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Study the Modelling and Process of PE Polymers

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ABSTRACT

The concept of Modeling and process of Polymers contribute a lot towards the streams of polymer science and engineering community. These inventions help in precise study of the fields like dynamics, thermodynamics, microscopic and macroscopic materialistic properties. The study of such processes should be handled out with proper care and all the precautions must be taken. The best practice methods, analysis of polymers, choice of polymer, best quality of polymer should be taken under consideration. With the growth of technology in computer sciences the pp polymers can be systematically simulated to meet the demands of in-vitro materials with ease. Now days, companies and people associated with polymer simulation are educated by letting them know and understand different methods to improve validity, usefulness and impact of polymers.

Introduction

PE polymers exhibit a complex structure and unique phenomena which cover large areas like monomers, radius of gyration and many times related phenomena which can exist from few seconds to even many years(Pruitt, 2011). Many phenomena of PE polymerization have been cracked but there are still some fields which require more study. With the advent of technology, simulations can be performed easily even on a device like smartphone. With all such inventions we can say that simulation of polymers is at fingertips, and it will provide us more detailed study of PP polymers(Ding et al., 2001).

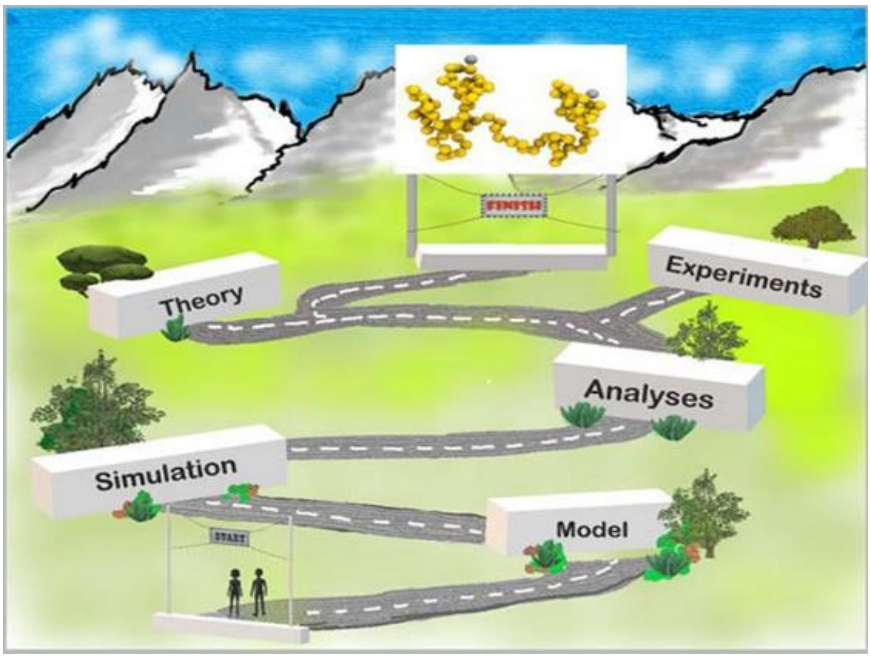

Figure 1: Image Briefing the process of modelling and simulation of polymers.

In-vitro experiments are considered the best experiments to perform such experiments. These experiments further inspire other novel experiments for simulating polymers. Sometimes it is difficult to differentiate between realistic and unrealistic result of simulation, therefor it is important to take proper care while carrying out such operations(McKeen, 2010). To correctly differentiate between the realistic and unrealistic result scientists must choose between the correct models of simulating polymers.

Experimental Evaluation

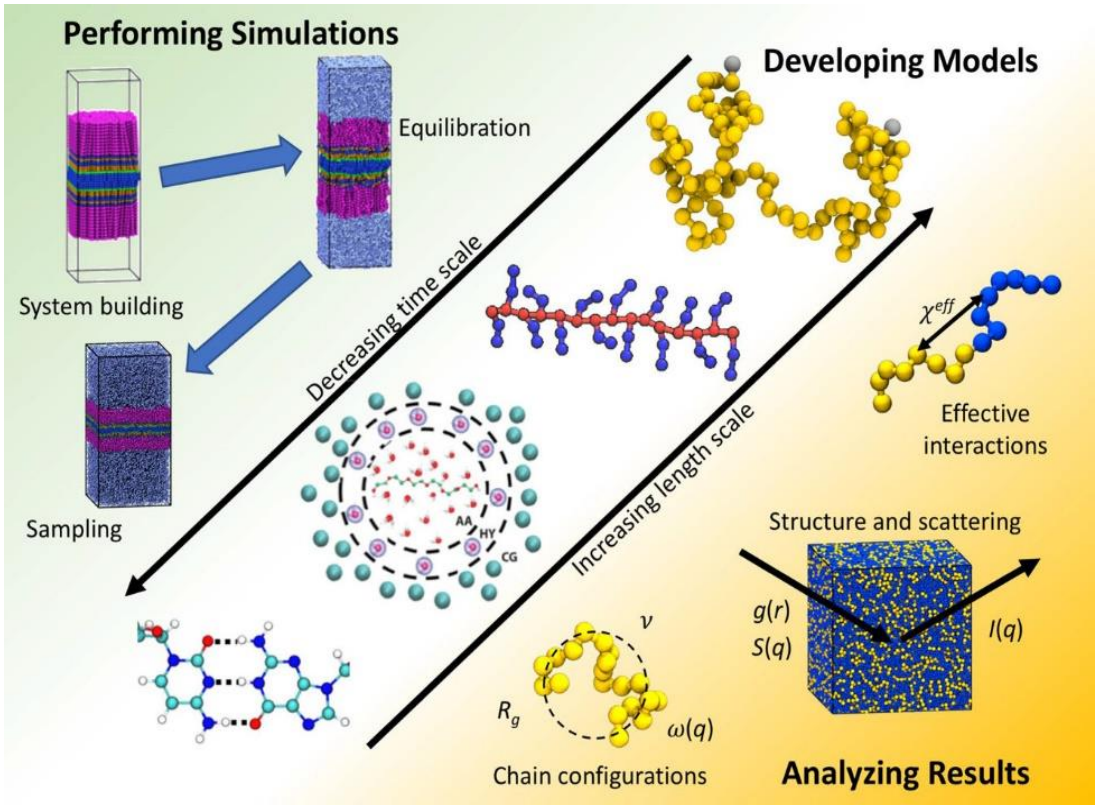

Figure 2: Key steps involved in PE- polymer simulation

Here we are going to discuss about two major models regarding simulation of PE-polymers which are:

- ATOMISTIC MODEL
- COARSE-GRAINED(CG) MODEL.

A) ATOMISTIC MODEL

Atomistic model principles are aplicaple only on those in which a polymer chain(polyethylene,PE) and a monomer(Ethylene, ET) are present.In such a model the result depends on various conditions such as temperature, pressure and concentration(McKeen, 2012). Such simulations are performed to know:

- Atomic level interactions.
- Inter-molecular interactions of a crustalline polymer.
- Interactions between two polymers that bind each other.

Atomistic models are used in the cases of a polymer chain which is usually small than a standard polymer chain.

The first step while calculating the result is to choose the correct force field from the availaible polymer set. Each field will consist of an unique set of parameters which will differ from each other on the grounds of functional forms. There are some equations to study the atomistic model of PE-polymers.

Equation 1) : U(R) = Ui bond+ U angle+ U dihedral+ U Coulomb+ U dispersion

Equation 2): R)=∑ j(l−l0)2+∑ j(θ−θ0)2k l jjk θ Ndihedrals kφ N qqN b o n d s i2jj2jj+ ∑ j (1 − cos(φ)) + ∑ i j 2rÄÉ ÅjÑj Åiσy iσyÑ i,j=1

In above stated equations Ri represent the coordinates of atoms in the model , l represends the bond length of atoms in the model, kθj and θ0j are the bond angle constant and equilibrium angle of bond angle, q is the charge on the atom and I and j represent the contact distance between the two atoms(Giles et al., 2005).

B) COARSE-GRAINED MODEL

A coarse-grained model will consist of polymer chain beads. Length of such beads can vary widly from atomistic model thus we have to choose very carefully to make a perfect CG model(Singh et al., 2017). In a CG model the beads represent some specific atoms within a monomer(intermediate monomer), a complete monomer(CG monomer), a group of monomers(Mesoscale monomers).

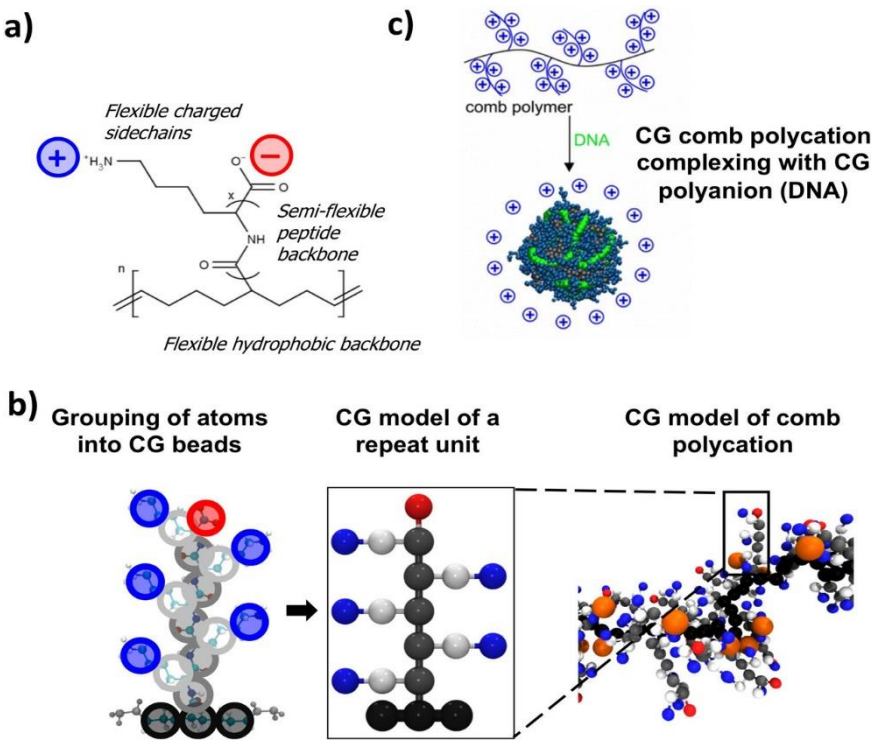

Figure 3: Diagramatic representation of a CG model pf PE-polymerisation.

Conjugated polymers like alkylthiophenes and alkyl side chains can be best simulated using CG model.

It can be said that for a new polymer to be simulated regarding which there is no previous knowledge the CG model technique is best suited and Atomistic approach should be avoided.

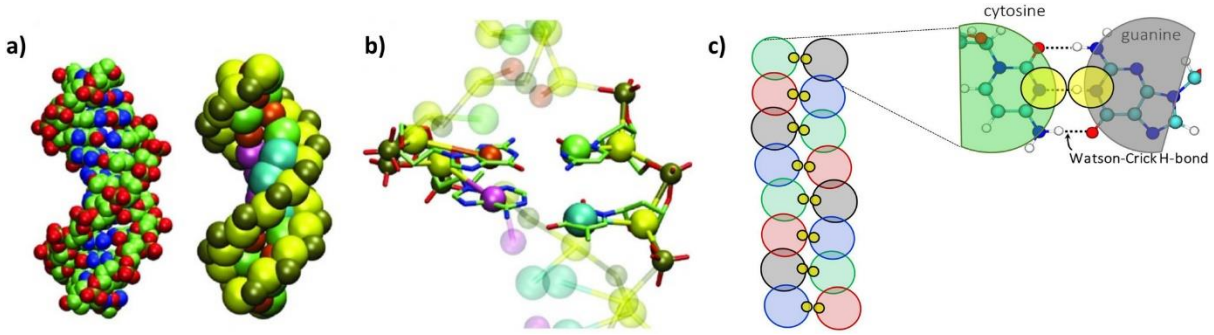

Figure 4: a shows all atoms and CG elements of a double stranded DNA helix. b shows nucleotide of a CG model being stick to the atoms. c shows mapping between the beads of a CG strand to the nucleotides with a formation of strong hydrogen bonding.

Performing Simulations

After choosing the best model for polymer simulation we need to decide the method to perform simulations. The two best methods are:

- Monte Carlo(MC)
- Molecular Dynamics(MD)

A) MONTE CARLO METHOD-:

The monte carlo method works upon the configurations created by stochastic displacement of beads and their acceptance or rejection depends upon the total potential energy exhibited by old and new configurations.Probability of their acceptance is high but proper care must be taken while developing MC moves.If a stochastic moment occurs within a single monomer chain then the process is slow where as if the cinfigurations are pivoted, bridges and helps in configurational regrowth then polymer can witness a drastic change(Arshady, 1992).

B) MOLECULAR DYNAMIC METHOD-:

MD methods use newton's law of equations to find the directions of atoms.MD method is more efficient than MC method as it can be easily implemented and is best suited for large systems. It is easily parallelizable.

MD configurations are easy to trap in kinetic states as they exhibit slow relaxation state of polymer chain. In such situations MC moves are preffered. In some cases MC moves are interspersed with MD confifurations to relax the configurational state of a polymer kinetically trapped(*Dispersion Polymerization in Organic Media*, 1975).

Both MD or MC simulations have three stages which are-:

- Creation of a sysytem and it's initialization
- Setting up an equilibrium
- Sampling

While creating a system, setting up it's equilibrium and providing it's sample one needs to make sure that the results obtained are not biased. These days mostly the MD techniques are being used to simulate the polyners but still it's the choice of a simulator to choose the best suited method for simulation.

After the choice has been made on the method of simulation, the thermodynamic esemble is added to the sample. In a MD simulation it forms a micro-canonical or NVE esemble where number of prticles, volume and energy of simulation box are constant.

MC method enables us to study Polymer bends by addding Gibbs ensemble or Grand canonical ensemble. Both MD and MC methods have contributed a lot in simulatory studies of a polymer as the do not tend to increase the gap between phases.

Conclusion

Stable polmer formation is the target of many chemcial reactions. Catayst are used to either slow the reaction or provide appropriate rate if interest. This work demonstrate two of the most common atomistic and coarse grain for forming polymers. Stable polymers will be formed in case all the requirments corresponding to temperatre and pressure are satisfied. By examining all of the above stated situations and the kind of polymer is chosen for simulation one can make out the best decision on the choice of method that is best suited fot PE Polymer simulation.

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