0atm for 1500 picoseconds and was plotted in Figure 14. Globule formation occurred at the intersection of the curved and straight lines. The polymer chains reached a minimum energy state after re-orienting to a globule formation from the straight chain construction established in the initial coordinates. As the chain length increases, a significant initial reduction in energy becomes more and more prominent. Individual energy plots for each chain length can be found in Appendix A. The key to the right of Figure 14 corresponds to chain length in terms of pseudo atoms.

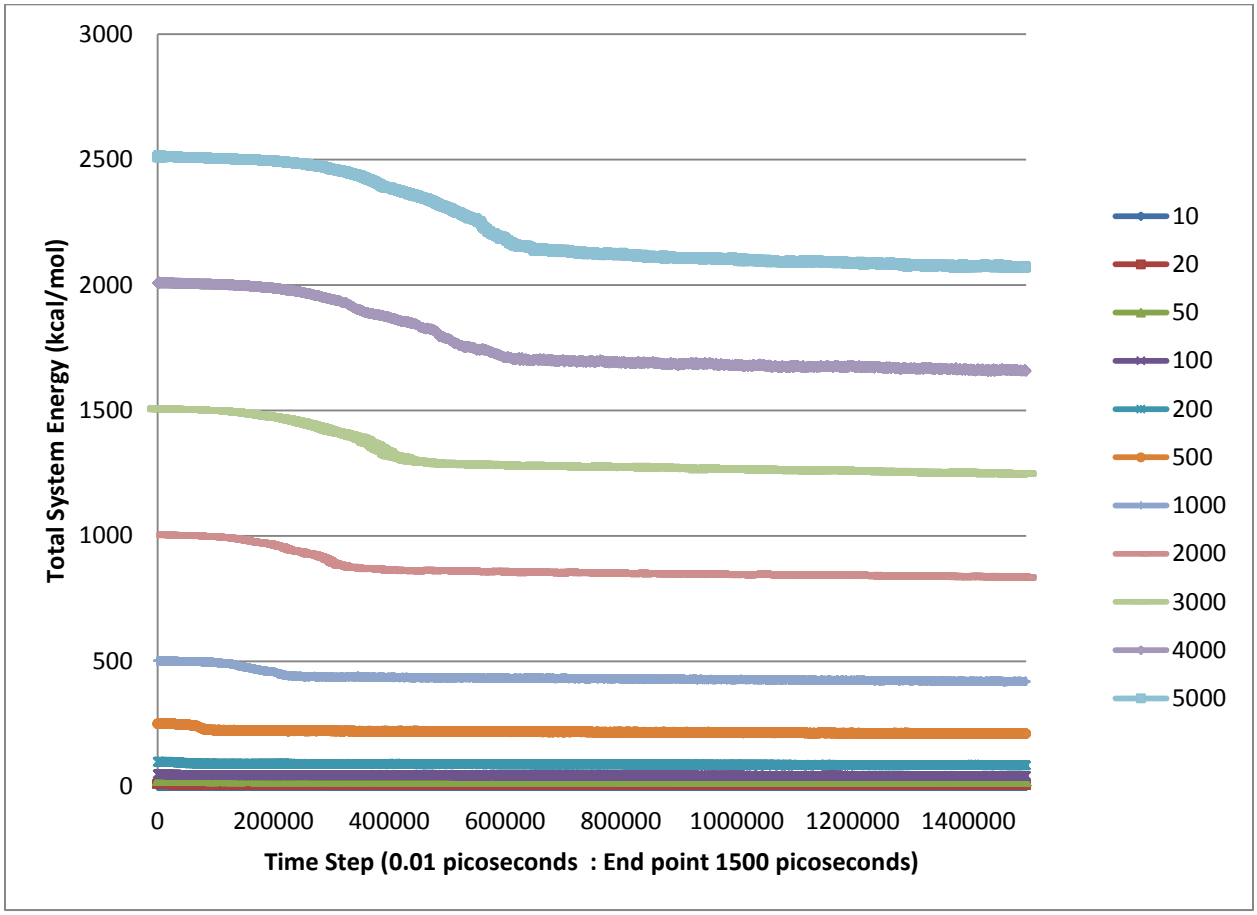

Figure 14: Total System Energy of HDPE for various chain lengths

Polymer Structure - Branching Effects (300K)

Figure 15 below shows the globule formation times of HDPE, PP, and LDPE on a per atom basis. Four chains of 2000 pseudo atoms in main chain length of each polymer type were simulated at 300K and 0atm for 3000 picoseconds. The figure shows a dramatic drop in time per atom between the non-branched HDPE and the side group/branched polymers PP and LDPE.

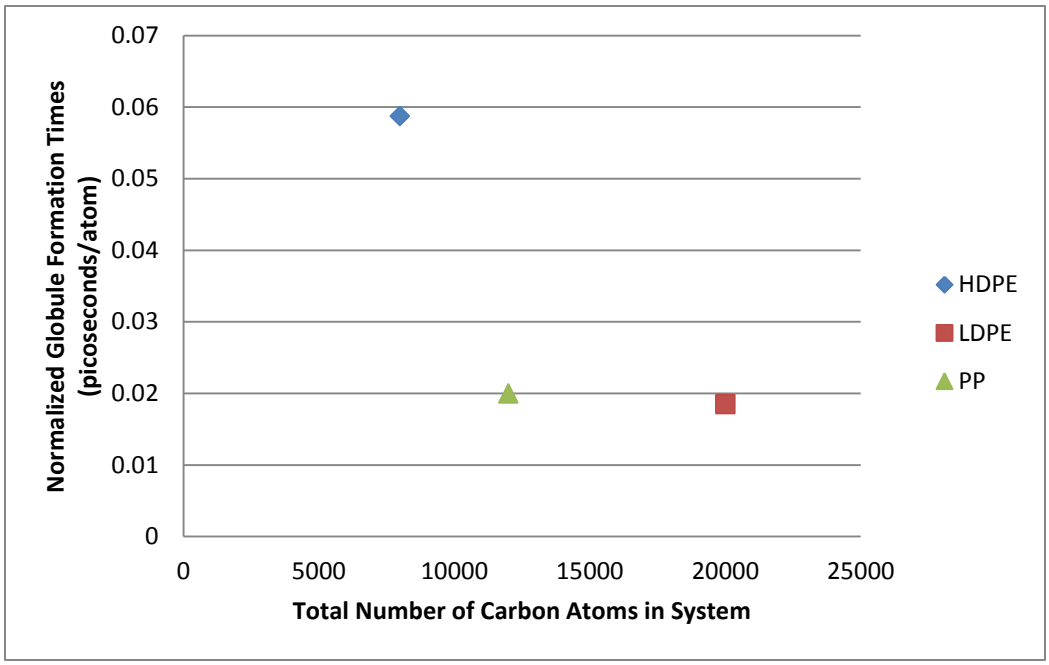

Figure 15: Branching Effects on Globule Formation Time

Figure 16, Figure 17, and Figure 18 are images of HDPE, PP, and LDPE simulations at 130 picoseconds during a 3000 picosecond simulation at 300K and 0atm for each. The scrunching of the chains is more prevalent with increased branching. As branching is increased, the lateral movement of the entire chain is decreased. The straight chains of HDPE show the complete lengths of the chains folding in on themselves to form a globule, whereas the chains of LDPE are seen to climb in on themselves in an elastic-like manner.

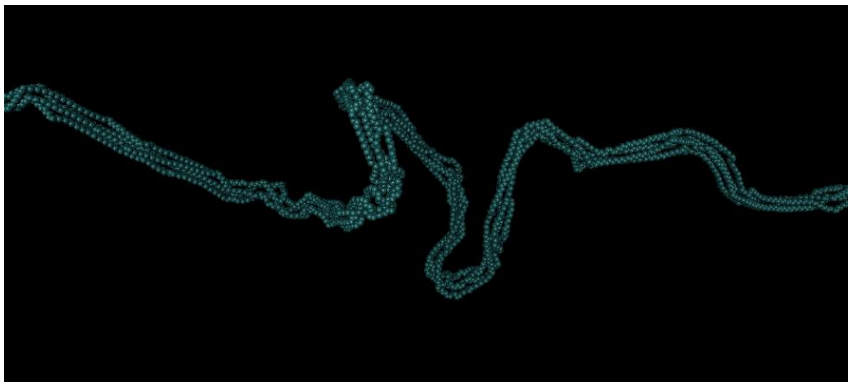

Figure 16: Image HDPE (130 picoseconds)

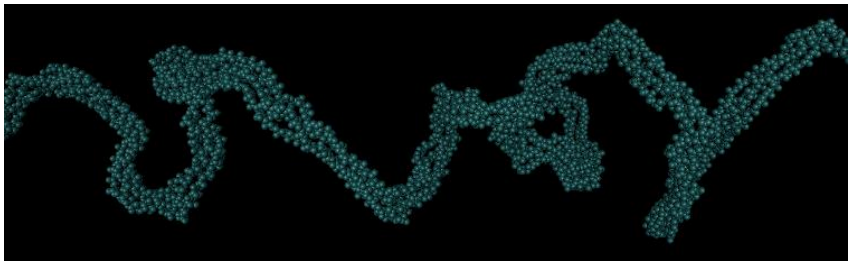

Figure 17: Image of Polyethylene (130 picoseconds)

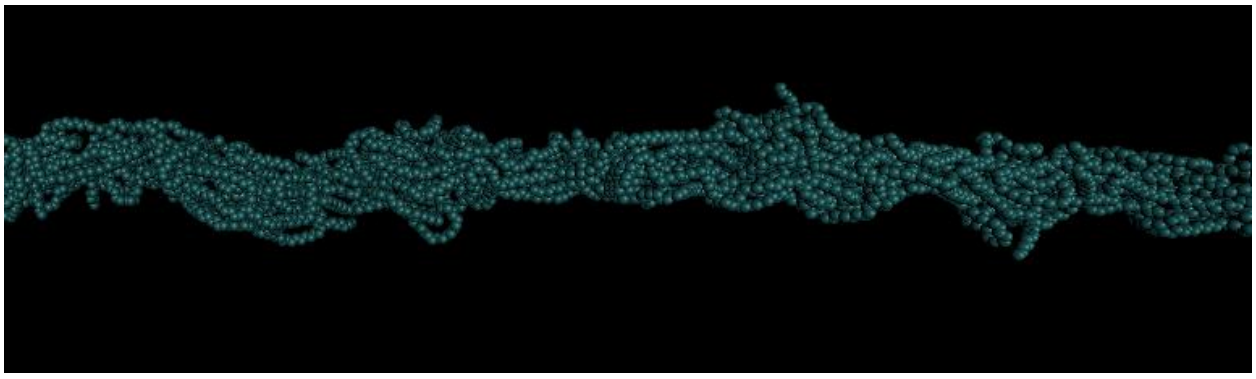

Figure 18: Image of LDPE (130 picoseconds)

Polymer Structure – Temperature Effects

Figure 19 below shows globule formation times for HDPE at various temperatures. The simulations were of four chains of 2000 pseudo atoms run for 3000 picoseconds at 300K and 0atm. As the temperature of the system was increased the time for the polymer to ball up and assume a globule shape decreased.

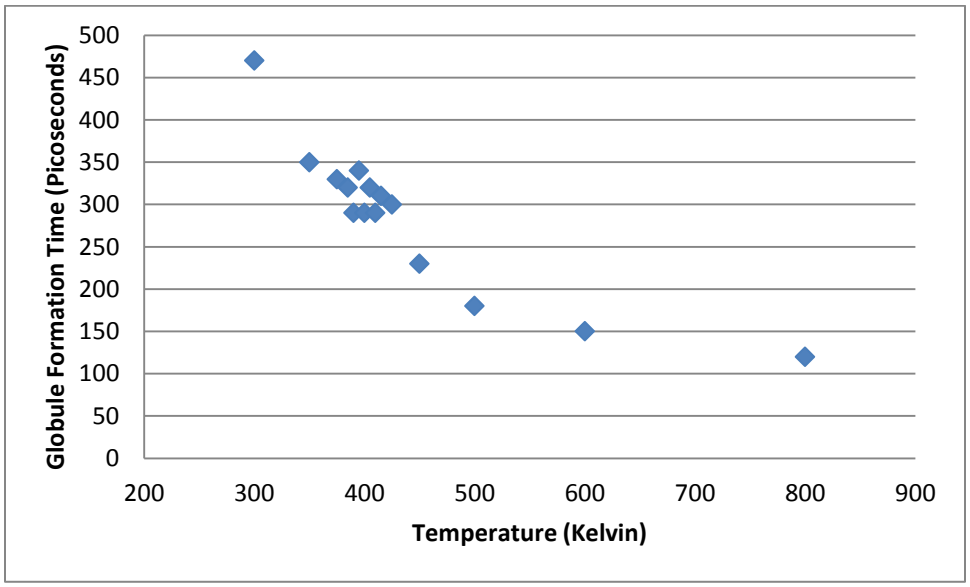

Figure 19: HDPE Globule Formation Times at Various Temperatures

Density

Pressure and Simulation Time Effects

Table 5 below shows the effect of simulation time, pressure, and chain length on the density of the polymer system. Simulations were run for single polymer systems at 300K. Experimental density of HDPE (0% branching; molecular weight 83100 $^{g}/_{mol}$) is 0.947g/cm^3. (Liu, Wang, & He, 2002)

Column	1	2	3	4
Simulation Duration (picoseconds)	150	1500	1500	1500
Polymer Chain Length (Number of Carbons)	1000	1000	1000	2000
Pressure (atm)	0	0	1	0
Temperature (Kelvin)	300	300	300	300
Density	1.0612	0.873	0.867	0.868

Table 5: Density of HDPE

Table 5 above, shows that for different simulation times (column 1 and 2), the longer simulation resulted in the more accurate density calculation. Pressure differences (column 2 and 3) had little effect on the density of the system, although the simulation with 0atm pressure was closer to literature values. The length of the polymer chain (columns 3 and 4) also had an insignificant effect on the density of the system.

Chain Length and Number of Chain Effects

Simulations shown in Table 6 were run for 3000 picoseconds at 300K and 0atm. Table 6 displays the density data for simulations of different chain lengths and quantities. Despite the previously stated findings of the critical molecular weight being 2000 carbons long for HDPE (Figure 6), the simulations of the chains of 100 and 200 pseudo atoms long produced the most accurate density data.

Number of Chains	**1**	**4**	**25**	**50**
Chain Length – Number of Atoms	2000	2000	200	100
Density (g/cm3)	0.868	0.886	0.951	0.944

Table 6: HDPE density data for different chain lengths and number of chains

Figure 20 and Figure 21 below, are images of HDPE for a 50 chain system of 100 pseudo atoms long and a 20 chain system of 500 pseudo atoms long respectively. The images were taken during 3000 picosecond long NPT simulations at 300K and 0atm. Voids can be seen in Figure 21 in the simulation of a longer chain system of lesser quantity.

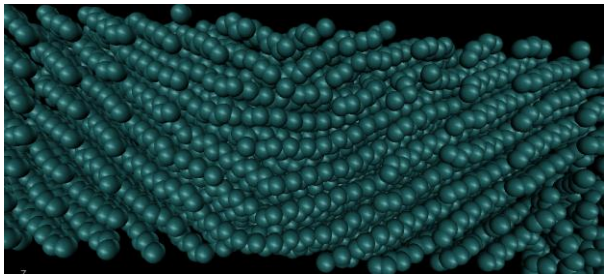

Figure 20: Image of HDPE 50 Chain System (100 atoms long)

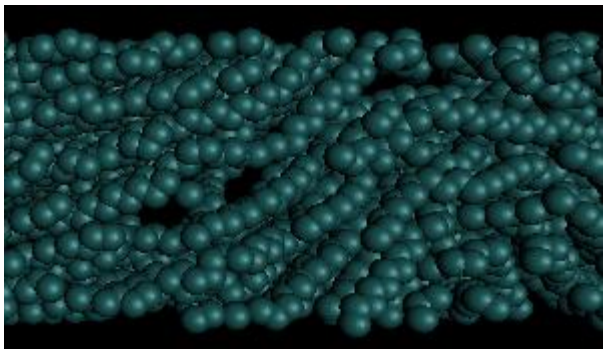

Figure 21: Image of HDPE 20 Chain System (500 atoms long)

Equilibration Effects

Initial NVT and NPT simulations in Table 7 were run for 3000 picoseconds at 300K and 0atm. Subsequent continuation simulations (NPT post equilibration) were run for 1500 picoseconds at 300K and 0atm. Table 6 Table 7 displays the results of six simulations that assessed the effects of equilibrating the system before running a NPT simulation to calculate the density. Equilibration is shown to affect the density minimally.

Type of Simulation	NPT - (no NVT equilibration	NPT – (with NVT equilibration
HDPE 50 Chains – 100 atoms long	0.942	0.944
HDPE 25 Chains – 200 atoms long	0.948	0.951

Table 7: Equilibrium/non-equilibrium HDPE density values (g/cm3)

Branching Effects

Densities of HDPE, PP, and LDPE are shown in Table 8. Simulations were performed for four chain systems at 300K and 0atm for 3000 picoseconds. A general trend can be seen where density increases with decreasing branching.

Polymer Type	HDPE	PP	LDPE
Density (g/cm3)	0.886	0.845	0.734

Table 8: Density of Four Chain Polymer systems (main chain length 2000 atoms)

Crystallization / Melting

A series of simulations were run at various temperatures under no periodic boundary conditions. Four chains of HDPE with chain lengths of 2000 pseudo atoms comprised each system. Each simulation was run at 0atm for 3000 picoseconds.

Figure 22 and Figure 23 below show a low temperature simulation which resulted in the polymer chains aligning themselves into ordered structures.

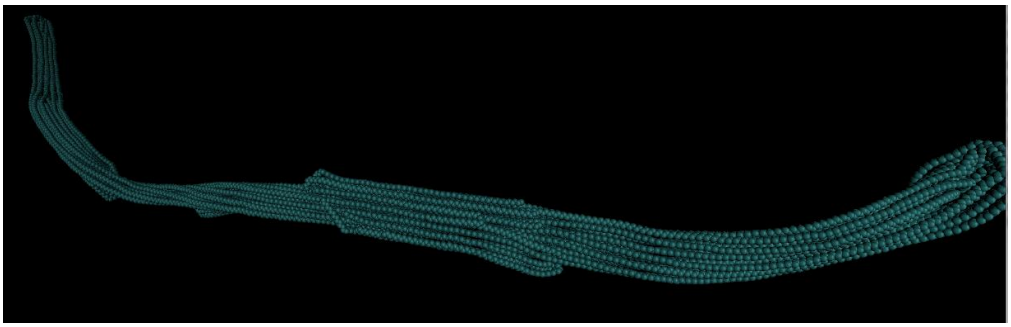

Figure 22: Image of HDPE 100K (3000 picoseconds)

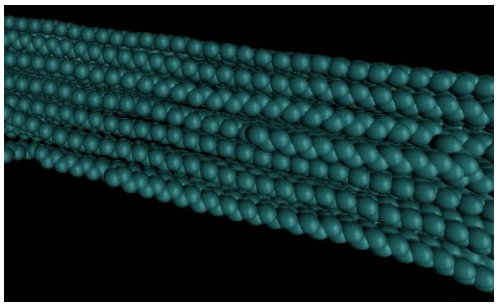

Figure 23: Image of HDPE 100K enlargement (3000 picoseconds)

Figure 24, Figure 25, and Figure 26 show room temperature simulations at 300K. These resulted in the formation of a globular structure. The chains stayed together in the globule formation process as seen in Figure 25.

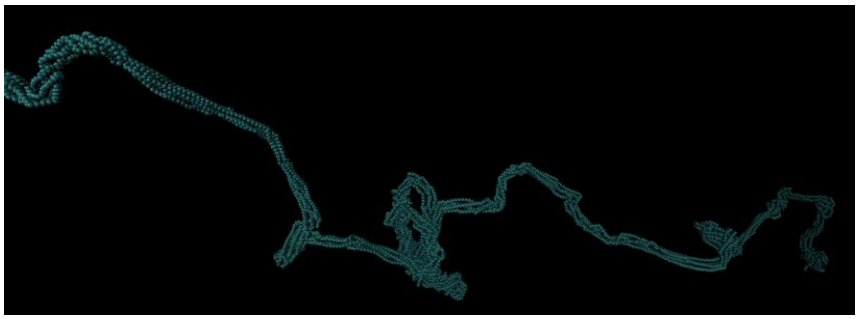

Figure 24: Image of HDPE 300K (220 picoseconds)

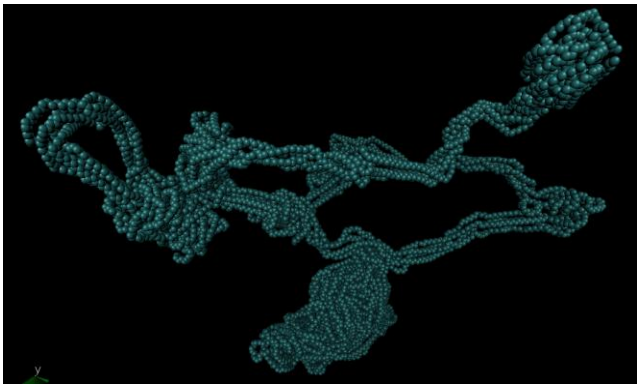

Figure 25: Image of HDPE 300K (340 picoseconds)

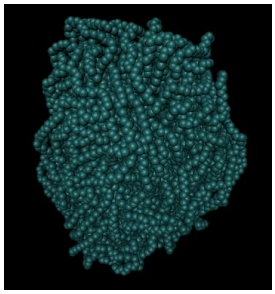

Figure 26: Image of HDPE 300K (3000 picoseconds)

As the temperature starts to increase, the chains do not stay together as well as seen by the large chain separation in Figure 27. Figure 28 and Figure 29 show singular chains stemming out from the globule which have parted from group of four from which they started.

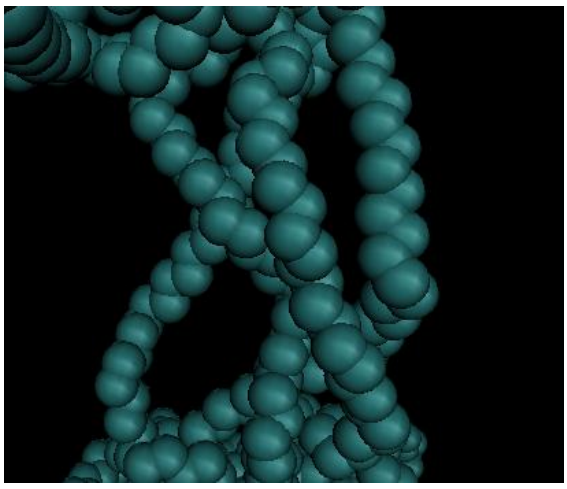

Figure 27: Image of HDPE 500K (130 picoseconds)

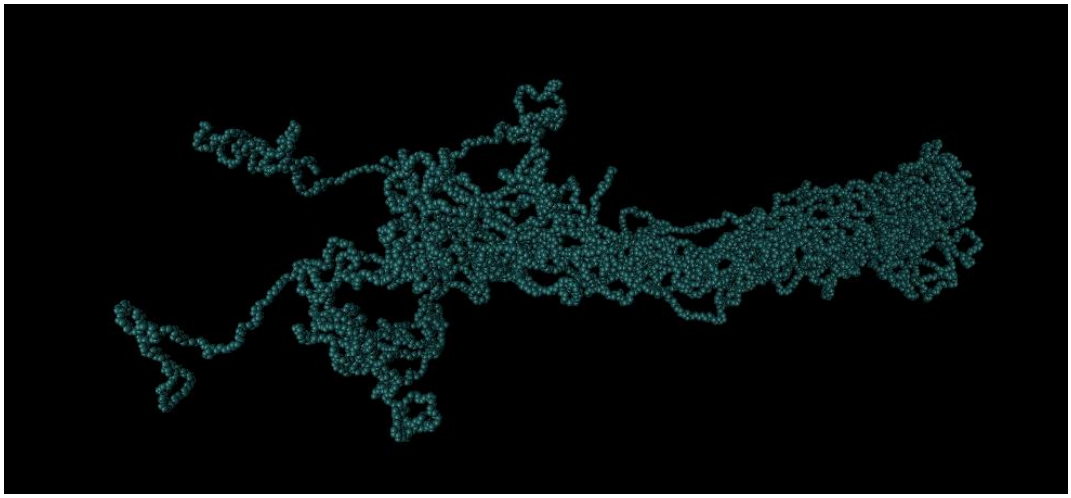

Figure 28: Image of HDPE 800K (210 picoseconds)

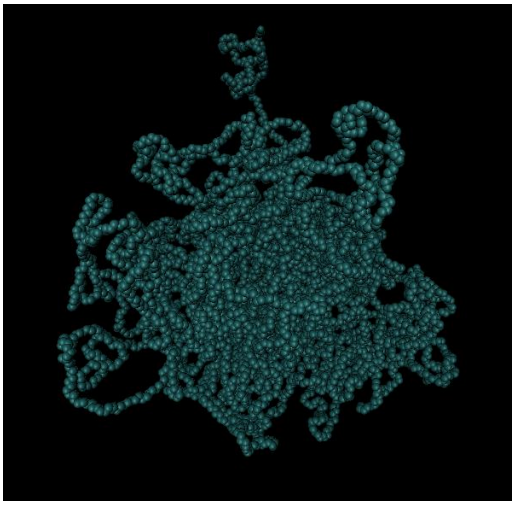

Figure 29: Image of HDPE 800K (3000 picoseconds)

Melting Point Determination

Density data for HDPE and PP at various temperatures are shown in Figure 30 and Figure 31 below. Four chains of 2000 pseudo atoms in length were simulated (NVT) for 3000 picoseconds with no periodic boundary conditions to equilibrate the system and then run (NPT) for an additional 1500 picoseconds. The pressure for all simulations was 0 atm. The melting point/glass transition temperatures were estimated by the vertical dotted lines placed between the two density values of differing slopes. The glass transition temperature is estimated for HDPE in Figure 30 as the system is mostly amorphous, while the melting point is estimated for PP in Figure 31 as the system is more crystalline.

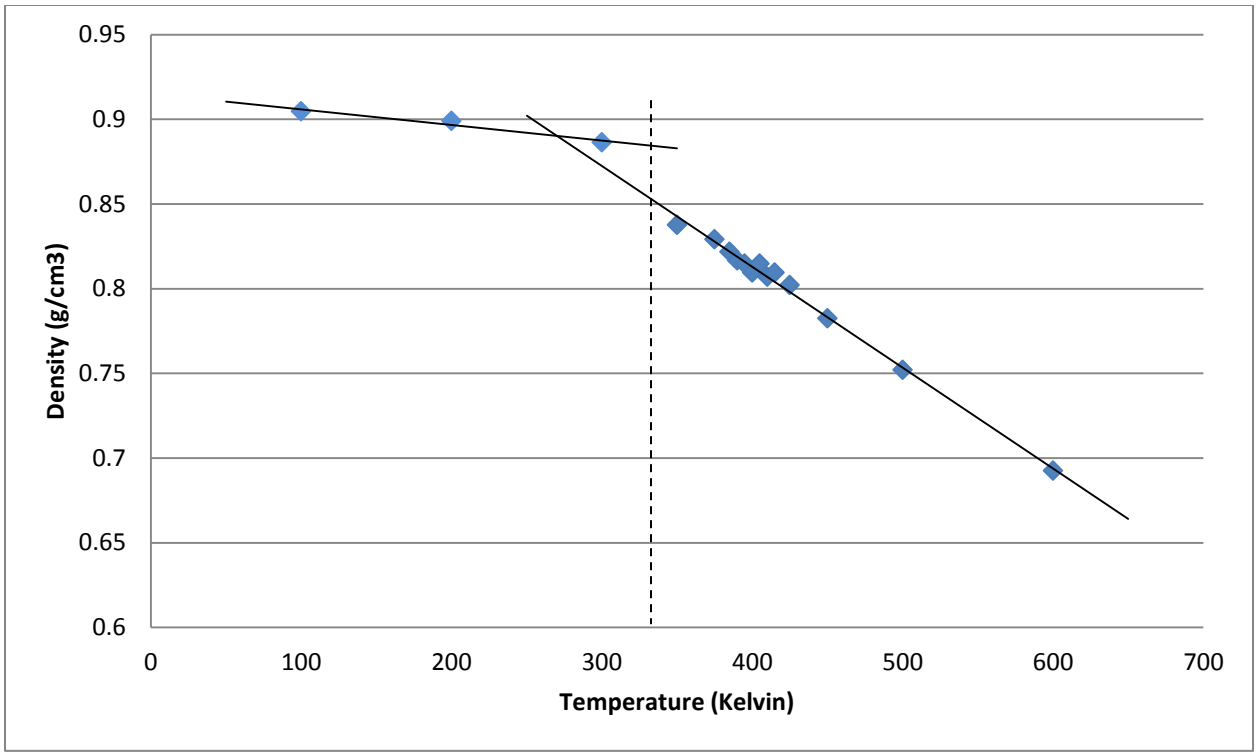

Figure 30: Density of HDPE at various temperatures

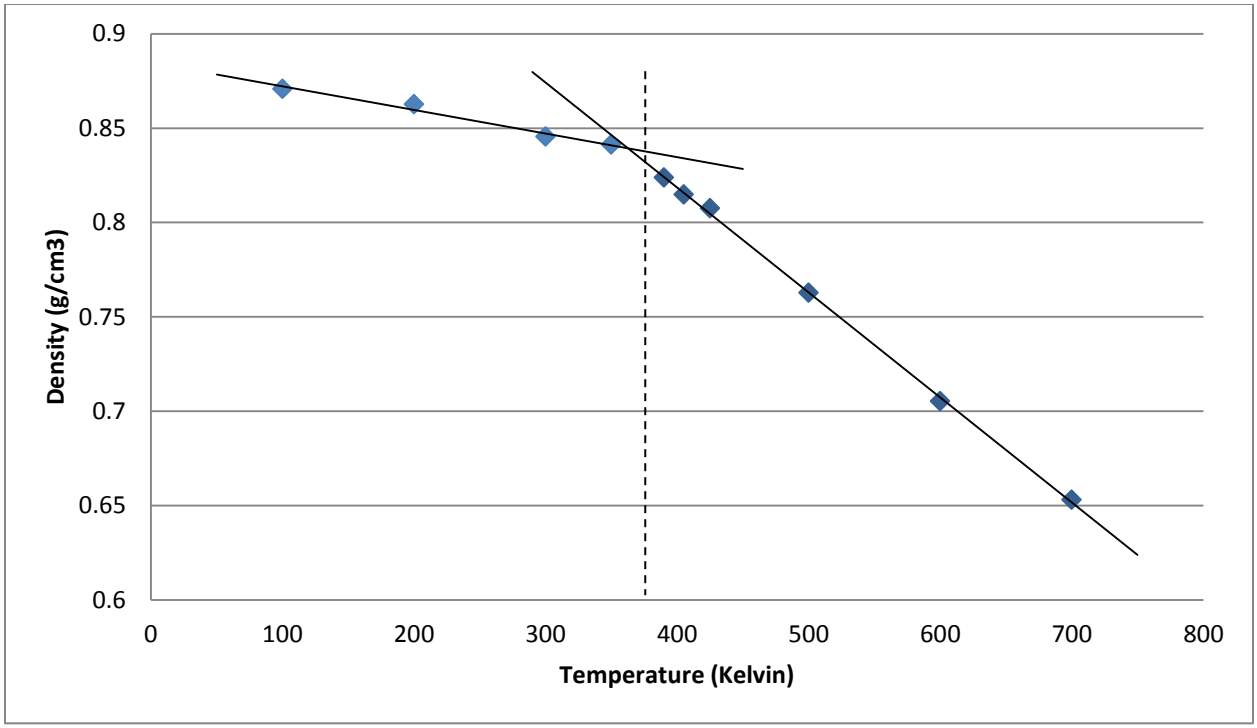

Figure 31: PP Density Data at Various Temperatures

Figure 32 below shows the volume data for polypropylene extracted from Figure 31. The plot shows a change in expansion rate of the polymer system when plotted for various temperatures.

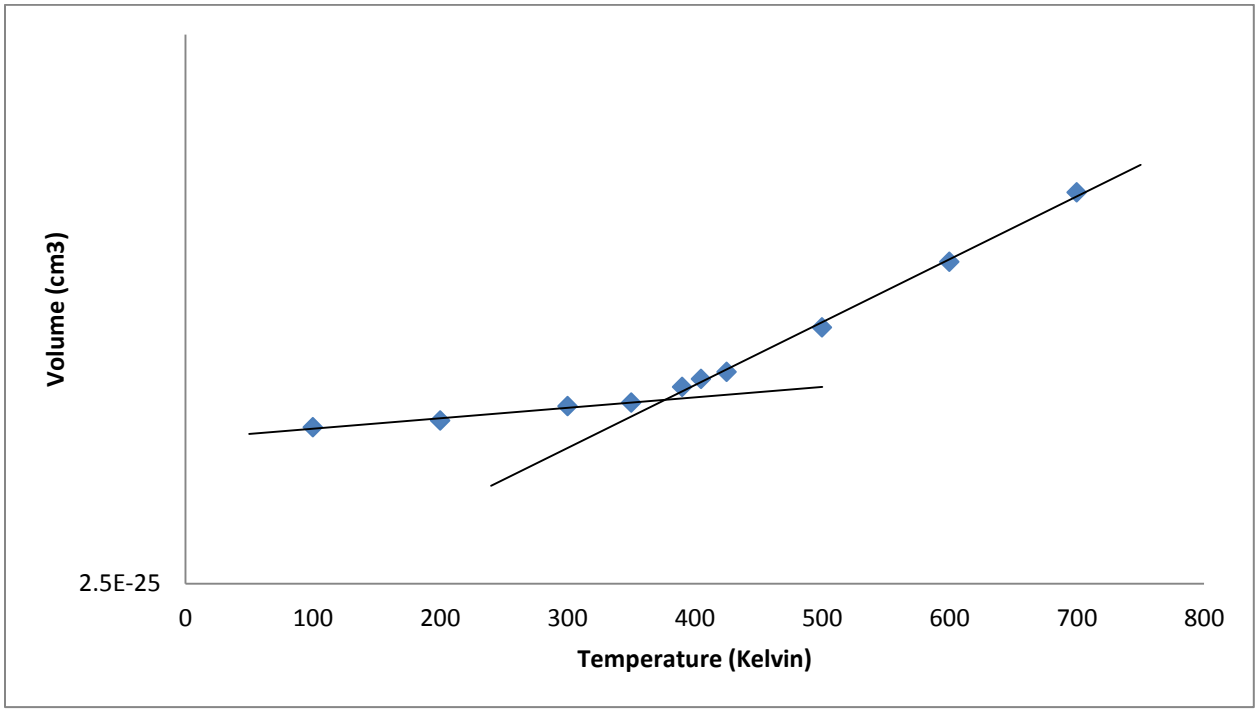

Figure 32: PP Volume data at various temperatures

Four chains of HDPE and PP were simulated for 3000 picoseconds at 0 atmospheres for various temperatures around the respective melting points of each polymer. Figure 33 and Figure 34 below, show the configurational energy change with increasing temperature. Figure 35 and Figure 36 below, show the van der Waals forces plotted against temperature. A slight inflection point can be seen around the melting temperatures of each polymer for these two types of system energy.

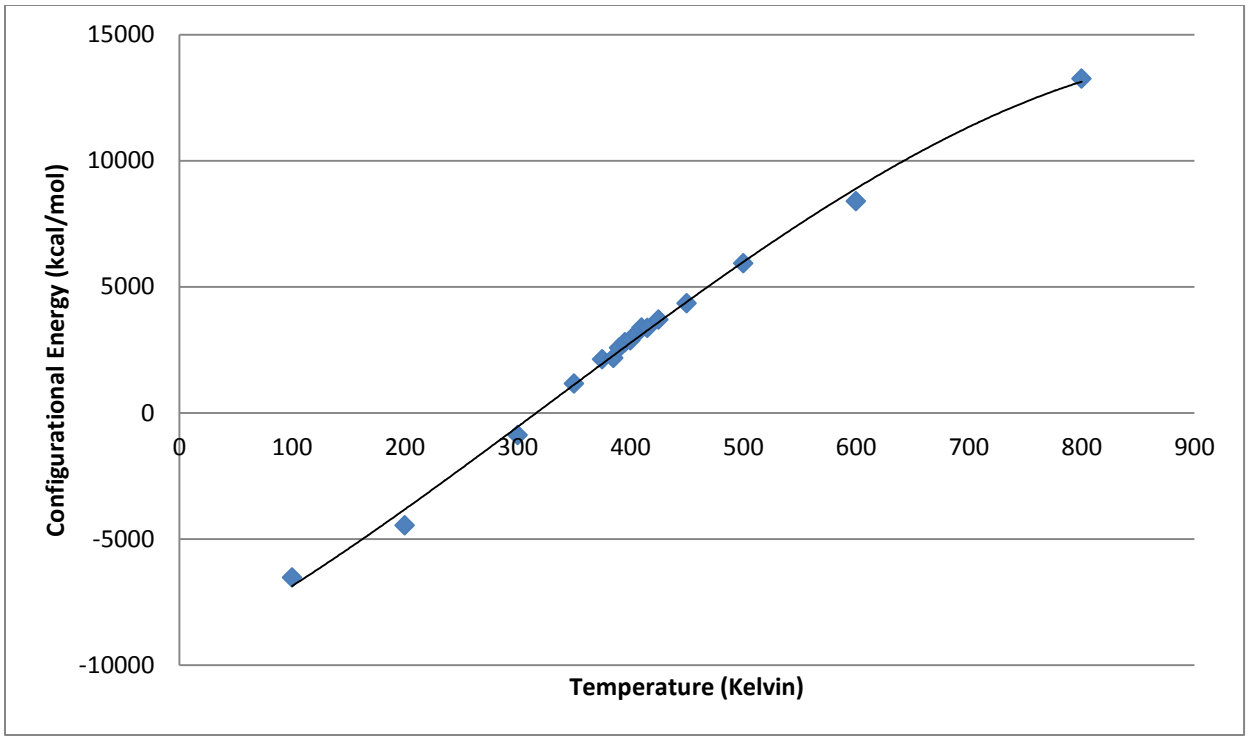

Figure 33: HDPE Configurational Energy Temperature Data

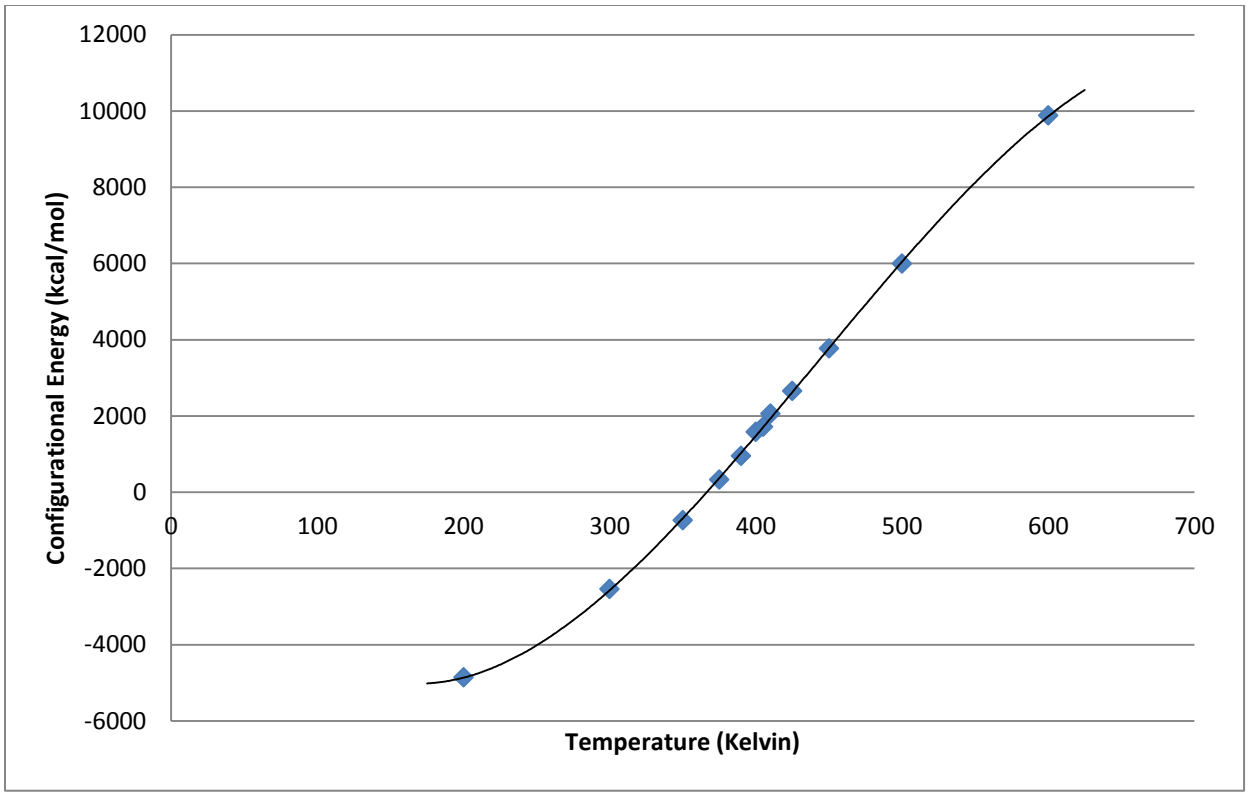

Figure 34: PP Configurational Energy Temperature Data

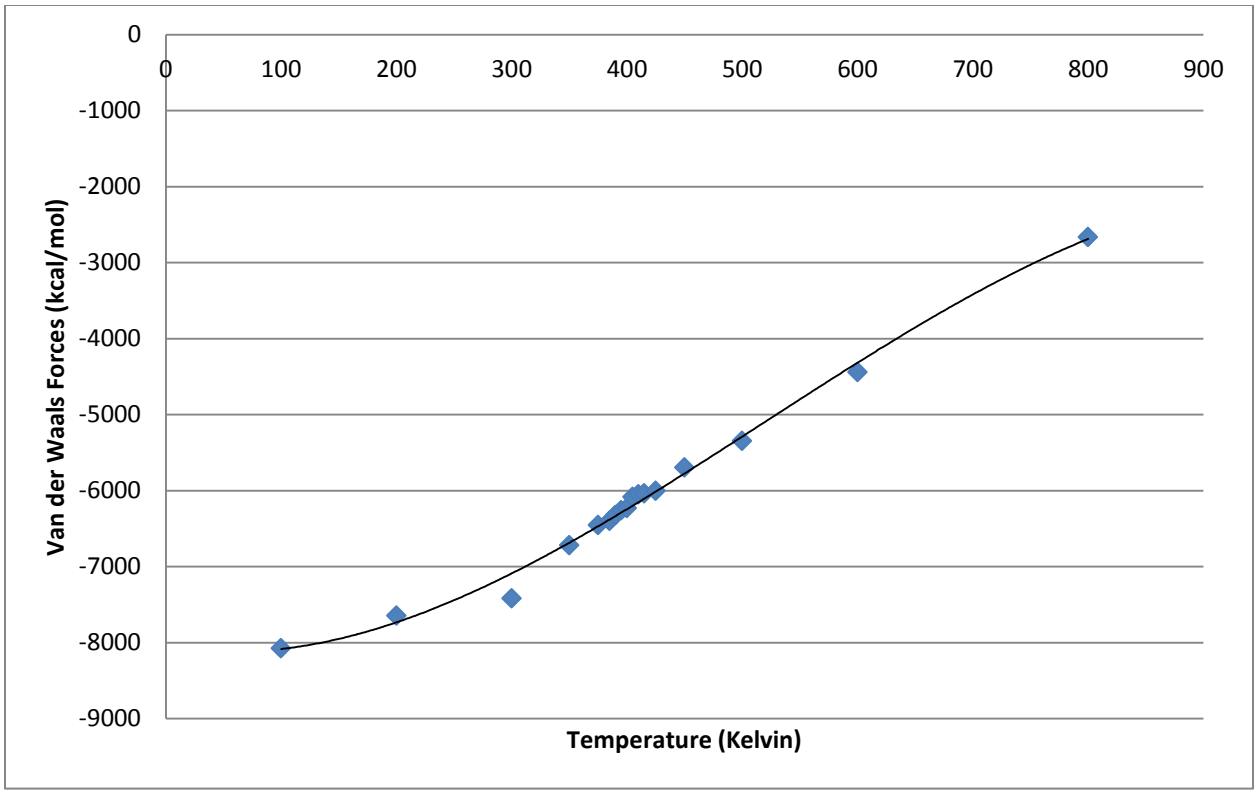

Figure 35: Van der Waals Forces of HDPE at Various Temperatures

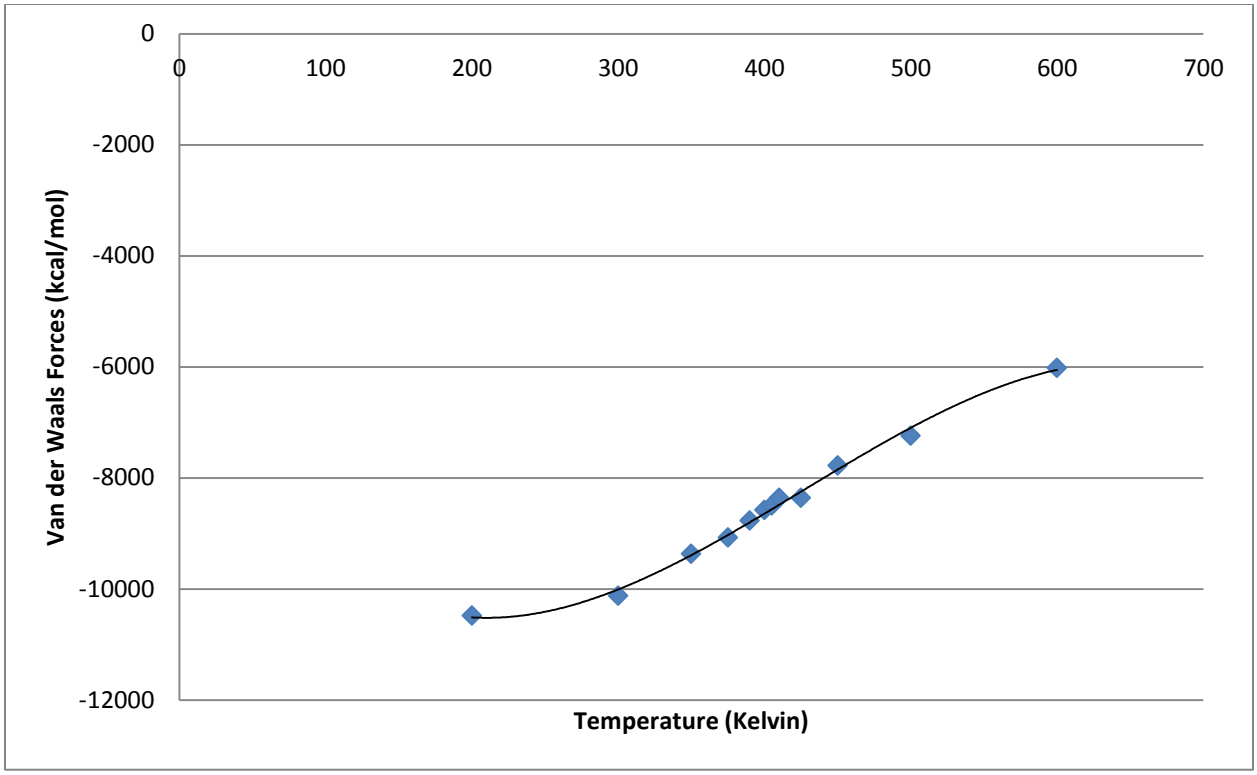

Figure 36: Van der Waals Forces of Polypropylene at Various Temperatures

Discussion

Globule Formation

As the time values were visually determined they are therefore approximate. The CONTROL file specifies the number of steps recorded to the HISTORY file. In order to keep the HISTORY file to a reasonable size, the steps logged were taken every X amount of steps. For longer simulations, this number increased. For a three million step simulation, steps recorded every 10,000 steps would produce 300 entries in the HISTORY file. Depending on the fraction of steps recorded, the instant that the globule may have appeared to form could possibly be some time after the actual formation. The globule formation times were used to assess trends and should not be taken as exact formation times.

Exact globule formation times could be more accurately determined through recording a larger percentage of the simulation steps. Using the coordinates of the HISTORY file, the McVol program could also be employed to calculate the volume of the molecule at every step. A more exact globule formation time could then be extracted based on the volume change. This would be a very tedious and time consuming process, and so was not used for the general purposes of this work.

The energy data was referenced when determining the globule formation times. The intersection of the curved dramatic energy drop with the linear, such as seen in Figure 14, also describes the globule formation time. The values extracted from the energy graph such as this were on the same level of accuracy as visual interpretation.

Figure 6, Figure 7, and Figure 8 display the globule formation times at various chain lengths. As chain length increases, so does the time it takes to form a globule. This is expected as the ends of long chains are further from each other than the ends of short chains, and so will take longer to come together as there is a greater distance to travel.

Figure 9, Figure 10, and Figure 11 display the globule formation times on a per atom basis. These plots show that as the size of the chain increases, the globule formation times on a per atom basis achieve constant values. When a constant value is reached, the van der Waals forces act proportionally on each atom in the polymer. This means that there is a minimum chain length for the van der Waals forces to be consistent. The minimum chain length corresponds to the critical molecular weight of a polymer.

The critical molecular weight values extracted from the plots were approximately 2000, 1700, and 1500 pseudo atoms long for HDPE, PP, and LDPE respectively. As HDPE is the most flexible out of the polymers tested, it is expected that the critical molecular weight will be highest, and therefore the chain length will be longest as it does not have side groups. The side groups of polypropylene stiffen the chain making it more rigid, promoting entanglement and van der Waals attractive forces. The branching of LDPE entangles the chain to an even higher degree, promoting van der Waals attractive forces also. As a result, polymer chains of 2000 pseudo-atoms long formed the standard chain length for all subsequent simulations in this work.

Figure 15 shows the effects of branching on globule formation time. The plot shows that globules are formed much more quickly when the chains have any amount of side groups or degree of branching.

The dramatic drop in time from the HDPE to the fairly equal values of both polypropylene and LDPE demonstrates this. The HDPE molecules are able to slide over one another more easily than the branched molecules do. The branching helps promote quicker globule formation due to increased entanglement of the chains.

Volume

The volume on a per atom basis shown in Figure 13 reaches an asymptotic value as the chain length increases beyond a certain point. The van der Waals forces from other parts of the chain promote bond angle bending to wrap the polymer in tightly and form a globule. The straight chain volume is larger than the volume of the globule. This can be seen as the shorter chains have larger volumes and are not able to collapse in on themselves to form globules but instead remain quite straight. The spheres encompassing each pseudo atom have large radii as specified by the McVol program. These radii are able to overlap and do so when attractive van der Walls forces bring distant parts of the chain together. The folding and tangling process promotes overlapping and therefore a decrease in volume. As bond angles can only vary so much, shorter chains are not able to exhibit McVol radii overlap, and therefore display a larger volume per atom.

Energy

The total system energy plot of HDPE, Figure 14, shows that as the chain length increases, the difficulty in maintaining a linear chain also increases. The energy needed to keep the polymer chain in this straight state is much higher and so becomes increasingly less ideal. This is described by the initial dramatic energy drop followed by the steady state straight line with minimal slope. The straight chain reaches a much lower energy state upon formation of a globule which occurs at the end of the dramatic energy drop. The globule undergoes a steady state energy minimization as it reorients itself to find the most stable conformation. This reorientation is described by the straight part of the line with minimal slope on the energy plot.

Density

The results in Table 6 show that the number of chains simulated is more important than the length of chain. The more chains that are simulated, the closer the density becomes to the actual value. The shorter polymers with the larger number of simulated chains were able to fill the simulation box more thoroughly as seen in Figure 20, depicting a more accurate polymeric environment with more precise bulk properties. The 1 and 4 chain systems may have created voids within the simulation box due to a large degree of chain folding, which resulted in a decreased density.

The results from Table 8 show an accurate trend. HDPE has a higher density than LDPE. The side groups and branching do not allow adjacent chains to lie as closely to one another as would linear chains. The inefficient packing results in voids within the system, effectively lowering the density.

Crystallization/Melting

Qualitative observations of crystallization and melting were made when running simulations at various temperatures.

Figure 22 and Figure 23 show crystallization. Four polymer chains were initially simulated at 100K for 3000 picoseconds. The figures reveal that the chains folded over onto one another in an ordered manner multiple times.

Figure 28 and Figure 29 depict melting as there are singular chains extending out from the center. The increased energy in the system has overpowered the attractive van der Waals forces allowing the chains to move independently. Only the bulk of the globule has enough mass to keep the chains centered in a globule type sphere, but they are held together much less tightly than the globules simulated at lower temperatures.

Melting Point/Glass Transition Temperature Determination

Figure 30 and Figure 31 show the densities of HDPE and polypropylene respectively as a function of temperature. Two lines were drawn on each figure that represented the general sloped trend of the data. A third dotted line was drawn in the middle of the two density values at the intersection of the two previous lines. This dotted line describes the melting points for crystalline systems and the glass transition temperatures for amorphous systems. Both systems were comprised of four chains and could be described to have portions of both crystalline and amorphous. As mentioned earlier, the temperatures of molecular simulations may not correspond perfectly to those in the lab. (Jobic, Smirnov, & Bougeard, 2001) For this added reason, the current work is more interested in the qualitative results produced by the simulations. The 'melting point' therefore of polypropylene is seen to be higher than that of HDPE which is expected. The methyl side groups of polypropylene act as barriers that hinder chain slippage and promote entanglement.

The intersection of the two lines with the dotted line describes the breaking point of the attractive van der Waals forces. Figure 32 displays the volumes of PP at various temperatures and can be thought of as the distances between neighboring molecules. This plot demonstrates how the VDW forces have a certain distance where the attraction is fairly consistent. When adjacent molecules exceed this distance, the attraction diminishes quickly, as seen by the rapid volume expansion, and therefore rapid separation of adjacent chains.

The melting point values for both plots are lower than literature values. These simulations were performed with four chains of 2000 pseudo atoms in length. As mentioned earlier in regards to density, simulations with larger numbers of molecules proved to be more accurate. As the melting points were calculated via a density change method, simulations with larger numbers of molecules may provide more precise results.

Figure 33 and Figure 34 show the configurational energy of a four chain system of HDPE and PP respectively. Figure 35 and Figure 36 show the van der Waals attractive forces of the same HDPE and PP systems. The slight inflection point shows the energy change corresponding to chain slippage or melting. The inflection point may have been more defined if simulations of a larger number of polymers were used.

Conclusions

The phenomenon of crystallization was qualitatively observed in the low temperature simulations. Chains were seen to form ordered structures through folding. Melting was also qualitatively observed at high temperatures. Chains were seen to separate from the four adjacent chains from which they initially started.

In agreement with Zhan & Mattice, globule formation was seen in all polymers simulated at temperatures at and above 300K. This depicted van der Walls attractive forces as a result of dipole-dipole interactions. As temperatures increased the chains were seen to break away from the central globules, showing that the increased energy of the system overpowered the attractive forces.

Physical properties were seen to differ between polymers of branched and linear structures. This was in accordance with the findings of Jabbarzadeh et al. The trend of critical molecular weights of all polymers modeled was accurately predicted. Polymers with the least branching exhibited the largest values, while polymers with the most branching displayed the lowest values.

The TraPPE-UA force field did accurately predict the density of high density polyethylene at room temperature, when simulated with a large number of chains. The simulations with four chains at and over the critical molecular weight had densities that deviated from experimental data more so than much shorter chains simulated with a large quantity. The density values corresponded to experimental data. This concludes that the number of chains in the simulation is more important than the length of the chains when studying density of a polymeric system. The current work used longer polymer chains and a larger number of chains during density simulations and expectedly reported densities more accurate than those of de Pablo et al.

Various accurate polymer property trends were observed in the current work. It is concluded that the same trends can be witnessed with a wide variety of polymer systems including those of special interest to the running shoe industry. Careful considerations need to be made in choosing how to model polymer systems of importance. Optimizations of these design parameters will produce more accurate data for predicted properties. Exploration of other force fields not used in this work may provide more precise values for both the properties examined in this work and other properties useful in assessing running shoe polymers.

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Appendix A

Total System Energy Plots for HDPE of Various Chain Lengths

Figure 37 through Figure 47 show the total system energy of HDPE at various chain lengths. Simulations were performed at 0atm and 300K for 1500 picoseconds. All figures in this appendix have Y-axis energy units of kcal/mol and X-axis units of time steps (0.01 picoseconds, where the end point time is 1500 picoseconds).

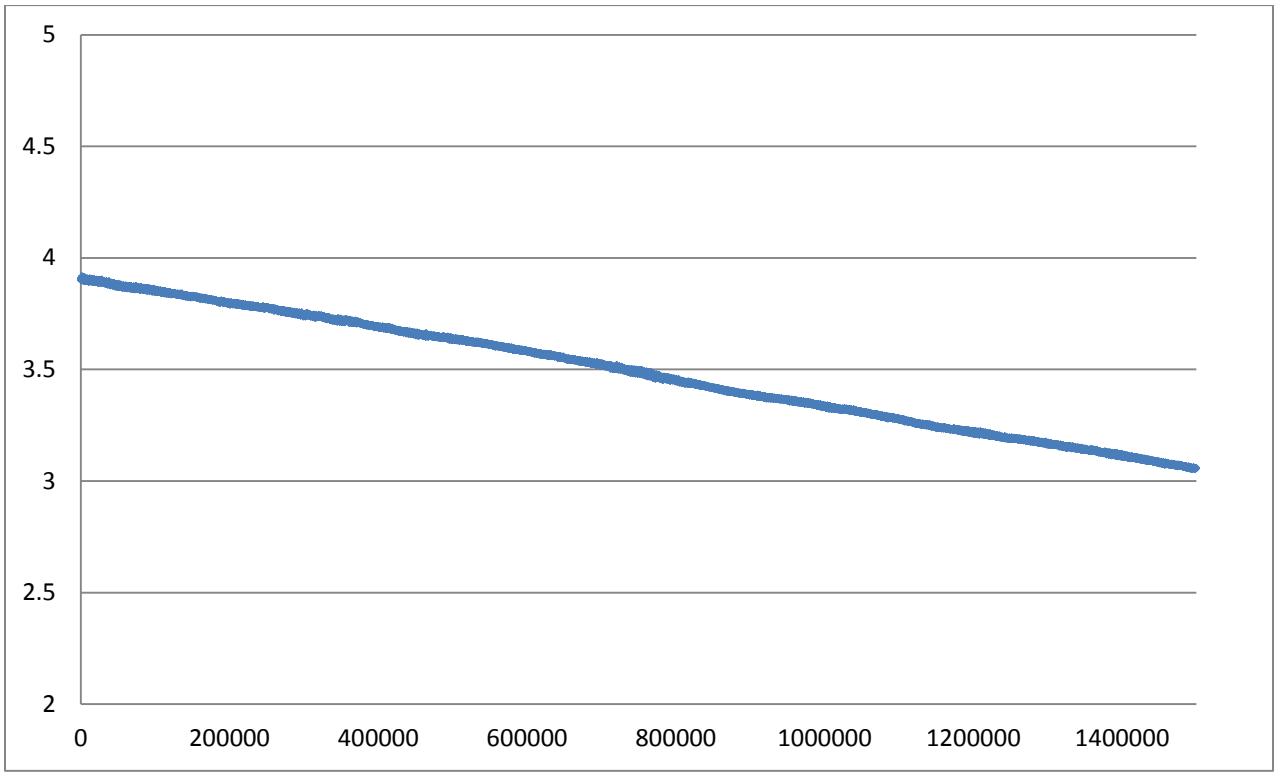

Figure 37: HDPE Chain Length 10 pseudo atoms

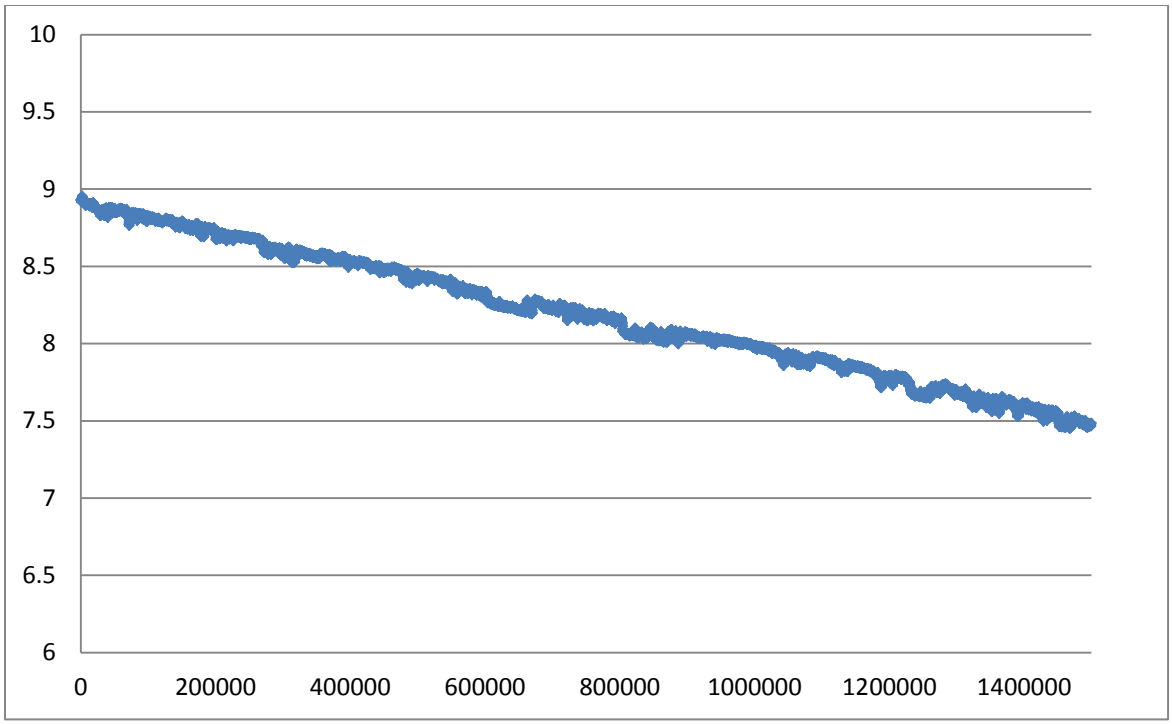

Figure 38: HDPE Chain Length 20 pseudo atoms

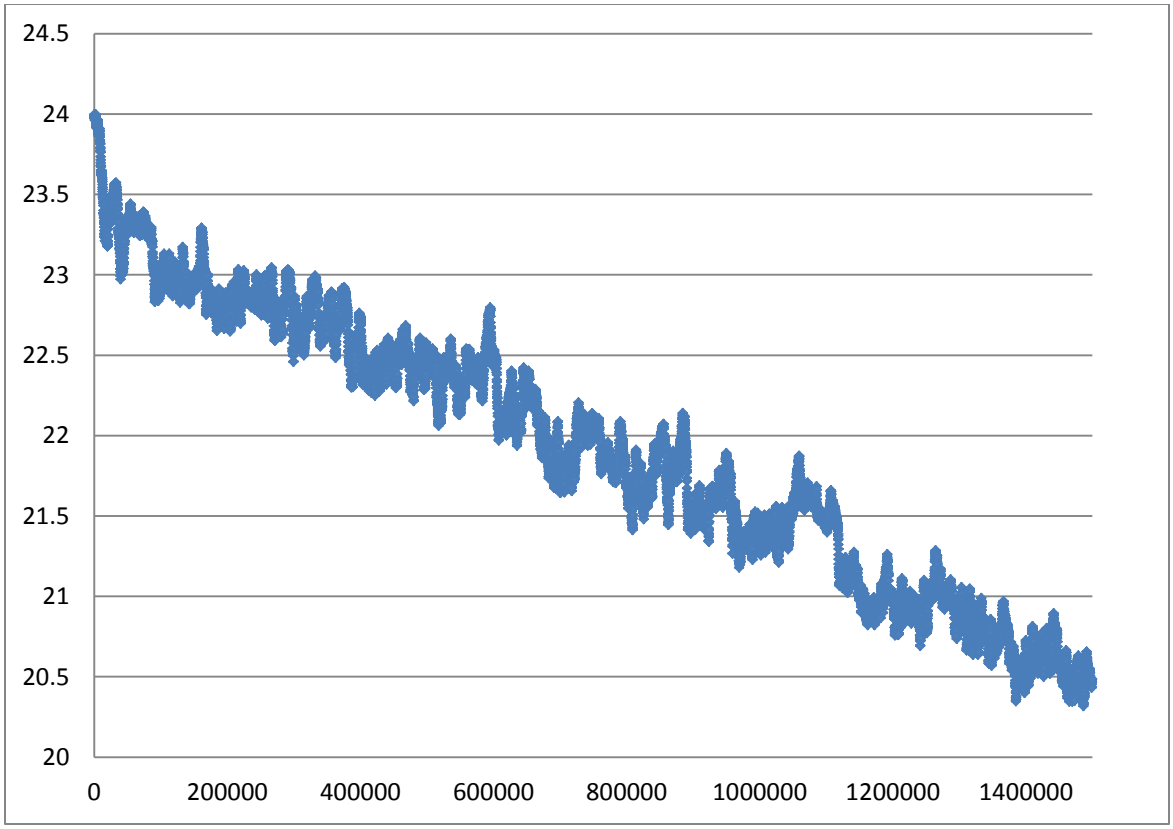

Figure 39: HDPE Chain Length 50 pseudo atoms

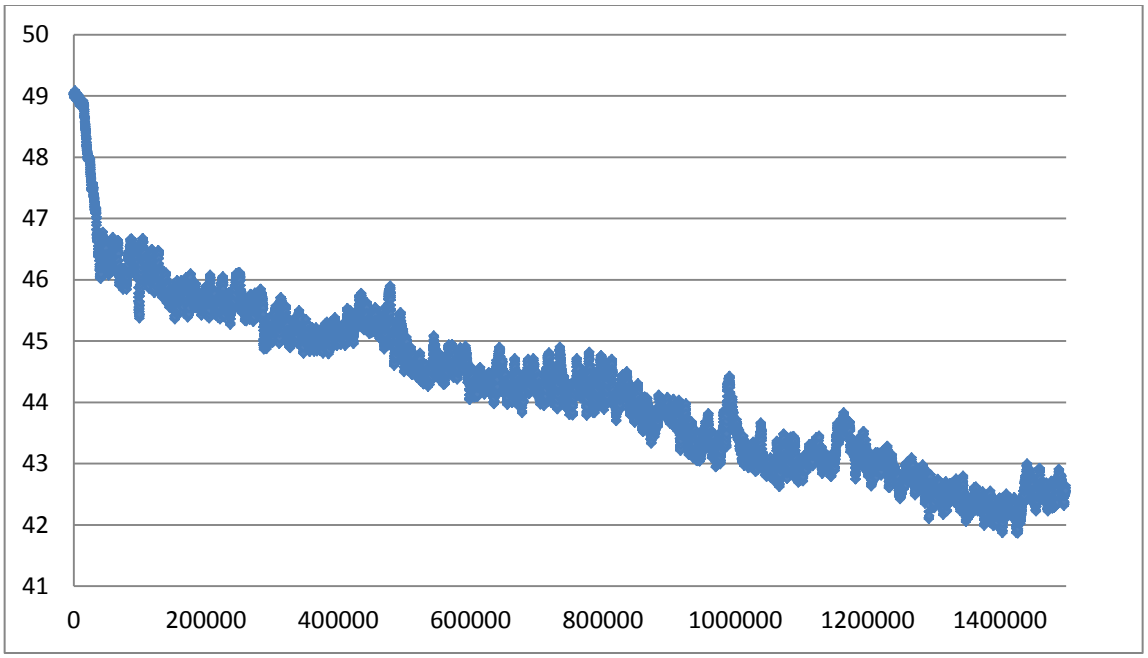

Figure 40: HDPE Chain Length 100 pseudo atoms

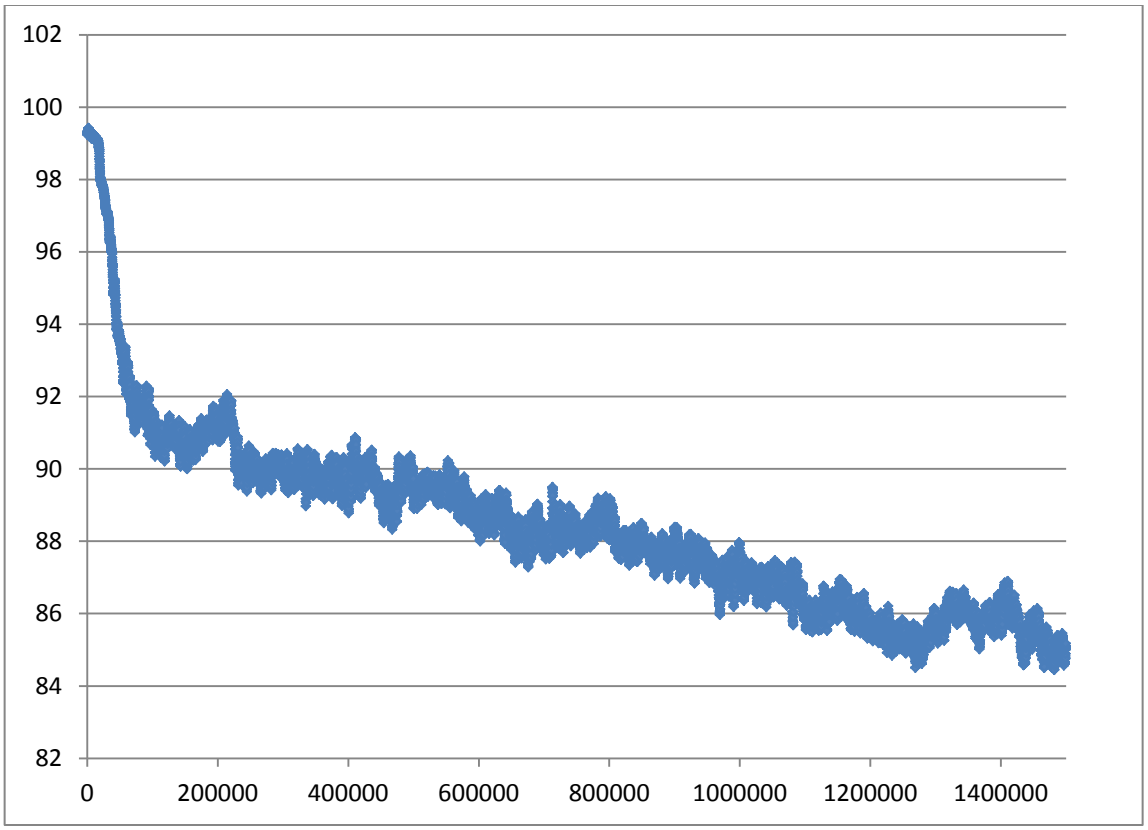

Figure 41: HDPE Chain Length 200 pseudo atoms

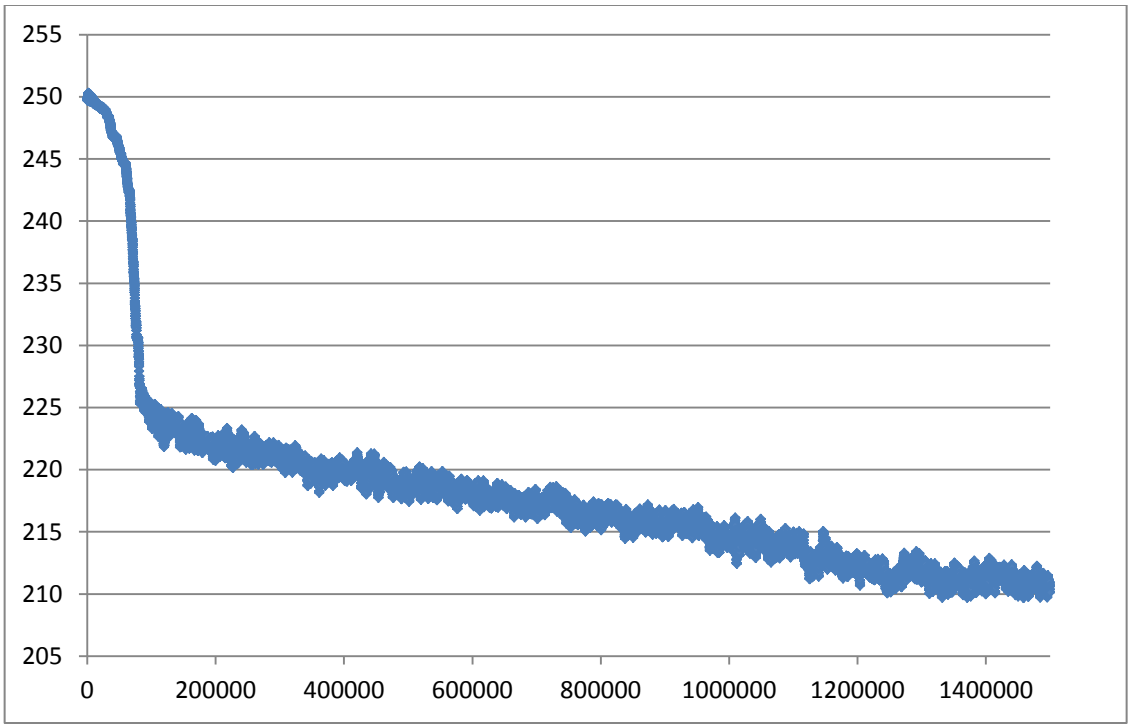

Figure 42: HDPE Chain Length 500 pseudo atoms

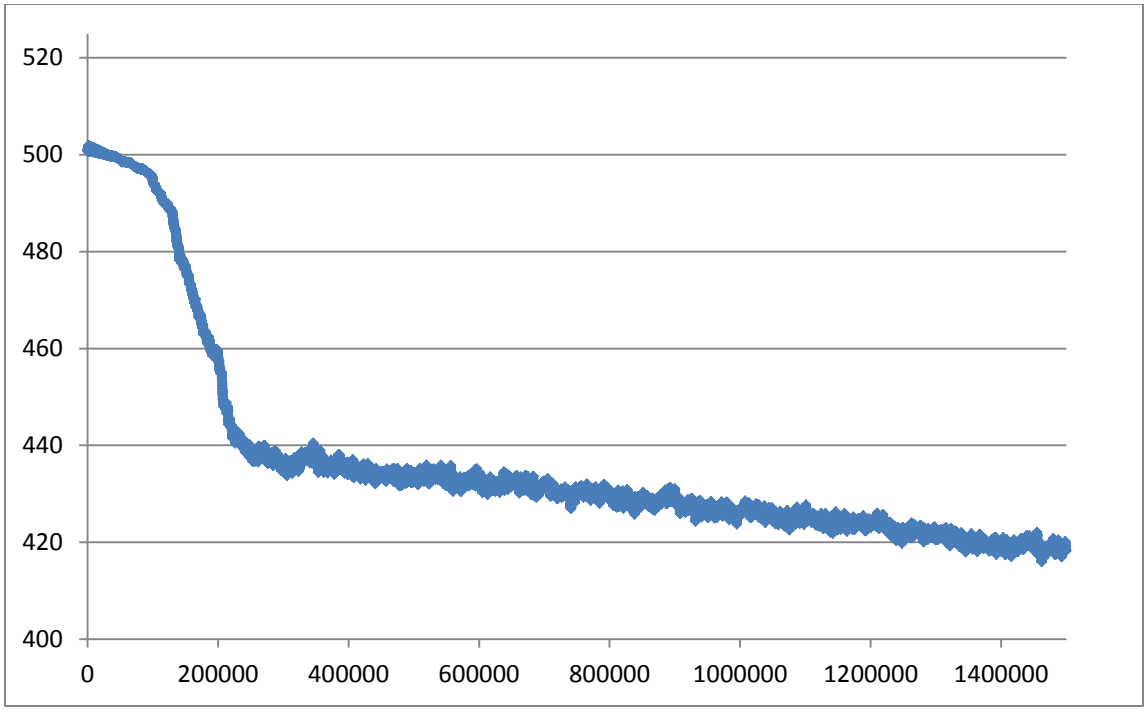

Figure 43: HDPE Chain Length 1000 pseudo atoms

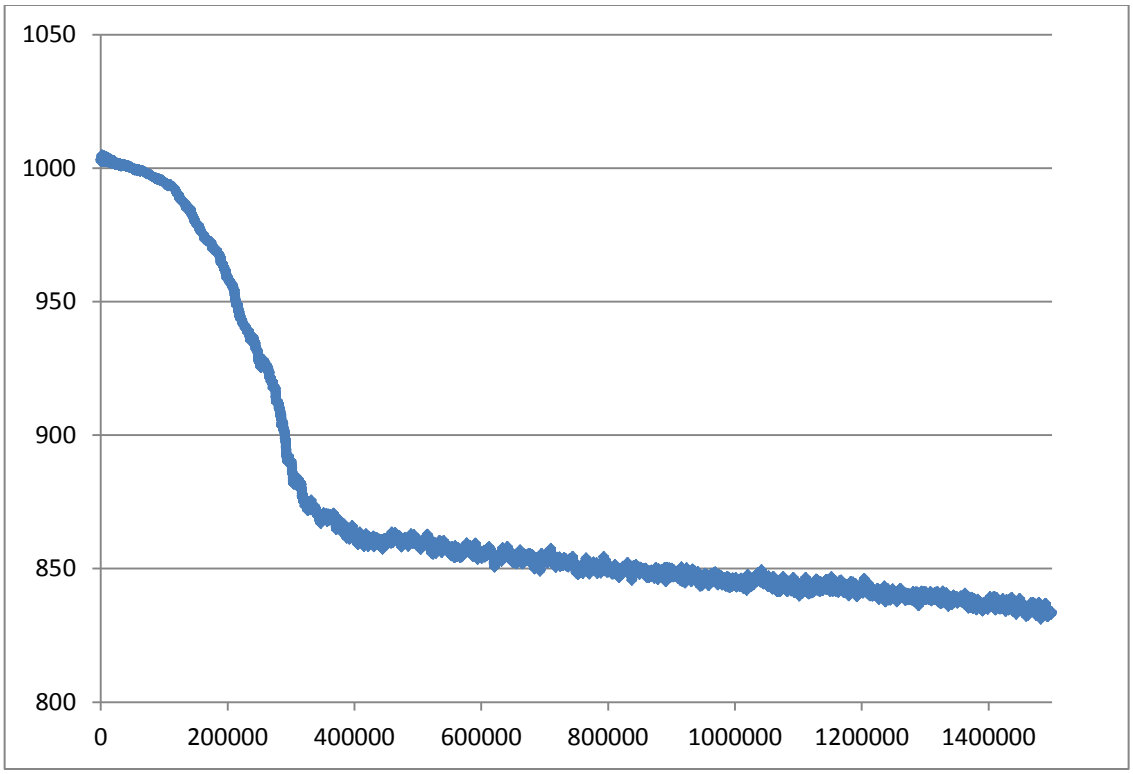

Figure 44: HDPE Chain Length 2000 pseudo atoms

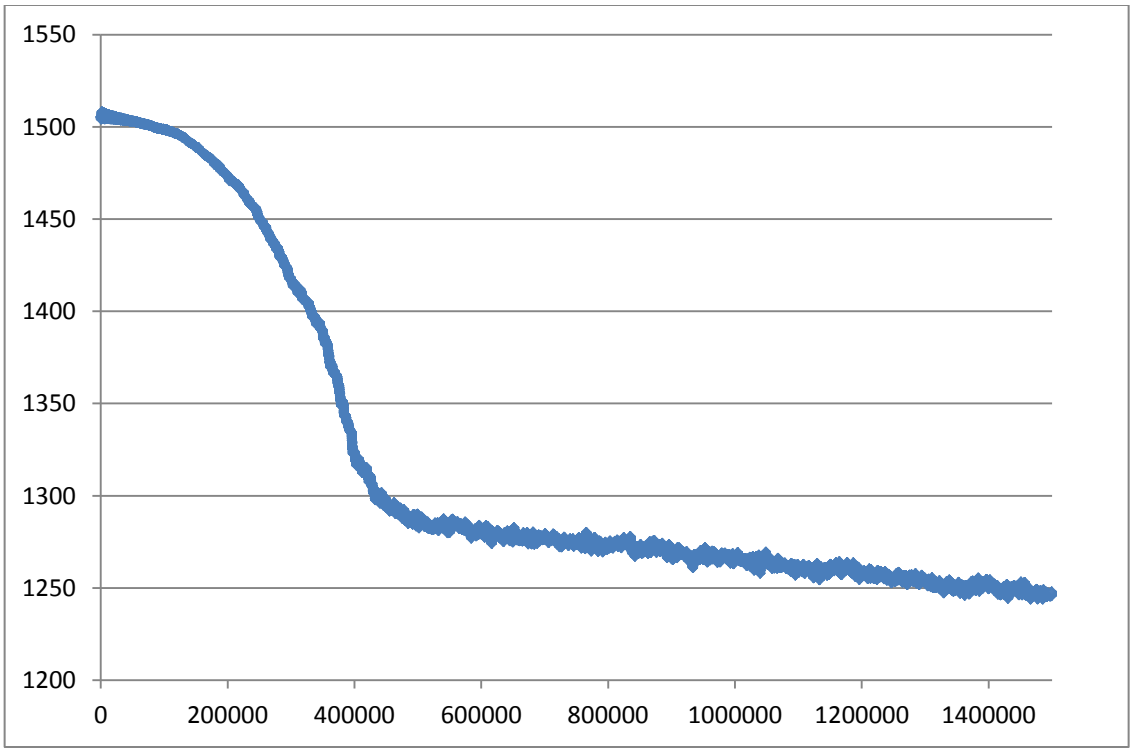

Figure 45: HDPE Chain Length 3000 pseudo atoms

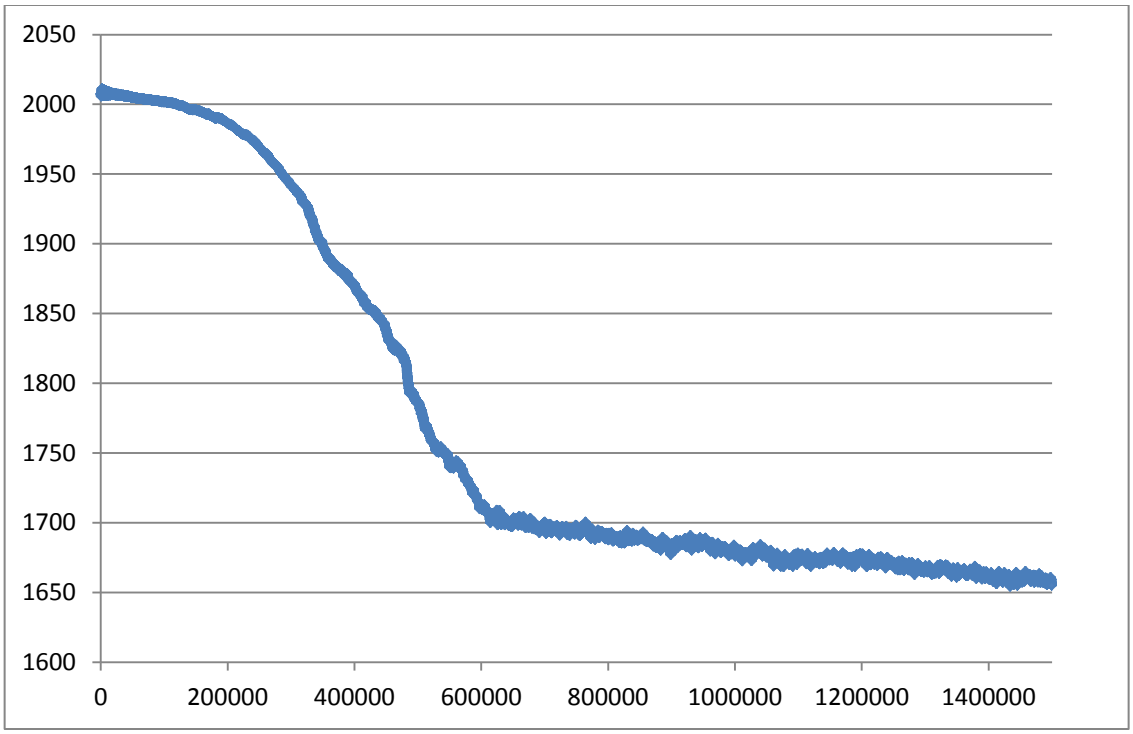

Figure 46: HDPE Chain Length 4000 pseudo atoms

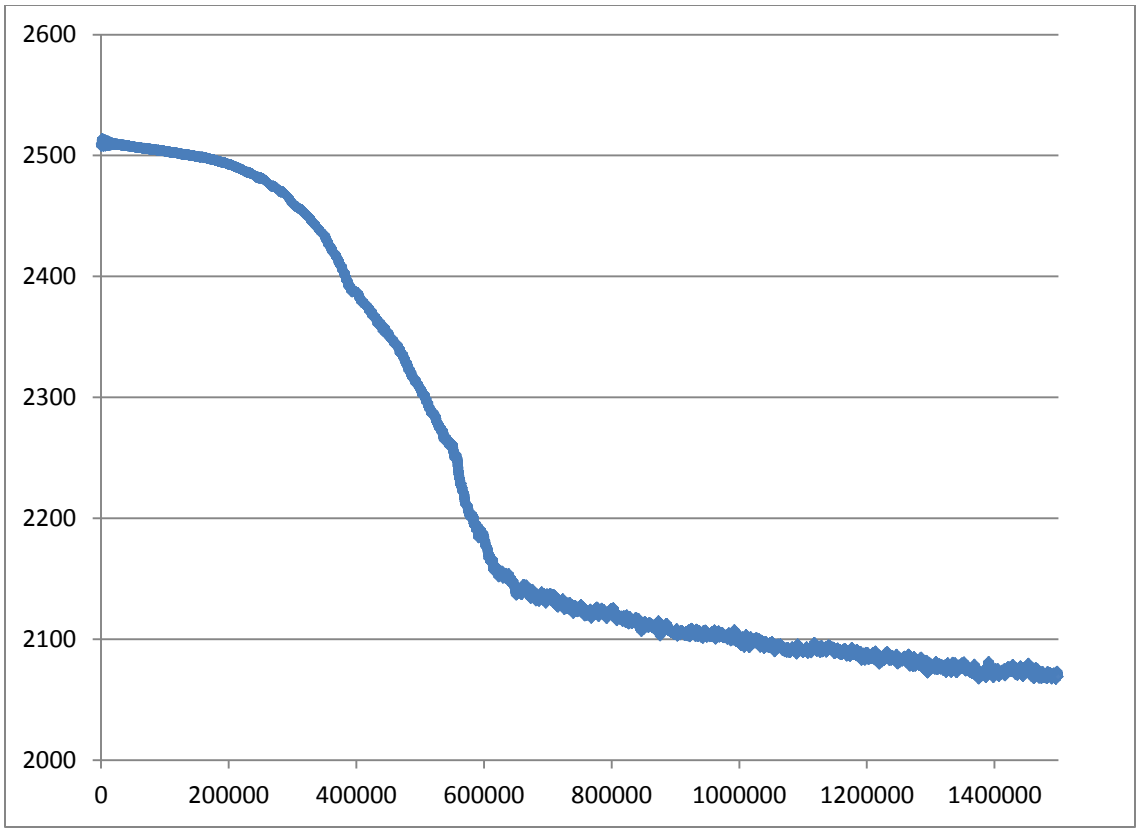

Figure 47: HDPE Chain Length 5000 pseudo atoms

Appendix B

Branching Effects of Polymer Structure

Low Density Polyethylene (LDPE)

Figure 48 through Figure 51 below, were images taken from one simulation of LDPE. Four chains of 2000 pseudo atoms in length were simulated at 0atm and 300K for 2000 picoseconds. The figures show the entanglement effects of the branching as the polymer chains form a globule over time.

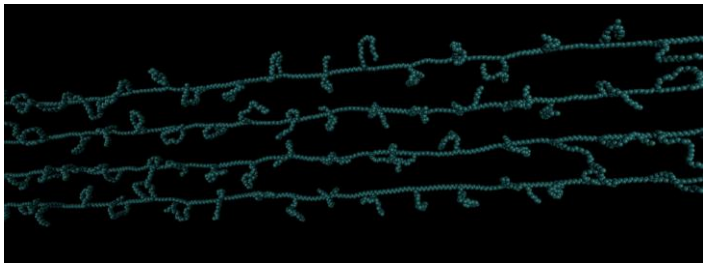

Figure 48: LDPE Initial Structure (Four Chains with Main Chain Length of 2000 pseudo atoms)

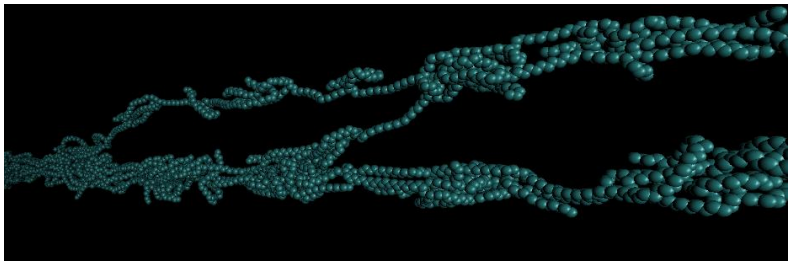

Figure 49: LDPE (60 picoseconds) (Four Chains with Main Chain Length of 2000 pseudo atoms)

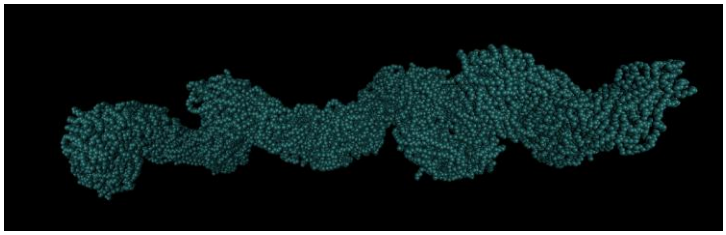

Figure 50: LDPE (310 picoseconds) (Four Chains with Main Chain Length of 2000 pseudo atoms)

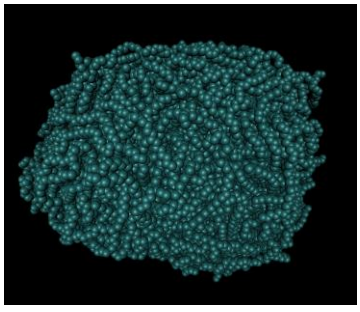

Figure 51: LDPE (2000 picoseconds) (Four Chains with Main Chain Length of 2000 pseudo atoms)

Polypropylene (PP)

The figure below was an image taken from one simulation of PP. Four chains of 2000 pseudo atoms in length were simulated at 0 atm and 300K for 3000 picoseconds. The figure shows the four straight adjacent chains beginning to interact. This demonstrates the attractive van der Waals forces.

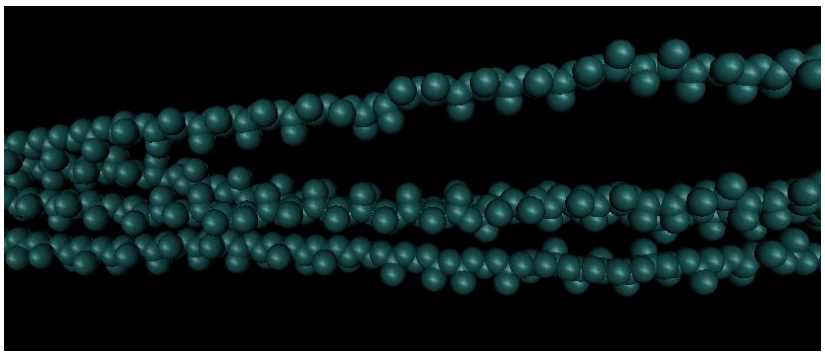

Figure 52: PP Initial Structure (Four Chains with Main Chain Length of 2000 pseudo atoms)

Appendix C

Final HDPE Temperature Variation Geometries (3000 picoseconds)

Figure 53 through Figure 60below, show four polymer chains of 2000 pseudo atoms long at various temperatures at 3000 picoseconds. The NVT simulations were run with no periodic boundary conditions at 0 atm. The progression of temperatures ranges from 100K to 800K.

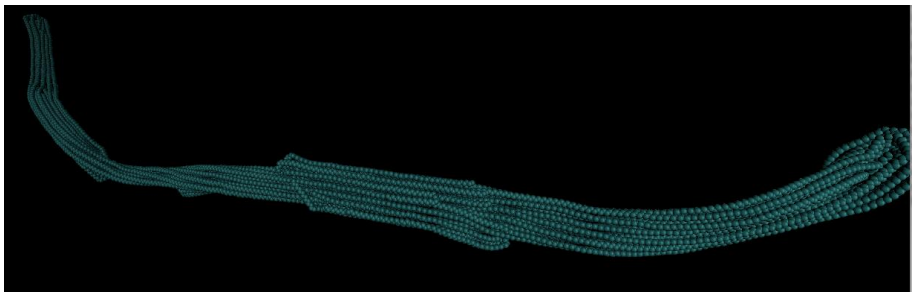

Figure 53: 100K

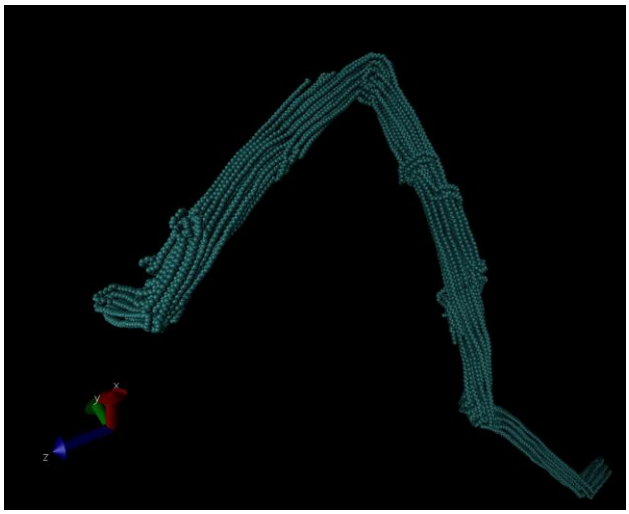

Figure 54: 200K

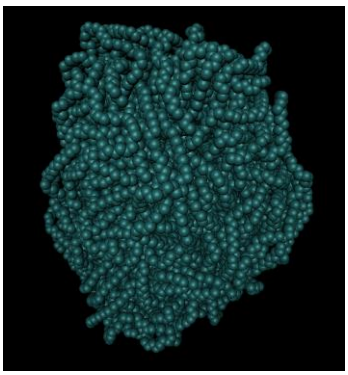

Figure 55: 300K

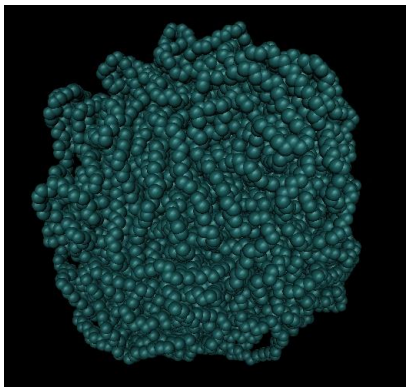

Figure 56: 350K

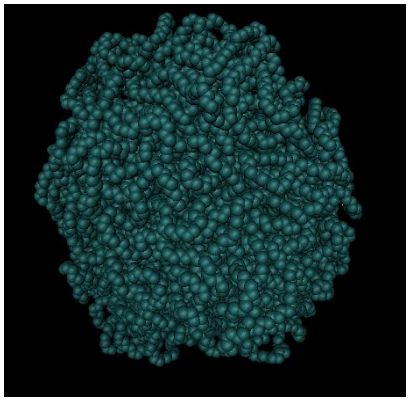

Figure 57: 400K

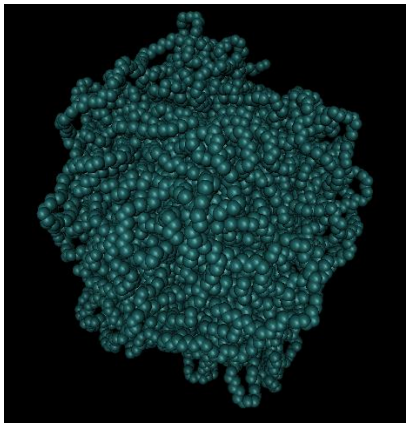

Figure 58: 500K

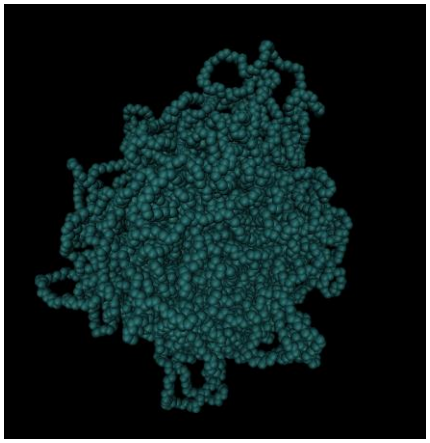

Figure 59: 600K

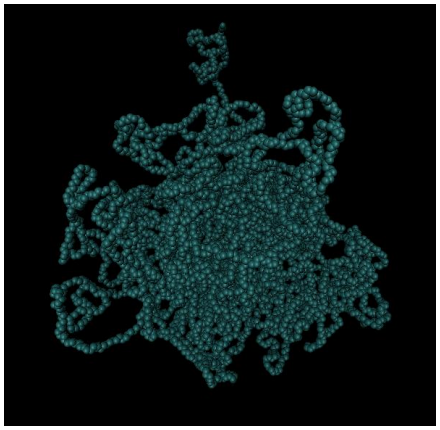

Figure 60: 800K

Appendix D

Density Calculations

Sample calculations are provided that detail how the box size values from the simulations were used to find the polymer density. Lengths of the X, Y, and Z sides of the simulation box were extracted from the REVCON file of completed NPT simulations.

Conversions

$1\ atomic\ mass\ unit = 1.6605389217 * 10^{-30} grams$

$1\ picometer = 10^{-10} centimeters$

$HDPE\ 1000 = 14028.95594 amu$

$Polymer\ Mass = (14028.95594 amu * 1.6605389217 * 10^{-30} g) = 2.32956274 * 10^{-26} grams$

$HDPE\ 2000 = 28057.91188 amu$

$Polymer\ Mass = (28057.91188 amu * 1.6605389217 * 10^{-30} g) = 5.3646 * 10^{-26} grams$

$$Density = \frac{mass}{volume}$$

Single Chain Simulations

150 Picosecond Simulation, 0atm, HDPE1000, 300K

$Polymer\ Volume = (28 * 10^{-10} cm)^3 = 2.1952 * 10^{-26} cm^3$

$$Density = \frac{2.32956274 * 10^{-26} grams}{2.1952 * 10^{-26} cm^3} = 1.061 \frac{g}{cm^3}$$

1500 Picosecond Simulation, 0atm, HDPE1000, 300K

$Polymer\ Volume = (29.8827 * 10^{-10} cm)^3 = 2.66845267 * 10^{-26} cm^3$

$$Density = \frac{2.32956274 * 10^{-26} grams}{2.66845267 * 10^{-26} cm^3} = 0.873 \frac{g}{cm^3}$$

1500 Picosecond Simulation, 1atm, HDPE1000, 300K

$Polymer\ Volume = (29.946329 * 10^{-10} cm)^3 = 2.6855 * 10^{-26} cm^3$

$$Density = \frac{2.32956274 * 10^{-26} grams}{2.6855 * 10^{-26} cm^3} = 0.867 \frac{g}{cm^3}$$

1500 Picosecond Simulation, 0atm, HDPE2000, 300K

$$Polymer\ Volume = (405278 * 10^{-10} cm)(37.5258 * 10^{-10} cm)(35.2742 * 10^{-10} cm)$$
$$= 5.3646 * 10^{-26} cm^3$$

$$Density = \frac{4.659125 * 10^{-26} grams}{5.3646 * 10^{-26} cm^3} = 0.868 \frac{g}{cm^3}$$

Appendix D

Globule Formation at Various Temperatures

The figures of this appendix are images at various time intervals of HDPE simulations. Four chains of 2000 pseudo atoms long were simulated at temperatures ranging from 300K to 800K at 0atm for 3000 picoseconds.

350 Kelvin Simulation

Figure 61, Figure 62, and Figure 63 below show the structure of the four chains simulated at 350K during the formation of a globule.

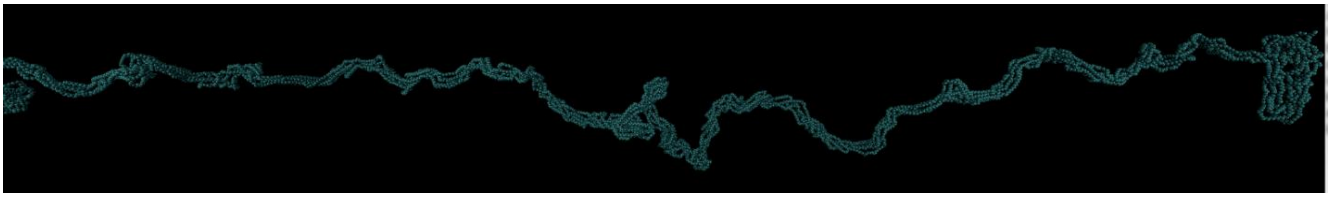

Figure 61: HDPE 350K (150 picoseconds)

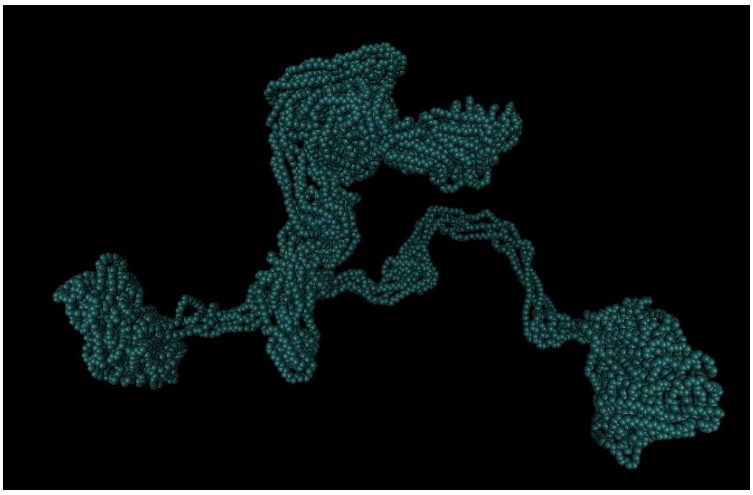

Figure 62: HDPE 350K (250 picoseconds)

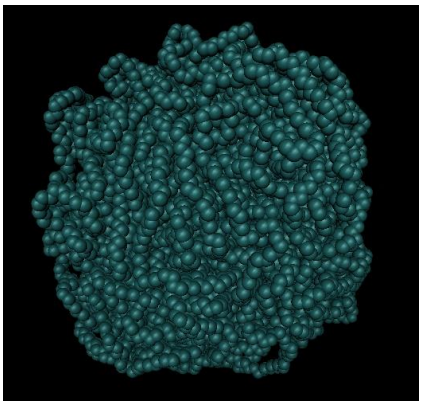

Figure 63: HDPE 350K (3000 picoseconds)

400 Kelvin Simulation

Figure 64, Figure 65, and Figure 66 below, show the structure of the four chains simulated at 400K.

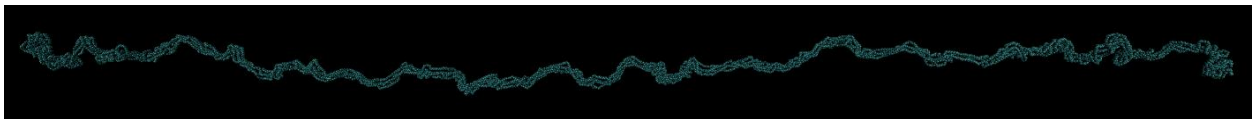

Figure 64: HDPE 400K (90 picoseconds)

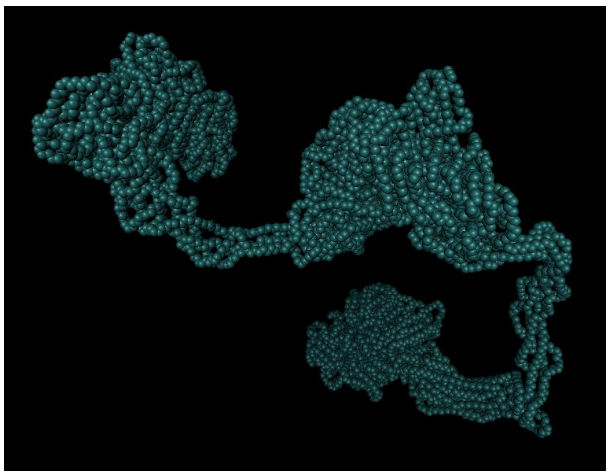

Figure 65: HDPE 400K (210 picoseconds)

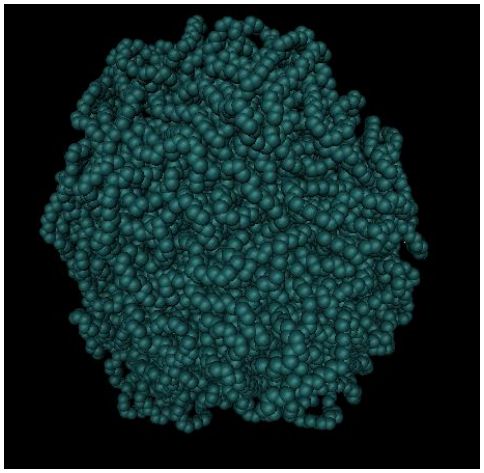

Figure 66: HDPE 400K (3000 picoseconds)

500 Kelvin Simulation

Figure 67, Figure 68, and Figure 69 below, show the structure of the four chains simulated at 500K.

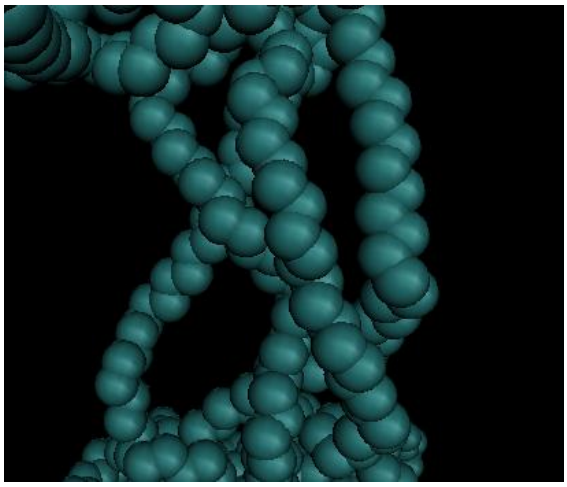

Figure 67: HDPE 500K (130 picoseconds)

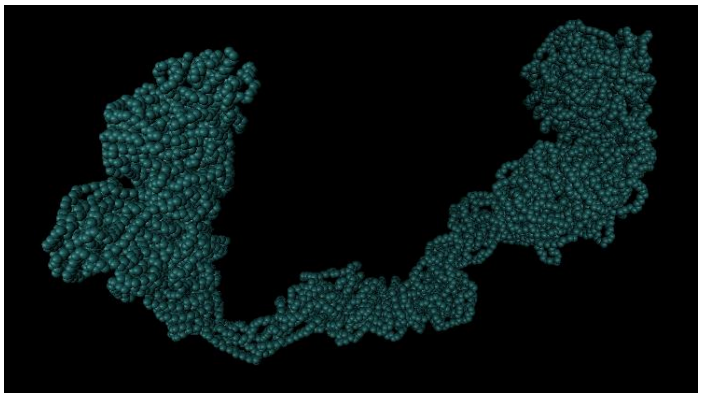

Figure 68: HDPE 500K (160 picoseconds)

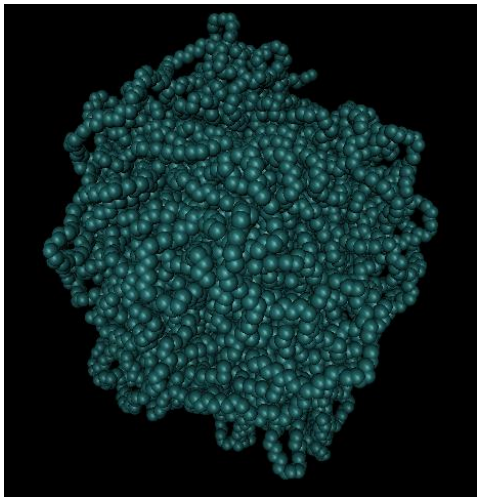

Figure 69: HDPE 500K (3000 picoseconds)

600 Kelvin Simulation

Figure 70 through Figure 74 below, show the structure of the four chains simulated at 600K. Figure 71 shows the initial point of globule formation. There is an abundance of kinetic energy in the system that prevents the globule from staying together at first pass. The momentum of the chains coming together only allows the globule to form for a brief moment before it starts to break apart. There is some oscillation between the globule state and the non-globule state as seen by the progression of Figure 70 to Figure 74.

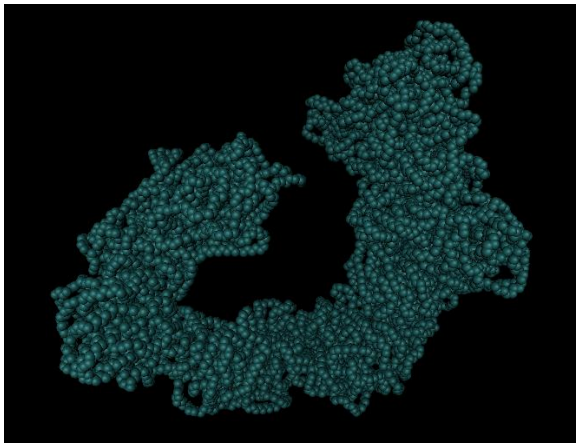

Figure 70: HDPE 600K (140 picoseconds)

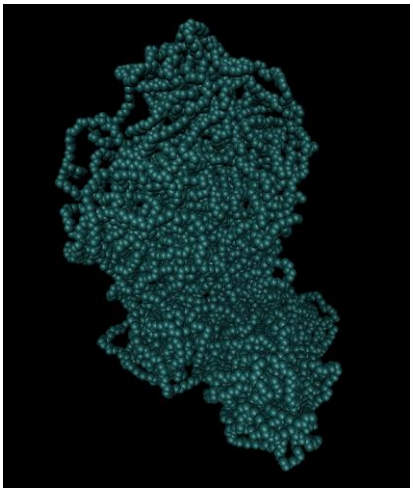

Figure 71: HDPE 600K (150 picoseconds)

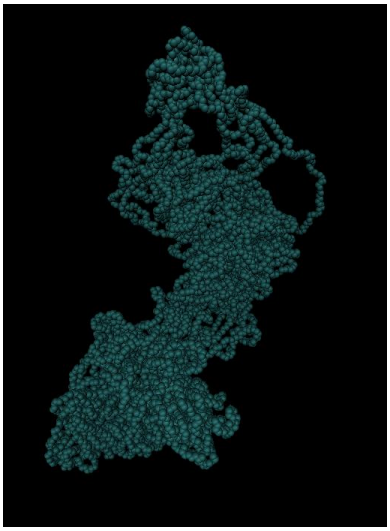

Figure 72: HDPE 600K (170 picoseconds)

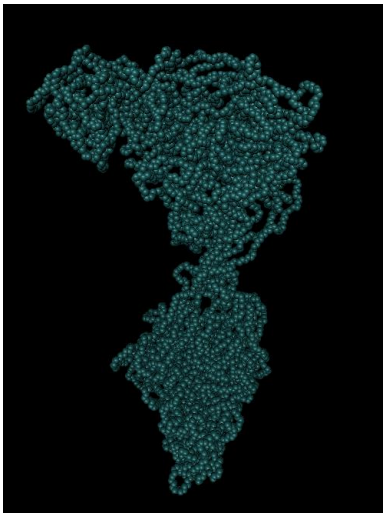

Figure 73: HDPE 600K (200 picoseconds)

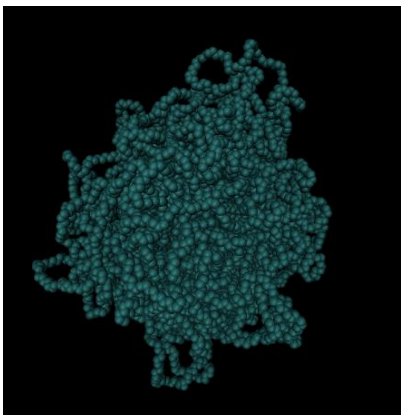

Figure 74: HDPE 600K (3000 picoseconds)

800 Kelvin Simulation

Figure 75 through Figure 78 below, show the structure of the four chains simulated at 800K. The oscillatory effect is seen as the momentum of the chains initially coming together overpowered the VDW attractive forces that hold together the globule. Figure 77 and Figure 78 depict melting as singular chains have broken away from the four adjacent chains from which they started, as well as from the globule as a whole.

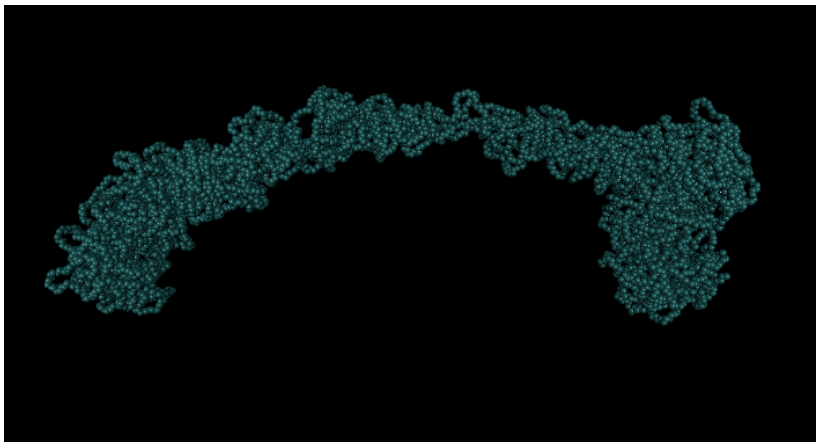

Figure 75: HDPE 800K (100 picoseconds)

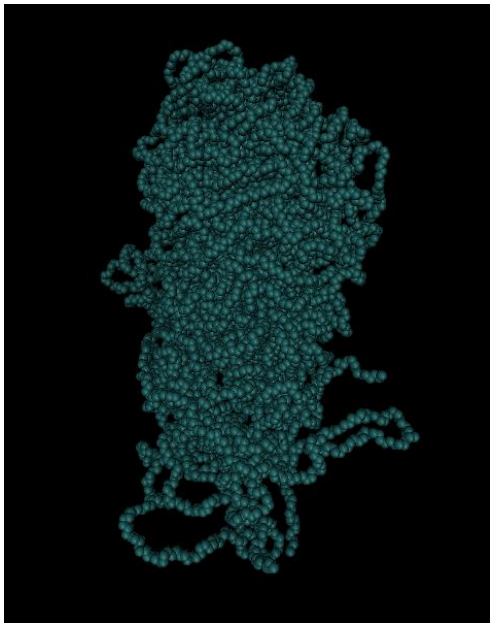

Figure 76: HDPE 800K (120 picoseconds)

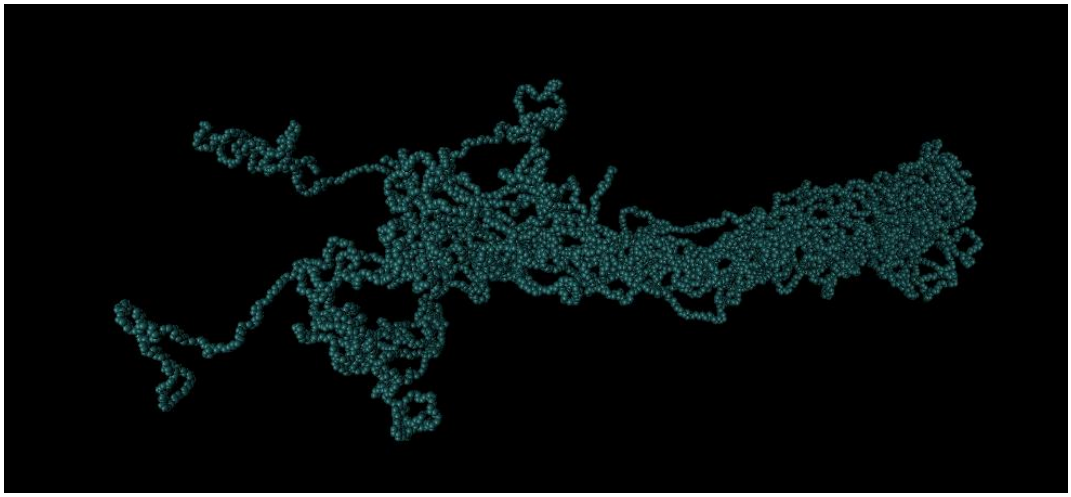

Figure 77: HDPE 800K (210 picoseconds)

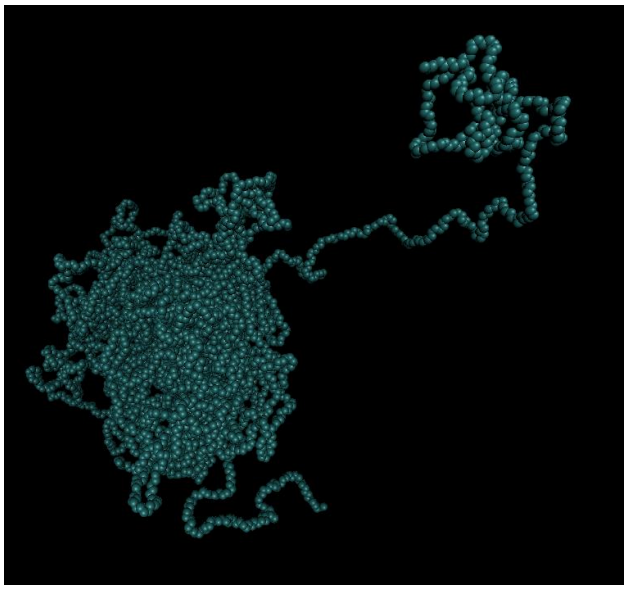

Figure 78: HDPE 800K (670 picoseconds)

Appendix E

DL_POLY2 Input Files

CONTROL, FIELD, and CONFIG input files are provided for the DL_POLY2 program below. HDPE files of one and four chain systems of 20 pseudo atoms long, PP files of a one chain system 50 pseudo atoms long, and LDPE files of a one chain system 200 pseudo atoms long were chosen.

CONTROL File

```
#zero
temperature                300 kelvin
pressure                     0 katm
equilibration steps        100 steps
timestep                 0.001 ps
#multiple timestep           1 steps
scale every                  1 steps
shake tolerance  1.0E-5


cutoff                 10.00 angstroms
#all pairs
no link
coul
rvdw                   10.00

delr                       .50 angstroms

print every              100 steps
#mxlist                   2.5
rdf sampling every       100 steps
print rdf

job time             500000000 seconds
close time              1000 seconds
#ewald precision          1d-6
cap forces in equilibration mode  1000 kT/A

ensemble    nvt hoover 0.5 0.5
stats                    10000
stats every              10000 steps
trajectory nstraj=0 istraj=10000 keytrj=0
stack                      100 deep
steps                  3000000 steps
#restart
finish
```

FIELD Files

High Density Polyethylene (HDPE)

One Chain – 20 Pseudo Atoms Long

```
Units kcal
Molecular types 1
Molecule name test
nummols 1
atoms  20
C3          15.03470     0.00000   1   0
C2          14.02680     0.00000   1   0
C2          14.02680     0.00000   1   0
C2          14.02680     0.00000   1   0
C2          14.02680     0.00000   1   0
C2          14.02680     0.00000   1   0
C2          14.02680     0.00000   1   0
C2          14.02680     0.00000   1   0
C2          14.02680     0.00000   1   0
C2          14.02680     0.00000   1   0
C2          14.02680     0.00000   1   0
C2          14.02680     0.00000   1   0
C2          14.02680     0.00000   1   0
C2          14.02680     0.00000   1   0
C2          14.02680     0.00000   1   0
C2          14.02680     0.00000   1   0
C2          14.02680     0.00000   1   0
C2          14.02680     0.00000   1   0
C2          14.02680     0.00000   1   0
C3          15.03470     0.00000   1   0
CONSTRAINTS     19
    1   2  1.54000000
    2   3  1.54000000
    3   4  1.54000000
    4   5  1.54000000
    5   6  1.54000000
    6   7  1.54000000
    7   8  1.54000000
    8   9  1.54000000
    9   10  1.54000000
    10   11  1.54000000
    11   12  1.54000000
    12   13  1.54000000
    13   14  1.54000000
    14   15  1.54000000
    15   16  1.54000000
    16   17  1.54000000
    17   18  1.54000000
    18   19  1.54000000
    19   20  1.54000000
angles  18
harm      1     2     3   124.19700   112.40000
harm      2     3     4   124.19700   112.40000
harm      3     4     5   124.19700   112.40000
harm      4     5     6   124.19700   112.40000
harm      5     6     7   124.19700   112.40000
harm      6     7     8   124.19700   112.40000
harm      7     8     9   124.19700   112.40000
harm      8     9     10   124.19700   112.40000
```

```
harm      9     10     11   124.19700   112.40000
harm      10     11     12   124.19700   112.40000
harm      11     12     13   124.19700   112.40000
harm      12     13     14   124.19700   112.40000
harm      13     14     15   124.19700   112.40000
harm      14     15     16   124.19700   112.40000
harm      15     16     17   124.19700   112.40000
harm      16     17     18   124.19700   112.40000
harm      17     18     19   124.19700   112.40000
harm      18     19     20   124.19700   112.40000
dihedral  17
OPLS  1 2 3 4  0.0000000 1.41100000 -0.27100000  3.145000000 0.00000000
OPLS  2 3 4 5  0.0000000 1.41100000 -0.27100000  3.145000000 0.00000000
OPLS  3 4 5 6  0.0000000 1.41100000 -0.27100000  3.145000000 0.00000000
OPLS  4 5 6 7  0.0000000 1.41100000 -0.27100000  3.145000000 0.00000000
OPLS  5 6 7 8  0.0000000 1.41100000 -0.27100000  3.145000000 0.00000000
OPLS  6 7 8 9  0.0000000 1.41100000 -0.27100000  3.145000000 0.00000000
OPLS  7 8 9 10  0.0000000 1.41100000 -0.27100000  3.145000000 0.00000000
OPLS  8 9 10 11  0.0000000 1.41100000 -0.27100000  3.145000000 0.00000000
OPLS  9 10 11 12  0.0000000 1.41100000 -0.27100000  3.145000000 0.00000000
OPLS  10 11 12 13  0.0000000 1.41100000 -0.27100000  3.145000000 0.00000000
OPLS  11 12 13 14  0.0000000 1.41100000 -0.27100000  3.145000000 0.00000000
OPLS  12 13 14 15  0.0000000 1.41100000 -0.27100000  3.145000000 0.00000000
OPLS  13 14 15 16  0.0000000 1.41100000 -0.27100000  3.145000000 0.00000000
OPLS  14 15 16 17  0.0000000 1.41100000 -0.27100000  3.145000000 0.00000000
OPLS  15 16 17 18  0.0000000 1.41100000 -0.27100000  3.145000000 0.00000000
OPLS  16 17 18 19  0.0000000 1.41100000 -0.27100000  3.145000000 0.00000000
OPLS  17 18 19 20  0.0000000 1.41100000 -0.27100000  3.145000000 0.00000000
finish
vdw 3
C3      C3      lj        0.1947      3.7500
C2      C3      lj        0.1334      3.8500
C2      C2      lj        0.0914      3.9500
close
```

Four Chains – 20 Pseudo Atoms Long

```
Units kcal
Molecular types 1
Molecule name test
nummols 4
atoms  20
C3          15.03470     0.00000   1   0
C2          14.02680     0.00000   1   0
C2          14.02680     0.00000   1   0
C2          14.02680     0.00000   1   0
C2          14.02680     0.00000   1   0
C2          14.02680     0.00000   1   0
C2          14.02680     0.00000   1   0
C2          14.02680     0.00000   1   0
C2          14.02680     0.00000   1   0
C2          14.02680     0.00000   1   0
C2          14.02680     0.00000   1   0
C2          14.02680     0.00000   1   0
C2          14.02680     0.00000   1   0
C2          14.02680     0.00000   1   0
C2          14.02680     0.00000   1   0
C2          14.02680     0.00000   1   0
C2          14.02680     0.00000   1   0
```

```
C2          14.02680     0.00000   1   0
C2          14.02680     0.00000   1   0
C3          15.03470     0.00000   1   0
CONSTRAINTS     19
    1   2  1.54000000
    2   3  1.54000000
    3   4  1.54000000
    4   5  1.54000000
    5   6  1.54000000
    6   7  1.54000000
    7   8  1.54000000
    8   9  1.54000000
    9   10  1.54000000
    10   11  1.54000000
    11   12  1.54000000
    12   13  1.54000000
    13   14  1.54000000
    14   15  1.54000000
    15   16  1.54000000
    16   17  1.54000000
    17   18  1.54000000
    18   19  1.54000000
    19   20  1.54000000
angles  18
harm      1     2     3   124.19700   112.40000
harm      2     3     4   124.19700   112.40000
harm      3     4     5   124.19700   112.40000
harm      4     5     6   124.19700   112.40000
harm      5     6     7   124.19700   112.40000
harm      6     7     8   124.19700   112.40000
harm      7     8     9   124.19700   112.40000
harm      8     9     10   124.19700   112.40000
harm      9     10     11   124.19700   112.40000
harm      10     11     12   124.19700   112.40000
harm      11     12     13   124.19700   112.40000
harm      12     13     14   124.19700   112.40000
harm      13     14     15   124.19700   112.40000
harm      14     15     16   124.19700   112.40000
harm      15     16     17   124.19700   112.40000
harm      16     17     18   124.19700   112.40000
harm      17     18     19   124.19700   112.40000
harm      18     19     20   124.19700   112.40000
dihedral  17
OPLS  1 2 3 4  0.0000000 1.41100000 -0.27100000  3.145000000 0.00000000
OPLS  2 3 4 5  0.0000000 1.41100000 -0.27100000  3.145000000 0.00000000
OPLS  3 4 5 6  0.0000000 1.41100000 -0.27100000  3.145000000 0.00000000
OPLS  4 5 6 7  0.0000000 1.41100000 -0.27100000  3.145000000 0.00000000
OPLS  5 6 7 8  0.0000000 1.41100000 -0.27100000  3.145000000 0.00000000
OPLS  6 7 8 9  0.0000000 1.41100000 -0.27100000  3.145000000 0.00000000
OPLS  7 8 9 10  0.0000000 1.41100000 -0.27100000  3.145000000 0.00000000
OPLS  8 9 10 11  0.0000000 1.41100000 -0.27100000  3.145000000 0.00000000
OPLS  9 10 11 12  0.0000000 1.41100000 -0.27100000  3.145000000 0.00000000
OPLS  10 11 12 13  0.0000000 1.41100000 -0.27100000  3.145000000 0.00000000
OPLS  11 12 13 14  0.0000000 1.41100000 -0.27100000  3.145000000 0.00000000
OPLS  12 13 14 15  0.0000000 1.41100000 -0.27100000  3.145000000 0.00000000
OPLS  13 14 15 16  0.0000000 1.41100000 -0.27100000  3.145000000 0.00000000
OPLS  14 15 16 17  0.0000000 1.41100000 -0.27100000  3.145000000 0.00000000
OPLS  15 16 17 18  0.0000000 1.41100000 -0.27100000  3.145000000 0.00000000
OPLS  16 17 18 19  0.0000000 1.41100000 -0.27100000  3.145000000 0.00000000
OPLS  17 18 19 20  0.0000000 1.41100000 -0.27100000  3.145000000 0.00000000
finish
vdw 3
C3      C3      lj        0.1947      3.7500
```

```
C2       C3       lj         0.1334      3.8500
C2       C2       lj         0.0914      3.9500
close
```

Low Density Polyethylene (LDPE)

One Chain – 200 Pseudo Atoms Long

```
Generated by DL_FIELD v2.00
Units kcal
Molecular types 1
Molecule name test
nummols 1
atoms  501
C3          15.03470     0.00000   1    0    1HEX
C1          13.01864     0.00000   1    0    1HEX
C2          14.02680     0.00000   1    0    1HEX
C2          14.02680     0.00000   1    0    1HEX
C2          14.02680     0.00000   1    0    1HEX
C2          14.02680     0.00000   1    0    1HEX
C2          14.02680     0.00000   1    0    1HEX
C2          14.02680     0.00000   1    0    1HEX
C2          14.02680     0.00000   1    0    1HEX
C2          14.02680     0.00000   1    0    1HEX
C2          14.02680     0.00000   1    0    1HEX
C2          14.02680     0.00000   1    0    1HEX
C2          14.02680     0.00000   1    0    1HEX
C2          14.02680     0.00000   1    0    1HEX
C2          14.02680     0.00000   1    0    1HEX
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harm     497     498     499   124.19700   114.00000
harm     498     499     500   124.19700   114.00000
harm     499     500     501   124.19700   114.00000
dihedral  368
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OPLS  43 44 45 46  0.0000000 1.41100000 -0.27100000  3.145000000 0.00000000
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```

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OPLS  280 281 282 283  -0.4989000 1.70390800 -0.44453000  1.753745000 0.00000000
OPLS  282 283 284 285  -0.4989000 1.70390800 -0.44453000  1.753745000 0.00000000
OPLS  284 285 286 287  -0.4989000 1.70390800 -0.44453000  1.753745000 0.00000000
OPLS  286 287 288 289  -0.4989000 1.70390800 -0.44453000  1.753745000 0.00000000
OPLS  288 289 290 291  0.0000000 1.41100000 -0.27100000  3.145000000 0.00000000
OPLS  61 62 292 293  -0.4989000 1.70390800 -0.44453000  1.753745000 0.00000000
OPLS  63 62 292 293  -0.4989000 1.70390800 -0.44453000  1.753745000 0.00000000
OPLS  62 292 293 294  0.0000000 1.41100000 -0.27100000  3.145000000 0.00000000
OPLS  292 293 294 295  -0.4989000 1.70390800 -0.44453000  1.753745000 0.00000000
OPLS  294 295 296 297  -0.4989000 1.70390800 -0.44453000  1.753745000 0.00000000
OPLS  296 297 298 299  -0.4989000 1.70390800 -0.44453000  1.753745000 0.00000000
OPLS  298 299 300 301  -0.4989000 1.70390800 -0.44453000  1.753745000 0.00000000
OPLS  300 301 302 303  -0.4989000 1.70390800 -0.44453000  1.753745000 0.00000000
OPLS  302 303 304 305  -0.4989000 1.70390800 -0.44453000  1.753745000 0.00000000
OPLS  304 305 306 307  -0.4989000 1.70390800 -0.44453000  1.753745000 0.00000000
OPLS  306 307 308 309  -0.4989000 1.70390800 -0.44453000  1.753745000 0.00000000
OPLS  308 309 310 311  -0.4989000 1.70390800 -0.44453000  1.753745000 0.00000000
OPLS  310 311 312 313  -0.4989000 1.70390800 -0.44453000  1.753745000 0.00000000
OPLS  312 313 314 315  -0.4989000 1.70390800 -0.44453000  1.753745000 0.00000000
OPLS  314 315 316 317  -0.4989000 1.70390800 -0.44453000  1.753745000 0.00000000
OPLS  316 317 318 319  -0.4989000 1.70390800 -0.44453000  1.753745000 0.00000000
OPLS  318 319 320 321  0.0000000 1.41100000 -0.27100000  3.145000000 0.00000000
OPLS  81 82 322 323  -0.4989000 1.70390800 -0.44453000  1.753745000 0.00000000
OPLS  83 82 322 323  -0.4989000 1.70390800 -0.44453000  1.753745000 0.00000000
OPLS  82 322 323 324  0.0000000 1.41100000 -0.27100000  3.145000000 0.00000000
OPLS  322 323 324 325  -0.4989000 1.70390800 -0.44453000  1.753745000 0.00000000
OPLS  324 325 326 327  -0.4989000 1.70390800 -0.44453000  1.753745000 0.00000000
OPLS  326 327 328 329  -0.4989000 1.70390800 -0.44453000  1.753745000 0.00000000
OPLS  328 329 330 331  -0.4989000 1.70390800 -0.44453000  1.753745000 0.00000000
OPLS  330 331 332 333  -0.4989000 1.70390800 -0.44453000  1.753745000 0.00000000
OPLS  332 333 334 335  -0.4989000 1.70390800 -0.44453000  1.753745000 0.00000000
OPLS  334 335 336 337  -0.4989000 1.70390800 -0.44453000  1.753745000 0.00000000
OPLS  336 337 338 339  -0.4989000 1.70390800 -0.44453000  1.753745000 0.00000000
OPLS  338 339 340 341  -0.4989000 1.70390800 -0.44453000  1.753745000 0.00000000
OPLS  340 341 342 343  -0.4989000 1.70390800 -0.44453000  1.753745000 0.00000000
OPLS  342 343 344 345  -0.4989000 1.70390800 -0.44453000  1.753745000 0.00000000
OPLS  344 345 346 347  -0.4989000 1.70390800 -0.44453000  1.753745000 0.00000000
OPLS  346 347 348 349  -0.4989000 1.70390800 -0.44453000  1.753745000 0.00000000
OPLS  348 349 350 351  0.0000000 1.41100000 -0.27100000  3.145000000 0.00000000
OPLS  101 102 352 353  -0.4989000 1.70390800 -0.44453000  1.753745000 0.00000000
OPLS  103 102 352 353  -0.4989000 1.70390800 -0.44453000  1.753745000 0.00000000
OPLS  102 352 353 354  0.0000000 1.41100000 -0.27100000  3.145000000 0.00000000
OPLS  352 353 354 355  -0.4989000 1.70390800 -0.44453000  1.753745000 0.00000000
OPLS  354 355 356 357  -0.4989000 1.70390800 -0.44453000  1.753745000 0.00000000
OPLS  356 357 358 359  -0.4989000 1.70390800 -0.44453000  1.753745000 0.00000000
OPLS  358 359 360 361  -0.4989000 1.70390800 -0.44453000  1.753745000 0.00000000
OPLS  360 361 362 363  -0.4989000 1.70390800 -0.44453000  1.753745000 0.00000000
OPLS  362 363 364 365  -0.4989000 1.70390800 -0.44453000  1.753745000 0.00000000
OPLS  364 365 366 367  -0.4989000 1.70390800 -0.44453000  1.753745000 0.00000000
OPLS  366 367 368 369  -0.4989000 1.70390800 -0.44453000  1.753745000 0.00000000
OPLS  368 369 370 371  -0.4989000 1.70390800 -0.44453000  1.753745000 0.00000000
```

```
OPLS  370 371 372 373  -0.4989000 1.70390800 -0.44453000  1.753745000 0.00000000
OPLS  372 373 374 375  -0.4989000 1.70390800 -0.44453000  1.753745000 0.00000000
OPLS  374 375 376 377  -0.4989000 1.70390800 -0.44453000  1.753745000 0.00000000
OPLS  376 377 378 379  -0.4989000 1.70390800 -0.44453000  1.753745000 0.00000000
OPLS  378 379 380 381  0.0000000 1.41100000 -0.27100000  3.145000000 0.00000000
OPLS  121 122 382 383  -0.4989000 1.70390800 -0.44453000  1.753745000 0.00000000
OPLS  123 122 382 383  -0.4989000 1.70390800 -0.44453000  1.753745000 0.00000000
OPLS  122 382 383 384  0.0000000 1.41100000 -0.27100000  3.145000000 0.00000000
OPLS  382 383 384 385  -0.4989000 1.70390800 -0.44453000  1.753745000 0.00000000
OPLS  384 385 386 387  -0.4989000 1.70390800 -0.44453000  1.753745000 0.00000000
OPLS  386 387 388 389  -0.4989000 1.70390800 -0.44453000  1.753745000 0.00000000
OPLS  388 389 390 391  -0.4989000 1.70390800 -0.44453000  1.753745000 0.00000000
OPLS  390 391 392 393  -0.4989000 1.70390800 -0.44453000  1.753745000 0.00000000
OPLS  392 393 394 395  -0.4989000 1.70390800 -0.44453000  1.753745000 0.00000000
OPLS  394 395 396 397  -0.4989000 1.70390800 -0.44453000  1.753745000 0.00000000
OPLS  396 397 398 399  -0.4989000 1.70390800 -0.44453000  1.753745000 0.00000000
OPLS  398 399 400 401  -0.4989000 1.70390800 -0.44453000  1.753745000 0.00000000
OPLS  400 401 402 403  -0.4989000 1.70390800 -0.44453000  1.753745000 0.00000000
OPLS  402 403 404 405  -0.4989000 1.70390800 -0.44453000  1.753745000 0.00000000
OPLS  404 405 406 407  -0.4989000 1.70390800 -0.44453000  1.753745000 0.00000000
OPLS  406 407 408 409  -0.4989000 1.70390800 -0.44453000  1.753745000 0.00000000
OPLS  408 409 410 411  0.0000000 1.41100000 -0.27100000  3.145000000 0.00000000
OPLS  141 142 412 413  -0.4989000 1.70390800 -0.44453000  1.753745000 0.00000000
OPLS  143 142 412 413  -0.4989000 1.70390800 -0.44453000  1.753745000 0.00000000
OPLS  142 412 413 414  0.0000000 1.41100000 -0.27100000  3.145000000 0.00000000
OPLS  412 413 414 415  -0.4989000 1.70390800 -0.44453000  1.753745000 0.00000000
OPLS  414 415 416 417  -0.4989000 1.70390800 -0.44453000  1.753745000 0.00000000
OPLS  416 417 418 419  -0.4989000 1.70390800 -0.44453000  1.753745000 0.00000000
OPLS  418 419 420 421  -0.4989000 1.70390800 -0.44453000  1.753745000 0.00000000
OPLS  420 421 422 423  -0.4989000 1.70390800 -0.44453000  1.753745000 0.00000000
OPLS  422 423 424 425  -0.4989000 1.70390800 -0.44453000  1.753745000 0.00000000
OPLS  424 425 426 427  -0.4989000 1.70390800 -0.44453000  1.753745000 0.00000000
OPLS  426 427 428 429  -0.4989000 1.70390800 -0.44453000  1.753745000 0.00000000
OPLS  428 429 430 431  -0.4989000 1.70390800 -0.44453000  1.753745000 0.00000000
OPLS  430 431 432 433  -0.4989000 1.70390800 -0.44453000  1.753745000 0.00000000
OPLS  432 433 434 435  -0.4989000 1.70390800 -0.44453000  1.753745000 0.00000000
OPLS  434 435 436 437  -0.4989000 1.70390800 -0.44453000  1.753745000 0.00000000
OPLS  436 437 438 439  -0.4989000 1.70390800 -0.44453000  1.753745000 0.00000000
OPLS  438 439 440 441  0.0000000 1.41100000 -0.27100000  3.145000000 0.00000000
OPLS  161 162 442 443  -0.4989000 1.70390800 -0.44453000  1.753745000 0.00000000
OPLS  163 162 442 443  -0.4989000 1.70390800 -0.44453000  1.753745000 0.00000000
OPLS  162 442 443 444  0.0000000 1.41100000 -0.27100000  3.145000000 0.00000000
OPLS  442 443 444 445  -0.4989000 1.70390800 -0.44453000  1.753745000 0.00000000
OPLS  444 445 446 447  -0.4989000 1.70390800 -0.44453000  1.753745000 0.00000000
OPLS  446 447 448 449  -0.4989000 1.70390800 -0.44453000  1.753745000 0.00000000
OPLS  448 449 450 451  -0.4989000 1.70390800 -0.44453000  1.753745000 0.00000000
OPLS  450 451 452 453  -0.4989000 1.70390800 -0.44453000  1.753745000 0.00000000
OPLS  452 453 454 455  -0.4989000 1.70390800 -0.44453000  1.753745000 0.00000000
OPLS  454 455 456 457  -0.4989000 1.70390800 -0.44453000  1.753745000 0.00000000
OPLS  456 457 458 459  -0.4989000 1.70390800 -0.44453000  1.753745000 0.00000000
OPLS  458 459 460 461  -0.4989000 1.70390800 -0.44453000  1.753745000 0.00000000
OPLS  460 461 462 463  -0.4989000 1.70390800 -0.44453000  1.753745000 0.00000000
OPLS  462 463 464 465  -0.4989000 1.70390800 -0.44453000  1.753745000 0.00000000
OPLS  464 465 466 467  -0.4989000 1.70390800 -0.44453000  1.753745000 0.00000000
OPLS  466 467 468 469  -0.4989000 1.70390800 -0.44453000  1.753745000 0.00000000
OPLS  468 469 470 471  0.0000000 1.41100000 -0.27100000  3.145000000 0.00000000
OPLS  181 182 472 473  -0.4989000 1.70390800 -0.44453000  1.753745000 0.00000000
OPLS  183 182 472 473  -0.4989000 1.70390800 -0.44453000  1.753745000 0.00000000
OPLS  182 472 473 474  0.0000000 1.41100000 -0.27100000  3.145000000 0.00000000
OPLS  472 473 474 475  -0.4989000 1.70390800 -0.44453000  1.753745000 0.00000000
OPLS  474 475 476 477  -0.4989000 1.70390800 -0.44453000  1.753745000 0.00000000
OPLS  476 477 478 479  -0.4989000 1.70390800 -0.44453000  1.753745000 0.00000000
OPLS  478 479 480 481  -0.4989000 1.70390800 -0.44453000  1.753745000 0.00000000
```

```
OPLS  480 481 482 483  -0.4989000 1.70390800 -0.44453000  1.753745000 0.00000000
OPLS  482 483 484 485  -0.4989000 1.70390800 -0.44453000  1.753745000 0.00000000
OPLS  484 485 486 487  -0.4989000 1.70390800 -0.44453000  1.753745000 0.00000000
OPLS  486 487 488 489  -0.4989000 1.70390800 -0.44453000  1.753745000 0.00000000
OPLS  488 489 490 491  -0.4989000 1.70390800 -0.44453000  1.753745000 0.00000000
OPLS  490 491 492 493  -0.4989000 1.70390800 -0.44453000  1.753745000 0.00000000
OPLS  492 493 494 495  -0.4989000 1.70390800 -0.44453000  1.753745000 0.00000000
OPLS  494 495 496 497  -0.4989000 1.70390800 -0.44453000  1.753745000 0.00000000
OPLS  496 497 498 499  -0.4989000 1.70390800 -0.44453000  1.753745000 0.00000000
OPLS  498 499 500 501  0.0000000 1.41100000 -0.27100000  3.145000000 0.00000000
finish
vdw 6
C3      C3      lj        0.1947      3.7500
C2      C3      lj        0.1334      3.8500
C1      C3      lj        0.0622      4.2150
C2      C2      lj        0.0914      3.9500
C1      C2      lj        0.0426      4.3150
C1      C1      lj        0.0199      4.6800
close
```

Polypropylene

One Chain – 50 Pseudo Atoms Long

```
Generated by DL_FIELD v2.00
Units kcal
Molecular types 1
Molecule name test
nummols 1
atoms  76
C3          15.03470     0.00000   1   0    1HEX
C1          13.01864     0.00000   1   0    1HEX
C3          15.03470     0.00000   1   0    1HEX
C2          14.02680     0.00000   1   0    1HEX
C1          13.01864     0.00000   1   0    1HEX
C3          15.03470     0.00000   1   0    1HEX
C2          14.02680     0.00000   1   0    1HEX
C1          13.01864     0.00000   1   0    1HEX
C3          15.03470     0.00000   1   0    1HEX
C2          14.02680     0.00000   1   0    1HEX
C1          13.01864     0.00000   1   0    1HEX
C3          15.03470     0.00000   1   0    1HEX
C2          14.02680     0.00000   1   0    1HEX
C1          13.01864     0.00000   1   0    1HEX
C3          15.03470     0.00000   1   0    1HEX
C2          14.02680     0.00000   1   0    1HEX
C1          13.01864     0.00000   1   0    1HEX
C3          15.03470     0.00000   1   0    1HEX
C2          14.02680     0.00000   1   0    1HEX
C1          13.01864     0.00000   1   0    1HEX
C3          15.03470     0.00000   1   0    1HEX
C2          14.02680     0.00000   1   0    1HEX
C1          13.01864     0.00000   1   0    1HEX
C3          15.03470     0.00000   1   0    1HEX
C2          14.02680     0.00000   1   0    1HEX
C1          13.01864     0.00000   1   0    1HEX
```

```
C3          15.03470     0.00000   1   0    1HEX
C2          14.02680     0.00000   1   0    1HEX
C1          13.01864     0.00000   1   0    1HEX
C3          15.03470     0.00000   1   0    1HEX
C2          14.02680     0.00000   1   0    1HEX
C1          13.01864     0.00000   1   0    1HEX
C3          15.03470     0.00000   1   0    1HEX
C2          14.02680     0.00000   1   0    1HEX
C1          13.01864     0.00000   1   0    1HEX
C3          15.03470     0.00000   1   0    1HEX
C2          14.02680     0.00000   1   0    1HEX
C1          13.01864     0.00000   1   0    1HEX
C3          15.03470     0.00000   1   0    1HEX
C2          14.02680     0.00000   1   0    1HEX
C1          13.01864     0.00000   1   0    1HEX
C3          15.03470     0.00000   1   0    1HEX
C2          14.02680     0.00000   1   0    1HEX
C1          13.01864     0.00000   1   0    1HEX
C3          15.03470     0.00000   1   0    1HEX
C2          14.02680     0.00000   1   0    1HEX
C1          13.01864     0.00000   1   0    1HEX
C3          15.03470     0.00000   1   0    1HEX
C2          14.02680     0.00000   1   0    1HEX
C1          13.01864     0.00000   1   0    1HEX
C3          15.03470     0.00000   1   0    1HEX
C2          14.02680     0.00000   1   0    1HEX
C1          13.01864     0.00000   1   0    1HEX
C3          15.03470     0.00000   1   0    1HEX
C2          14.02680     0.00000   1   0    1HEX
C1          13.01864     0.00000   1   0    1HEX
C3          15.03470     0.00000   1   0    1HEX
C2          14.02680     0.00000   1   0    1HEX
C1          13.01864     0.00000   1   0    1HEX
C3          15.03470     0.00000   1   0    1HEX
C2          14.02680     0.00000   1   0    1HEX
C1          13.01864     0.00000   1   0    1HEX
C3          15.03470     0.00000   1   0    1HEX
C2          14.02680     0.00000   1   0    1HEX
C1          13.01864     0.00000   1   0    1HEX
C3          15.03470     0.00000   1   0    1HEX
C2          14.02680     0.00000   1   0    1HEX
C1          13.01864     0.00000   1   0    1HEX
C3          15.03470     0.00000   1   0    1HEX
C2          14.02680     0.00000   1   0    1HEX
C1          13.01864     0.00000   1   0    1HEX
C3          15.03470     0.00000   1   0    1HEX
C2          14.02680     0.00000   1   0    1HEX
C1          13.01864     0.00000   1   0    1HEX
C3          15.03470     0.00000   1   0    1HEX
C3          15.03470     0.00000   1   0    1HEX
CONSTRAINTS     75
    1   2  1.54000000
    2   3  1.54000000
    2   4  1.54000000
    4   5  1.54000000
    5   6  1.54000000
    5   7  1.54000000
    7   8  1.54000000
    8   9  1.54000000
    8   10  1.54000000
    10   11  1.54000000
    11   12  1.54000000
    11   13  1.54000000
```

13	14	1.54000000
14	15	1.54000000
14	16	1.54000000
16	17	1.54000000
17	18	1.54000000
17	19	1.54000000
19	20	1.54000000
20	21	1.54000000
20	22	1.54000000
22	23	1.54000000
23	24	1.54000000
23	25	1.54000000
25	26	1.54000000
26	27	1.54000000
26	28	1.54000000
28	29	1.54000000
29	30	1.54000000
29	31	1.54000000
31	32	1.54000000
32	33	1.54000000
32	34	1.54000000
34	35	1.54000000
35	36	1.54000000
35	37	1.54000000
37	38	1.54000000
38	39	1.54000000
38	40	1.54000000
40	41	1.54000000
41	42	1.54000000
41	43	1.54000000
43	44	1.54000000
44	45	1.54000000
44	46	1.54000000
46	47	1.54000000
47	48	1.54000000
47	49	1.54000000
49	50	1.54000000
50	51	1.54000000
50	52	1.54000000
52	53	1.54000000
53	54	1.54000000
53	55	1.54000000
55	56	1.54000000
56	57	1.54000000
56	58	1.54000000
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59	60	1.54000000
59	61	1.54000000
61	62	1.54000000
62	63	1.54000000
62	64	1.54000000
64	65	1.54000000
65	66	1.54000000
65	67	1.54000000
67	68	1.54000000
68	69	1.54000000
68	70	1.54000000
70	71	1.54000000
71	72	1.54000000
71	73	1.54000000
73	74	1.54000000
74	75	1.54000000
74	76	1.54000000

```
angles  99
harm      1     2     3   124.19700   112.00000
harm      1     2     4   124.19700   112.00000
harm      3     2     4   124.19700   112.00000
harm      2     4     5   124.19700   114.00000
harm      4     5     6   124.19700   112.00000
harm      4     5     7   124.19700   112.00000
harm      6     5     7   124.19700   112.00000
harm      5     7     8   124.19700   114.00000
harm      7     8     9   124.19700   112.00000
harm      7     8    10   124.19700   112.00000
harm      9     8    10   124.19700   112.00000
harm      8    10    11   124.19700   114.00000
harm     10    11    12   124.19700   112.00000
harm     10    11    13   124.19700   112.00000
harm     12    11    13   124.19700   112.00000
harm     11    13    14   124.19700   114.00000
harm     13    14    15   124.19700   112.00000
harm     13    14    16   124.19700   112.00000
harm     15    14    16   124.19700   112.00000
harm     14    16    17   124.19700   114.00000
harm     16    17    18   124.19700   112.00000
harm     16    17    19   124.19700   112.00000
harm     18    17    19   124.19700   112.00000
harm     17    19    20   124.19700   114.00000
harm     19    20    21   124.19700   112.00000
harm     19    20    22   124.19700   112.00000
harm     21    20    22   124.19700   112.00000
harm     20    22    23   124.19700   114.00000
harm     22    23    24   124.19700   112.00000
harm     22    23    25   124.19700   112.00000
harm     24    23    25   124.19700   112.00000
harm     23    25    26   124.19700   114.00000
harm     25    26    27   124.19700   112.00000
harm     25    26    28   124.19700   112.00000
harm     27    26    28   124.19700   112.00000
harm     26    28    29   124.19700   114.00000
harm     28    29    30   124.19700   112.00000
harm     28    29    31   124.19700   112.00000
harm     30    29    31   124.19700   112.00000
harm     29    31    32   124.19700   114.00000
harm     31    32    33   124.19700   112.00000
harm     31    32    34   124.19700   112.00000
harm     33    32    34   124.19700   112.00000
harm     32    34    35   124.19700   114.00000
harm     34    35    36   124.19700   112.00000
harm     34    35    37   124.19700   112.00000
harm     36    35    37   124.19700   112.00000
harm     35    37    38   124.19700   114.00000
harm     37    38    39   124.19700   112.00000
harm     37    38    40   124.19700   112.00000
harm     39    38    40   124.19700   112.00000
harm     38    40    41   124.19700   114.00000
harm     40    41    42   124.19700   112.00000
harm     40    41    43   124.19700   112.00000
harm     42    41    43   124.19700   112.00000
harm     41    43    44   124.19700   114.00000
harm     43    44    45   124.19700   112.00000
harm     43    44    46   124.19700   112.00000
harm     45    44    46   124.19700   112.00000
harm     44    46    47   124.19700   114.00000
harm     46    47    48   124.19700   112.00000
harm     46    47    49   124.19700   112.00000
```

```
harm      48     47     49   124.19700   112.00000
harm      47     49     50   124.19700   114.00000
harm      49     50     51   124.19700   112.00000
harm      49     50     52   124.19700   112.00000
harm      51     50     52   124.19700   112.00000
harm      50     52     53   124.19700   114.00000
harm      52     53     54   124.19700   112.00000
harm      52     53     55   124.19700   112.00000
harm      54     53     55   124.19700   112.00000
harm      53     55     56   124.19700   114.00000
harm      55     56     57   124.19700   112.00000
harm      55     56     58   124.19700   112.00000
harm      57     56     58   124.19700   112.00000
harm      56     58     59   124.19700   114.00000
harm      58     59     60   124.19700   112.00000
harm      58     59     61   124.19700   112.00000
harm      60     59     61   124.19700   112.00000
harm      59     61     62   124.19700   114.00000
harm      61     62     63   124.19700   112.00000
harm      61     62     64   124.19700   112.00000
harm      63     62     64   124.19700   112.00000
harm      62     64     65   124.19700   114.00000
harm      64     65     66   124.19700   112.00000
harm      64     65     67   124.19700   112.00000
harm      66     65     67   124.19700   112.00000
harm      65     67     68   124.19700   114.00000
harm      67     68     69   124.19700   112.00000
harm      67     68     70   124.19700   112.00000
harm      69     68     70   124.19700   112.00000
harm      68     70     71   124.19700   114.00000
harm      70     71     72   124.19700   112.00000
harm      70     71     73   124.19700   112.00000
harm      72     71     73   124.19700   112.00000
harm      71     73     74   124.19700   114.00000
harm      73     74     75   124.19700   112.00000
harm      73     74     76   124.19700   112.00000
harm      75     74     76   124.19700   112.00000
dihedral  96
OPLS  1 2 4 5  -0.4989000 1.70390800 -0.44453000  1.753745000 0.00000000
OPLS  2 4 5 7  -0.4989000 1.70390800 -0.44453000  1.753745000 0.00000000
OPLS  4 5 7 8  -0.4989000 1.70390800 -0.44453000  1.753745000 0.00000000
OPLS  5 7 8 10  -0.4989000 1.70390800 -0.44453000  1.753745000 0.00000000
OPLS  7 8 10 11  -0.4989000 1.70390800 -0.44453000  1.753745000 0.00000000
OPLS  8 10 11 13  -0.4989000 1.70390800 -0.44453000  1.753745000 0.00000000
OPLS  10 11 13 14  -0.4989000 1.70390800 -0.44453000  1.753745000 0.00000000
OPLS  11 13 14 16  -0.4989000 1.70390800 -0.44453000  1.753745000 0.00000000
OPLS  13 14 16 17  -0.4989000 1.70390800 -0.44453000  1.753745000 0.00000000
OPLS  14 16 17 19  -0.4989000 1.70390800 -0.44453000  1.753745000 0.00000000
OPLS  16 17 19 20  -0.4989000 1.70390800 -0.44453000  1.753745000 0.00000000
OPLS  17 19 20 22  -0.4989000 1.70390800 -0.44453000  1.753745000 0.00000000
OPLS  19 20 22 23  -0.4989000 1.70390800 -0.44453000  1.753745000 0.00000000
OPLS  20 22 23 25  -0.4989000 1.70390800 -0.44453000  1.753745000 0.00000000
OPLS  22 23 25 26  -0.4989000 1.70390800 -0.44453000  1.753745000 0.00000000
OPLS  23 25 26 28  -0.4989000 1.70390800 -0.44453000  1.753745000 0.00000000
OPLS  25 26 28 29  -0.4989000 1.70390800 -0.44453000  1.753745000 0.00000000
OPLS  26 28 29 31  -0.4989000 1.70390800 -0.44453000  1.753745000 0.00000000
OPLS  28 29 31 32  -0.4989000 1.70390800 -0.44453000  1.753745000 0.00000000
OPLS  29 31 32 34  -0.4989000 1.70390800 -0.44453000  1.753745000 0.00000000
OPLS  31 32 34 35  -0.4989000 1.70390800 -0.44453000  1.753745000 0.00000000
OPLS  32 34 35 37  -0.4989000 1.70390800 -0.44453000  1.753745000 0.00000000
OPLS  34 35 37 38  -0.4989000 1.70390800 -0.44453000  1.753745000 0.00000000
OPLS  35 37 38 40  -0.4989000 1.70390800 -0.44453000  1.753745000 0.00000000
OPLS  37 38 40 41  -0.4989000 1.70390800 -0.44453000  1.753745000 0.00000000
```

```
OPLS   38 40 41 43  -0.4989000 1.70390800 -0.44453000  1.753745000 0.00000000
OPLS   40 41 43 44  -0.4989000 1.70390800 -0.44453000  1.753745000 0.00000000
OPLS   41 43 44 46  -0.4989000 1.70390800 -0.44453000  1.753745000 0.00000000
OPLS   43 44 46 47  -0.4989000 1.70390800 -0.44453000  1.753745000 0.00000000
OPLS   44 46 47 49  -0.4989000 1.70390800 -0.44453000  1.753745000 0.00000000
OPLS   46 47 49 50  -0.4989000 1.70390800 -0.44453000  1.753745000 0.00000000
OPLS   47 49 50 52  -0.4989000 1.70390800 -0.44453000  1.753745000 0.00000000
OPLS   49 50 52 53  -0.4989000 1.70390800 -0.44453000  1.753745000 0.00000000
OPLS   50 52 53 55  -0.4989000 1.70390800 -0.44453000  1.753745000 0.00000000
OPLS   52 53 55 56  -0.4989000 1.70390800 -0.44453000  1.753745000 0.00000000
OPLS   53 55 56 58  -0.4989000 1.70390800 -0.44453000  1.753745000 0.00000000
OPLS   55 56 58 59  -0.4989000 1.70390800 -0.44453000  1.753745000 0.00000000
OPLS   56 58 59 61  -0.4989000 1.70390800 -0.44453000  1.753745000 0.00000000
OPLS   58 59 61 62  -0.4989000 1.70390800 -0.44453000  1.753745000 0.00000000
OPLS   59 61 62 64  -0.4989000 1.70390800 -0.44453000  1.753745000 0.00000000
OPLS   61 62 64 65  -0.4989000 1.70390800 -0.44453000  1.753745000 0.00000000
OPLS   62 64 65 67  -0.4989000 1.70390800 -0.44453000  1.753745000 0.00000000
OPLS   64 65 67 68  -0.4989000 1.70390800 -0.44453000  1.753745000 0.00000000
OPLS   65 67 68 70  -0.4989000 1.70390800 -0.44453000  1.753745000 0.00000000
OPLS   67 68 70 71  -0.4989000 1.70390800 -0.44453000  1.753745000 0.00000000
OPLS   68 70 71 73  -0.4989000 1.70390800 -0.44453000  1.753745000 0.00000000
OPLS   70 71 73 74  -0.4989000 1.70390800 -0.44453000  1.753745000 0.00000000
OPLS   71 73 74 76  -0.4989000 1.70390800 -0.44453000  1.753745000 0.00000000
OPLS   3 2 4 5  -0.4989000 1.70390800 -0.44453000  1.753745000 0.00000000
OPLS   6 5 4 2  -0.4989000 1.70390800 -0.44453000  1.753745000 0.00000000
OPLS   6 5 7 8  -0.4989000 1.70390800 -0.44453000  1.753745000 0.00000000
OPLS   9 8 7 5  -0.4989000 1.70390800 -0.44453000  1.753745000 0.00000000
OPLS   9 8 10 11  -0.4989000 1.70390800 -0.44453000  1.753745000 0.00000000
OPLS   12 11 10 8  -0.4989000 1.70390800 -0.44453000  1.753745000 0.00000000
OPLS   12 11 13 14  -0.4989000 1.70390800 -0.44453000  1.753745000 0.00000000
OPLS   15 14 13 11  -0.4989000 1.70390800 -0.44453000  1.753745000 0.00000000
OPLS   15 14 16 17  -0.4989000 1.70390800 -0.44453000  1.753745000 0.00000000
OPLS   18 17 16 14  -0.4989000 1.70390800 -0.44453000  1.753745000 0.00000000
OPLS   18 17 19 20  -0.4989000 1.70390800 -0.44453000  1.753745000 0.00000000
OPLS   21 20 19 17  -0.4989000 1.70390800 -0.44453000  1.753745000 0.00000000
OPLS   21 20 22 23  -0.4989000 1.70390800 -0.44453000  1.753745000 0.00000000
OPLS   24 23 22 20  -0.4989000 1.70390800 -0.44453000  1.753745000 0.00000000
OPLS   24 23 25 26  -0.4989000 1.70390800 -0.44453000  1.753745000 0.00000000
OPLS   27 26 25 23  -0.4989000 1.70390800 -0.44453000  1.753745000 0.00000000
OPLS   27 26 28 29  -0.4989000 1.70390800 -0.44453000  1.753745000 0.00000000
OPLS   30 29 28 26  -0.4989000 1.70390800 -0.44453000  1.753745000 0.00000000
OPLS   30 29 31 32  -0.4989000 1.70390800 -0.44453000  1.753745000 0.00000000
OPLS   33 32 31 29  -0.4989000 1.70390800 -0.44453000  1.753745000 0.00000000
OPLS   33 32 34 35  -0.4989000 1.70390800 -0.44453000  1.753745000 0.00000000
OPLS   36 35 34 32  -0.4989000 1.70390800 -0.44453000  1.753745000 0.00000000
OPLS   36 35 37 38  -0.4989000 1.70390800 -0.44453000  1.753745000 0.00000000
OPLS   39 38 37 35  -0.4989000 1.70390800 -0.44453000  1.753745000 0.00000000
OPLS   39 38 40 41  -0.4989000 1.70390800 -0.44453000  1.753745000 0.00000000
OPLS   42 41 40 38  -0.4989000 1.70390800 -0.44453000  1.753745000 0.00000000
OPLS   42 41 43 44  -0.4989000 1.70390800 -0.44453000  1.753745000 0.00000000
OPLS   45 44 43 41  -0.4989000 1.70390800 -0.44453000  1.753745000 0.00000000
OPLS   45 44 46 47  -0.4989000 1.70390800 -0.44453000  1.753745000 0.00000000
OPLS   48 47 46 44  -0.4989000 1.70390800 -0.44453000  1.753745000 0.00000000
OPLS   48 47 49 50  -0.4989000 1.70390800 -0.44453000  1.753745000 0.00000000
OPLS   51 50 49 47  -0.4989000 1.70390800 -0.44453000  1.753745000 0.00000000
OPLS   51 50 52 53  -0.4989000 1.70390800 -0.44453000  1.753745000 0.00000000
OPLS   54 53 52 50  -0.4989000 1.70390800 -0.44453000  1.753745000 0.00000000
OPLS   54 53 55 56  -0.4989000 1.70390800 -0.44453000  1.753745000 0.00000000
OPLS   57 56 55 53  -0.4989000 1.70390800 -0.44453000  1.753745000 0.00000000
OPLS   57 56 58 59  -0.4989000 1.70390800 -0.44453000  1.753745000 0.00000000
OPLS   60 59 58 56  -0.4989000 1.70390800 -0.44453000  1.753745000 0.00000000
OPLS   60 59 61 62  -0.4989000 1.70390800 -0.44453000  1.753745000 0.00000000
OPLS   63 62 61 59  -0.4989000 1.70390800 -0.44453000  1.753745000 0.00000000
```

```
OPLS  63 62 64 65  -0.4989000 1.70390800 -0.44453000  1.753745000 0.00000000
OPLS  66 65 64 62  -0.4989000 1.70390800 -0.44453000  1.753745000 0.00000000
OPLS  66 65 67 68  -0.4989000 1.70390800 -0.44453000  1.753745000 0.00000000
OPLS  69 68 67 65  -0.4989000 1.70390800 -0.44453000  1.753745000 0.00000000
OPLS  69 68 70 71  -0.4989000 1.70390800 -0.44453000  1.753745000 0.00000000
OPLS  72 71 70 68  -0.4989000 1.70390800 -0.44453000  1.753745000 0.00000000
OPLS  72 71 73 74  -0.4989000 1.70390800 -0.44453000  1.753745000 0.00000000
OPLS  75 74 73 71  -0.4989000 1.70390800 -0.44453000  1.753745000 0.00000000
finish
vdw 6
C3      C3      lj        0.1947      3.7500
C2      C3      lj        0.1334      3.8500
C1      C3      lj        0.0622      4.2150
C2      C2      lj        0.0914      3.9500
C1      C2      lj        0.0426      4.3150
C1      C1      lj        0.0199      4.6800
close
```

CONFIG Files

High Density Polyethylene

One Chain – 20 Pseudo Atoms Long

```
calc
         0         0
C3
          -1.920000             0.000000             0.422000
C2
          -0.641000             0.000000            -0.422000
C2
           0.641000             0.000000             0.422000
C2
           1.920000             0.000000            -0.422000
C2
           3.202000             0.000000             0.422000
C2
           4.481000             0.000000            -0.422000
C2
           5.763000             0.000000             0.422000
C2
           7.042000             0.000000            -0.422000
C2
           8.324000             0.000000             0.422000
C2
           9.603000             0.000000            -0.422000
C2
          10.885000             0.000000             0.422000
C2
          12.164000             0.000000            -0.422000
C2
          13.446000             0.000000             0.422000
C2
          14.725000             0.000000            -0.422000
C2
          16.007000             0.000000             0.422000
C2
          17.286000             0.000000            -0.422000
C2
          18.568000             0.000000             0.422000
C2
          19.847000             0.000000            -0.422000
C2
          21.129000             0.000000             0.422000
C3
          22.408000             0.000000            -0.422000
```

Four Chains – 20 Pseudo Atoms Long

```
calc
         0         0
C3
          -1.920000             0.000000             0.422000
C2
```

	-0.641000	0.000000	-0.422000
C2			
	0.641000	0.000000	0.422000
C2			
	1.920000	0.000000	-0.422000
C2			
	3.202000	0.000000	0.422000
C2			
	4.481000	0.000000	-0.422000
C2			
	5.763000	0.000000	0.422000
C2			
	7.042000	0.000000	-0.422000
C2			
	8.324000	0.000000	0.422000
C2			
	9.603000	0.000000	-0.422000
C2			
	10.885000	0.000000	0.422000
C2			
	12.164000	0.000000	-0.422000
C2			
	13.446000	0.000000	0.422000
C2			
	14.725000	0.000000	-0.422000
C2			
	16.007000	0.000000	0.422000
C2			
	17.286000	0.000000	-0.422000
C2			
	18.568000	0.000000	0.422000
C2			
	19.847000	0.000000	-0.422000
C2			
	21.129000	0.000000	0.422000
C3			
	22.408000	0.000000	-0.422000
C3			
	-1.920000	5.000000	0.422000
C2			
	-0.641000	5.000000	-0.422000
C2			
	0.641000	5.000000	0.422000
C2			
	1.920000	5.000000	-0.422000
C2			
	3.202000	5.000000	0.422000
C2			
	4.481000	5.000000	-0.422000
C2			
	5.763000	5.000000	0.422000
C2			
	7.042000	5.000000	-0.422000
C2			
	8.324000	5.000000	0.422000
C2			
	9.603000	5.000000	-0.422000
C2			
	10.885000	5.000000	0.422000
C2			
	12.164000	5.000000	-0.422000
C2			
	13.446000	5.000000	0.422000

C2	14.725000	5.000000	-0.422000
C2	16.007000	5.000000	0.422000
C2	17.286000	5.000000	-0.422000
C2	18.568000	5.000000	0.422000
C2	19.847000	5.000000	-0.422000
C2	21.129000	5.000000	0.422000
C3	22.408000	5.000000	-0.422000
C3	-1.920000	10.000000	0.422000
C2	-0.641000	10.000000	-0.422000
C2	0.641000	10.000000	0.422000
C2	1.920000	10.000000	-0.422000
C2	3.202000	10.000000	0.422000
C2	4.481000	10.000000	-0.422000
C2	5.763000	10.000000	0.422000
C2	7.042000	10.000000	-0.422000
C2	8.324000	10.000000	0.422000
C2	9.603000	10.000000	-0.422000
C2	10.885000	10.000000	0.422000
C2	12.164000	10.000000	-0.422000
C2	13.446000	10.000000	0.422000
C2	14.725000	10.000000	-0.422000
C2	16.007000	10.000000	0.422000
C2	17.286000	10.000000	-0.422000
C2	18.568000	10.000000	0.422000
C2	19.847000	10.000000	-0.422000
C2	21.129000	10.000000	0.422000
C3	22.408000	10.000000	-0.422000
C3	-1.920000	15.000000	0.422000
C2	-0.641000	15.000000	-0.422000
C2	0.641000	15.000000	0.422000
C2	1.920000	15.000000	-0.422000
C2			

```
            3.202000            15.000000             0.422000
C2
            4.481000            15.000000            -0.422000
C2
            5.763000            15.000000             0.422000
C2
            7.042000            15.000000            -0.422000
C2
            8.324000            15.000000             0.422000
C2
            9.603000            15.000000            -0.422000
C2
           10.885000            15.000000             0.422000
C2
           12.164000            15.000000            -0.422000
C2
           13.446000            15.000000             0.422000
C2
           14.725000            15.000000            -0.422000
C2
           16.007000            15.000000             0.422000
C2
           17.286000            15.000000            -0.422000
C2
           18.568000            15.000000             0.422000
C2
           19.847000            15.000000            -0.422000
C2
           21.129000            15.000000             0.422000
C3
           22.408000            15.000000            -0.422000
```

Low Density Polyethylene (LDPE)

One Chain – 200 Pseudo Atoms Long

```
calc
          0         0
C3
           -1.920000             0.000000             0.422000
C1
           -0.641000             0.000000            -0.422000
C2
            0.641000             0.000000             0.422000
C2
            1.920000             0.000000            -0.422000
C2
            3.202000             0.000000             0.422000
C2
            4.481000             0.000000            -0.422000
C2
            5.763000             0.000000             0.422000
C2
            7.042000             0.000000            -0.422000
C2
            8.324000             0.000000             0.422000
C2
```

	9.603000	0.000000	-0.422000
C2			
	10.885000	0.000000	0.422000
C2			
	12.164000	0.000000	-0.422000
C2			
	13.446000	0.000000	0.422000
C2			
	14.725000	0.000000	-0.422000
C2			
	16.007000	0.000000	0.422000
C2			
	17.286000	0.000000	-0.422000
C2			
	18.568000	0.000000	0.422000
C2			
	19.847000	0.000000	-0.422000
C2			
	21.129000	0.000000	0.422000
C2			
	22.408000	0.000000	-0.422000
C2			
	23.690000	0.000000	0.422000
C1			
	24.969000	0.000000	-0.422000
C2			
	26.251000	0.000000	0.422000
C2			
	27.530000	0.000000	-0.422000
C2			
	28.812000	0.000000	0.422000
C2			
	30.091000	0.000000	-0.422000
C2			
	31.373000	0.000000	0.422000
C2			
	32.652000	0.000000	-0.422000
C2			
	33.934000	0.000000	0.422000
C2			
	35.213000	0.000000	-0.422000
C2			
	36.495000	0.000000	0.422000
C2			
	37.774000	0.000000	-0.422000
C2			
	39.056000	0.000000	0.422000
C2			
	40.335000	0.000000	-0.422000
C2			
	41.617000	0.000000	0.422000
C2			
	42.896000	0.000000	-0.422000
C2			
	44.178000	0.000000	0.422000
C2			
	45.457000	0.000000	-0.422000
C2			
	46.739000	0.000000	0.422000
C2			
	48.018000	0.000000	-0.422000
C2			
	49.300000	0.000000	0.422000

C1	50.579000	0.000000	-0.422000
C2	51.861000	0.000000	0.422000
C2	53.140000	0.000000	-0.422000
C2	54.422000	0.000000	0.422000
C2	55.701000	0.000000	-0.422000
C2	56.983000	0.000000	0.422000
C2	58.262000	0.000000	-0.422000
C2	59.544000	0.000000	0.422000
C2	60.823000	0.000000	-0.422000
C2	62.105000	0.000000	0.422000
C2	63.384000	0.000000	-0.422000
C2	64.666000	0.000000	0.422000
C2	65.945000	0.000000	-0.422000
C2	67.227000	0.000000	0.422000
C2	68.506000	0.000000	-0.422000
C2	69.788000	0.000000	0.422000
C2	71.067000	0.000000	-0.422000
C2	72.349000	0.000000	0.422000
C2	73.628000	0.000000	-0.422000
C2	74.910000	0.000000	0.422000
C1	76.189000	0.000000	-0.422000
C2	77.471000	0.000000	0.422000
C2	78.750000	0.000000	-0.422000
C2	80.032000	0.000000	0.422000
C2	81.311000	0.000000	-0.422000
C2	82.593000	0.000000	0.422000
C2	83.872000	0.000000	-0.422000
C2	85.154000	0.000000	0.422000
C2	86.433000	0.000000	-0.422000
C2	87.715000	0.000000	0.422000
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	213.856523	0.000000	-19.888642
C2			
	215.135523	0.000000	-20.732642
C2			
	215.067248	0.000000	-22.145380
C2			
	216.346248	0.000000	-22.989380
C2			
	216.277973	0.000000	-24.402118
C2			
	217.556973	0.000000	-25.246118
C2			
	217.488698	0.000000	-26.658856
C2			
	218.767698	0.000000	-27.502856
C2			
	218.699422	0.000000	-28.915594
C2			
	219.978422	0.000000	-29.759594
C2			
	219.910147	0.000000	-31.172332
C2			
	221.189147	0.000000	-32.016332
C2			
	221.120872	0.000000	-33.429070
C3			
	222.399872	0.000000	-34.273070
C2			
	229.780725	0.000000	-1.834738
C2			
	231.059725	0.000000	-2.678738
C2			
	230.991450	0.000000	-4.091476
C2			
	232.270450	0.000000	-4.935476
C2			
	232.202174	0.000000	-6.348214
C2			
	233.481174	0.000000	-7.192214
C2			
	233.412899	0.000000	-8.604952
C2			
	234.691899	0.000000	-9.448952
C2			
	234.623624	0.000000	-10.861690
C2			
	235.902624	0.000000	-11.705690
C2			
	235.834349	0.000000	-13.118428

```
C2
        237.113349              0.000000          -13.962428
C2
        237.045074              0.000000          -15.375166
C2
        238.324074              0.000000          -16.219166
C2
        238.255798              0.000000          -17.631904
C2
        239.534798              0.000000          -18.475904
C2
        239.466523              0.000000          -19.888642
C2
        240.745523              0.000000          -20.732642
C2
        240.677248              0.000000          -22.145380
C2
        241.956248              0.000000          -22.989380
C2
        241.887973              0.000000          -24.402118
C2
        243.166973              0.000000          -25.246118
C2
        243.098698              0.000000          -26.658856
C2
        244.377698              0.000000          -27.502856
C2
        244.309422              0.000000          -28.915594
C2
        245.588422              0.000000          -29.759594
C2
        245.520147              0.000000          -31.172332
C2
        246.799147              0.000000          -32.016332
C2
        246.730872              0.000000          -33.429070
C3
        248.009872              0.000000          -34.273070
```

Polypropylene

One Chain – 50 Pseudo Atoms Long

```
calc
        0         0
C3
         -1.920000              0.000000            0.422000
C1
         -0.641000              0.000000           -0.422000
C3
         -0.641000              0.000000           -1.962000
C2
          0.641000              0.000000            0.422000
C1
          1.920000              0.000000           -0.422000
C3
          1.920000              0.000000           -1.962000
C2
```

	3.202000	0.000000	0.422000
C1			
	4.481000	0.000000	-0.422000
C3			
	4.481000	0.000000	-1.962000
C2			
	5.763000	0.000000	0.422000
C1			
	7.042000	0.000000	-0.422000
C3			
	7.042000	0.000000	-1.962000
C2			
	8.324000	0.000000	0.422000
C1			
	9.603000	0.000000	-0.422000
C3			
	9.603000	0.000000	-1.962000
C2			
	10.885000	0.000000	0.422000
C1			
	12.164000	0.000000	-0.422000
C3			
	12.164000	0.000000	-1.962000
C2			
	13.446000	0.000000	0.422000
C1			
	14.725000	0.000000	-0.422000
C3			
	14.725000	0.000000	-1.962000
C2			
	16.007000	0.000000	0.422000
C1			
	17.286000	0.000000	-0.422000
C3			
	17.286000	0.000000	-1.962000
C2			
	18.568000	0.000000	0.422000
C1			
	19.847000	0.000000	-0.422000
C3			
	19.847000	0.000000	-1.962000
C2			
	21.129000	0.000000	0.422000
C1			
	22.408000	0.000000	-0.422000
C3			
	22.408000	0.000000	-1.962000
C2			
	23.690000	0.000000	0.422000
C1			
	24.969000	0.000000	-0.422000
C3			
	24.969000	0.000000	-1.962000
C2			
	26.251000	0.000000	0.422000
C1			
	27.530000	0.000000	-0.422000
C3			
	27.530000	0.000000	-1.962000
C2			
	28.812000	0.000000	0.422000
C1			
	30.091000	0.000000	-0.422000

C3			
	30.091000	0.000000	-1.962000
C2			
	31.373000	0.000000	0.422000
C1			
	32.652000	0.000000	-0.422000
C3			
	32.652000	0.000000	-1.962000
C2			
	33.934000	0.000000	0.422000
C1			
	35.213000	0.000000	-0.422000
C3			
	35.213000	0.000000	-1.962000
C2			
	36.495000	0.000000	0.422000
C1			
	37.774000	0.000000	-0.422000
C3			
	37.774000	0.000000	-1.962000
C2			
	39.056000	0.000000	0.422000
C1			
	40.335000	0.000000	-0.422000
C3			
	40.335000	0.000000	-1.962000
C2			
	41.617000	0.000000	0.422000
C1			
	42.896000	0.000000	-0.422000
C3			
	42.896000	0.000000	-1.962000
C2			
	44.178000	0.000000	0.422000
C1			
	45.457000	0.000000	-0.422000
C3			
	45.457000	0.000000	-1.962000
C2			
	46.739000	0.000000	0.422000
C1			
	48.018000	0.000000	-0.422000
C3			
	48.018000	0.000000	-1.962000
C2			
	49.300000	0.000000	0.422000
C1			
	50.579000	0.000000	-0.422000
C3			
	50.579000	0.000000	-1.962000
C2			
	51.861000	0.000000	0.422000
C1			
	53.140000	0.000000	-0.422000
C3			
	53.140000	0.000000	-1.962000
C2			
	54.422000	0.000000	0.422000
C1			
	55.701000	0.000000	-0.422000
C3			
	55.701000	0.000000	-1.962000
C2			

	56.983000	0.000000	0.422000
C1			
	58.262000	0.000000	-0.422000
C3			
	58.262000	0.000000	-1.962000
C2			
	59.544000	0.000000	0.422000
C1			
	60.823000	0.000000	-0.422000
C3			
	60.823000	0.000000	-1.962000
C3			
	62.105000	0.000000	0.422000