TRENDS IN THE APPLICATION OF POLYMERS. HISTORICAL STAGES OF HIGH MOLECULAR COMPOUNDS AND PROSPECTS OF THEIR SYNTHESISIN THE 21ST CENTURY

Kravchenko D.V., Marzeniuk O.V., Kozhukhova M.M., Vilensky V.O.
Zhytomyr Ivan Franko State University, Zhytomyr, Ukraine, zu@zu.edu.ua

The ability of polymers to satisfy the demands of society, science and industry during the late 19th and 20th centuries made them a key player in the development of such defining areas of our lives as healthcare, transportation, preservation and distribution of food, construction, space exploration, and even interplanetary research.

The use of available methods for the synthesis of polymeric materials (PM) has led to a disruption of the balance between PMs that are utilized and those that were supposed to be disposed of, i.e., subjected to dissipation, the result of which was their conversion into substances that constitute them. Humanity did not realized this neither during the heyday of polymer chemistry in the 20-60s of the 20th century nor in the 90s when the balance between the use of polymers and their waste was almost catastrophically disrupted. Currently, the mass of waste exceeds 100 billion tons, and their volumes are measured in thousands of square kilometers.

Like any science, polymer chemistry is divided into several historical stages [1]. The first historical stage is associated with the synthesis of natural polymers, such as rubber, fibers, leather, and silk. The second stage is associated with the creation of polymers based on petroleum products. The first chemical reaction with completely synthetic polymer components, probably the nitration of polystyrene, dates back to 1845, which was an important step forward in the history of polymer chemistry. The third stage involves an increased interest in modifying existing market-available polymers to provide them with properties demanded by the economy. Thanks to the discovery of new methods for polymer synthesis and modification, higher quality materials became possible, such as those that are more Plastic, heat-resistant, have good conductivity, compatible with human physiology for medical treatment and prosthetics. This made it possible to apply such materials in new fields, such as electronics and biomedicine, increasing the demand for polymers.

The disposal of polymer waste is unfortunately a big problem for many countries, including Ukraine. Polymers account for approximately 20% with a growing trend up to 30% of the total mass of municipal waste in Ukraine, but only 10% of waste is recycled, with the rest accumulating in local landfills. The high costs of storage, processing, and disposal of polymer waste, as well as the negative impact on the environment, are serious problems for the world as a whole. One solution to this problem could be the development of new methods for processing and disposing of polymer waste, for example, by using recycled materials to produce new polymer materials. Attention could also be paid to the development of efficient technologies that use biological processes for the recycling of polymer waste.

To conclude this section, it is necessary to mention people who significantly contribute to solving the pollution of our planet with technological waste, such as Bill Gates, Jeff Bezos, and Elon Musk, who support international environmental protection projects. We are particularly attracted to the proposal made separately by B. Gates and J. Bezos to move energy-intensive and heat-emitting processes to "Technological Platforms" in nearby space.

Computer modeling of known and new substances that can be created on the desktop of the HyperChem software [2] is an attractive alternative to live experiments, as it allows for demanding experiments to be carried out and subcritical properties of model compounds to be established. Computer chemistry is a competitor to modern technologies and allows us to look beyond the boundaries that were previously inaccessible [3].

Another attractive aspect of computer modeling is that, in most cases, the cost of a good computer and the corresponding software is lower than conducting the necessary experiments involving specialized equipment, experts, chemical reagents, and many other research factors associated with hazardous conditions and substances.

Regarding computer chemistry tools, the main ones are five widely used programs. Molecular Mechanics (MM+), which is based on the model of a molecule as a collection of spheres (atoms) connected by springs (bonds). The energy of the collection of spheres and springs is calculated, which determines the energy of the molecule. Ab initio calculations, which are based on the Schrödinger equation. This is one of the fundamental equations of quantum physics that describes the behavior of electrons in a molecule. The Ab initio method approximately solves the Schrödinger equation for the molecule and provides the energy through the wave function of the molecule. Semiempirical Calculations (SE) - the next level of calculations, which also relies on the Schrödinger equation, but with greater approximations that involve complex integrals. The Molecular Dynamics method, which is used to determine the time dependence of the molecule's behavior in vibrational or Brownian motion. Typically, a certain number of molecules are assigned an initial position and velocity, and new positions are computed based on this motion after some time. Quantum Chemistry, which uses quantum mechanics to describe chemical processes and the electronic structure of molecules. It can solve the Schrödinger equation for chemical systems with high accuracy, but requires significantly more computational resources than other methods.

In this work, the MM+ and MD methods were employed to demonstrate their effective use in describing the characteristic properties of compounds that underwent molecular design and acquired properties that differ from the original ones.

For the study of drug models, we selected histamine (Fig. 1 *model*), which causes allergic symptoms in the human body, such as rash and discomfort around the eyes and nose, and brompheniramine (Fig. 2 *model*), which is a product of the design [4] of the structure of histamine. Brompheniramine reduces the symptoms of the disease and is a sleep aid. The HyperChem software package was chosen to build the models. In order to compare the properties of the initial sample and its design product, the optimization of the structure of the initial sample and the design product was carried out using the Molecular Mechanics of Force Fields (MM+) method. The corresponding eperimental curves (Fig. 3 (Change in the optimization energy of histamine) and Fig. 4 (Change in the optimization energy of brompheniramine)) indicate that the processes of achieving equilibrium state for compounds 1 and 2 are not similar and are accompanied by different deviations from exponential flow.

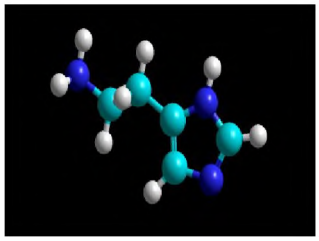

Fig.1

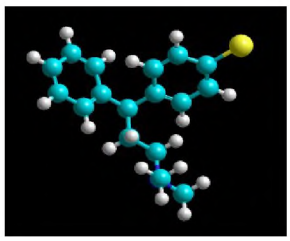

Fig. 2

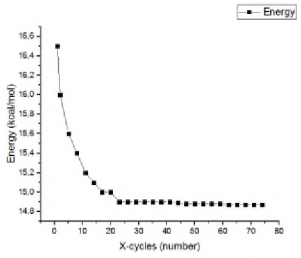

Fig.3

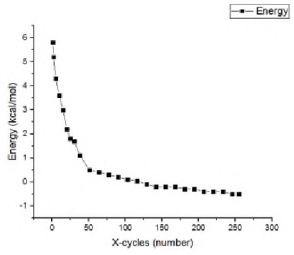

Fig.4

This conclusion is supported by the differences in the components of the initial Optimization Energy, its components, and Dipole Moments, which are presented in theTable:

E_{str}, kcal/mol	Bond	Angle	Dihidr	Vdw	Strech bend	Elecrtstatic	M_D
17.1-Hexam	0.25	13.7	2.2	0.11	0.2	-5.1	2.47
29.3-Bromphe	1.25	2.83	9.7	14.65	0.3	0.07	1.8

1. Chemical History. Edited C.A Russel; G.K Roberts. The Royal Society of Chemistry, 2005

2. HyperChem™, Release 8.0.8, Serial N 12-800159179999; Dealer: Vilensky

3. Lewars E.G. Computational Chemistry: Introduction to the Theory and Applications of Molecular and Quantum Mechanics. – Springer Science + Business Media B.V., 2011.

4. Chemical and Process-Design Handbook, James G. Speight. McGRAW-HILL.©2002