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A GREEN STRATEGY TOWARDS THE MISCIBILITY STUDIES OF STYROFOAM IN ORGANIC AND INORGANIC SOLVENTS BY USING MATERIALS MODELLING AND SIMULATION METHOD

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ABSTRACT

For chemical industries environmental consideration is an issue. It is required to control the operational inputs to reduce and minimize emissions including air pollutant and global warming gasses such as CO2 and Per-fluorinated chemicals/gasses (PFC's). Therefore we need to look for the solutions that aid to limit the waste (solid and liquid chemicals), and to reduce them by recycling methods. This paper focuses on the topic that introduces the miscibility studies of Styrofoam cup (polystyrene foam) in water (inorganic solvent) and in acetone (organic solvent) by using Materials Studio Software. The structures of Styrofoam cup, water and acetone were constructed prior to the calculation of miscibility. Optimization was carried out on the models and the energy of the built structures was reduced to the minimum levels in which the most stable state of the materials was achieved. Two miscibility tests, blending energy and mixing energy, were done on the optimized structures. In blending test, acetone was proven as a better solvent to dissolve the Styrofoam cup as compared to water. The temperature range of 0–56^{o} C was used in the mixing energy analysis. Results showed that the miscibility of the Styrofoam cup-acetone system was higher than the Styrofoam-water system at all temperatures. Besides, both systems also showed improvement of miscibility at elevated temperature.

KEYWORDS: Miscibility Studies, Environmental Impact Sustainability, Materials Studio, Styrofoam Decomposition Method, Binding Energy, Mixing Energy

INTRODUCTION

The implementation of green management strategies for sustainable development towards the chemical products has become the most essential lecture nowadays. Most of the manufacturing factories in the world nowadays dose not really meet the environmental guidelines as set by a government or a higher authority [1]. On the other hand the concept of Eco-materials was introduced in 1990s and so on. The purpose of ecomaterials was to serve the human life and activities in relation with fewer burdens to environment by considering the fitness of the earth and environment [2].

One of the unfriendly environmental products used extensively in world's food packaging business nowadays is Styrofoam. Its light weight property it a most famous product used for food packaging but its contents dose not decompose easily as compared with the food product that decomposes very easily. Styrofoam remains un-decomposed due to its organic structure known as polystyrene [3]. The primary research of this paper is to develop an idea for re-utilizing waste polystyrene. Therefore by analyzing the chemical tests practically in laboratories and their byproduct impacts on the environment gravely, a synthetic green management strategy to conduct a chemical reaction test can be formulated effectively by using a sustainable computer modelling and simulation method to study polystyrene properties.

In this article a research on miscibility of Styrofoam cup (polystyrene foam) in water (inorganic solvent) and in acetone (organic solvent) was studied by using software. The structures of Styrofoam, water and acetone molecules were constructed prior to the calculation of miscibility. Optimization was carried out on the models and the energy of the built structures was reduced to the minimum levels in which the most stable state of the materials was achieved and then the Miscibility tests were conducted upon the software model to demonstrate the miscible system virtually.

MISCIBILITY AND STYROFOAM

It is the property of liquids to mix in all proportions, forming a homogeneous solution, and it is also applied to other phases of materials (solid and gases) as well. But this research topic deals with the Miscibility studies of solid (Styrofoam cup) with a Liquid, in fact two states of matter in a mixture. To have a clear understanding on miscibility see Figure 1, where two solvent (A & B) are mixed to produce an immiscible system and a miscible system.

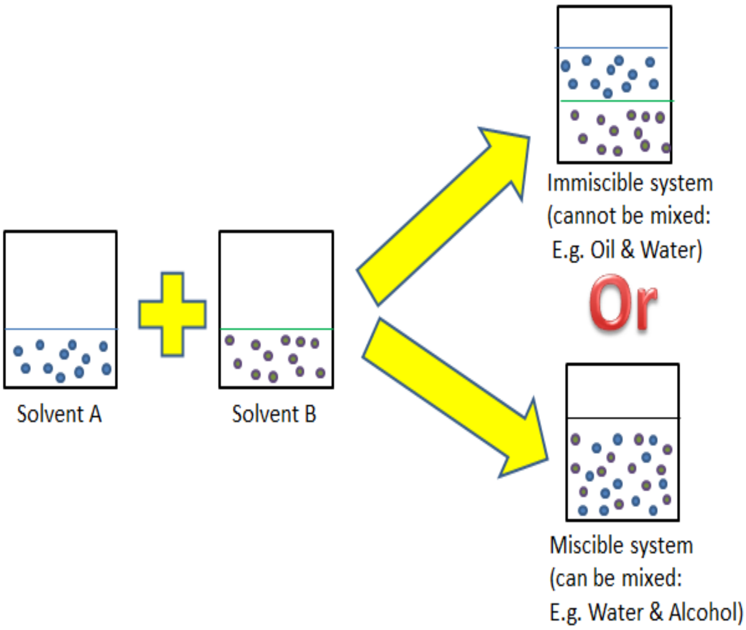


Figure 1: Miscible System Test

Styrofoam Material Environmental Hazards

In past few years the use of Styrofoam has reached to its maximum in food supplying products as drinking cups, food containers etc. and as illustrated in Figure 2 that the total estimated time for natural decomposition rate of Styrofoam containers is more than 1 million years, perhaps never. If it is recycled by heating and melting process, the toxic fumes are hazardous to environment. Therefore an innovative of decomposing such non-bio degradable product is presented to degrade and recycle it back again. This will not only save the recycling-time, but also the pollution created by the Styrofoam waste on the earth.

Figure 1: Daily Used Products Natural Decomposition

Penn State University, U.S. Bureau of Land Management

Taken from: http://www.earthlyissues.com/recycling.htm, (2014)

How the Styrofoam Decomposition Method Works?

Well to explain this scenario: Two tests were conducted on Styrofoam. In the first test the Styrofoam cup was mixed with an inorganic solvent (water) and as a result there was no reaction. In second test the Styrofoam was allowed to mix with an organic solvent (acetone) and as a result a miscible mixture was achieved, acetone dissolving solid state Styrofoam cup into a liquid state in just few second (see Figure 3). Perhaps by doing this the decomposition of Styrofoam cup in organic solvent was proved.

Figure 2: Acetone Dissolving Styrofoam Cup

What is Material Modelling and Why Simulation Method is Selected to Test Miscibility?

Chemical tests operated in laboratories now days have gone far most in advance reactions in their characteristics, properties and formulations. Conducting a chemical test may be dangerous, hazardous to health, environment and some time it is a cause of destructions and loss of human life. Then the wasted by-products of tests chemicals are also causing huge environmental problems, specially contaminating our drinking water resources (rivers); for example fertilizers chemical industries waste. And also to conduct a small test in laboratory requires chemicals to test, beakers, test tubes and other equipment etc. which consumes a lot of time while just preparing the setup for a small chemical test and the main fact is the cost of all the laboratory equipment and the safety procedures for just only a normal school labs, what about the R&D Labs of chemical industries, how much safety and cost of equipment they have to bare and a threat of tragedy, a single mistake in handling chemicals can cause them a huge lose economically and human wise.

Therefore, sustainable idea to conduct a chemical test and resolve all the problems addressed above, with the aid of Computerized Material Modelling and Simulation Method to conduct chemical test or reactions virtually to achieve the final result or product before going through a practical laboratory test is presented, in case the chemical reaction is dangerous, destructive, producing toxic fumes into the environment and causing human lab-attendants health issues, its cost and long testing time. This Sustainable idea of conducting chemical test is used by doing a miscibility test of Styrofoam and proving best miscible solvent for its decomposition.

Conventional Method vs. Simulation Method in Miscibility Studies

In conventional method, two laboratory tests were conducted (see Figure 4): In test 1, Styrofoam was mixed with an inorganic solvent, Water, and an immiscible system was achieved. And in test 2, Styrofoam was mixed with an organic solvent, Acetone, forming a miscible system.

Point to be noted here is that, both of these tests are conducted separately to test the miscibility of Styrofoam. *What will happen if there are 100s of solvents to test the miscibility practically in labs?*

Of course it would require a longer time to test and prepare the lab equipment, including the cost of test products and equipment.

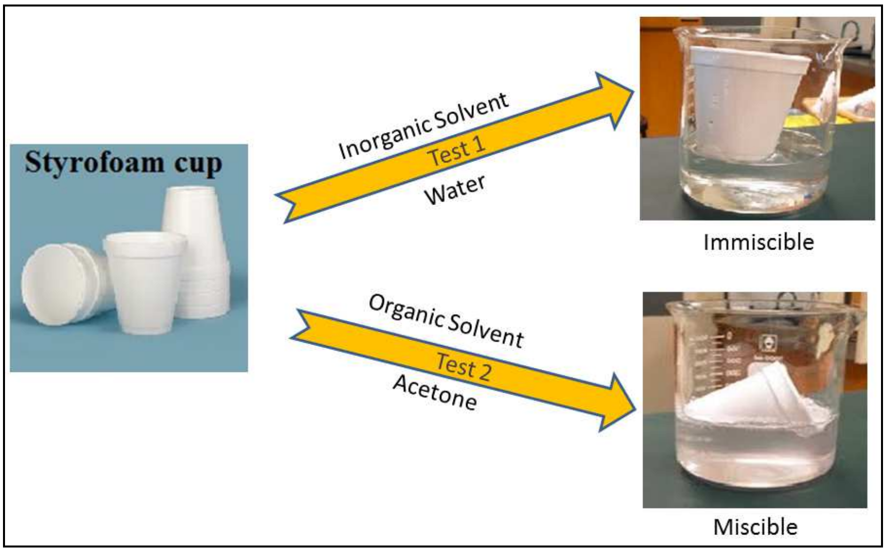
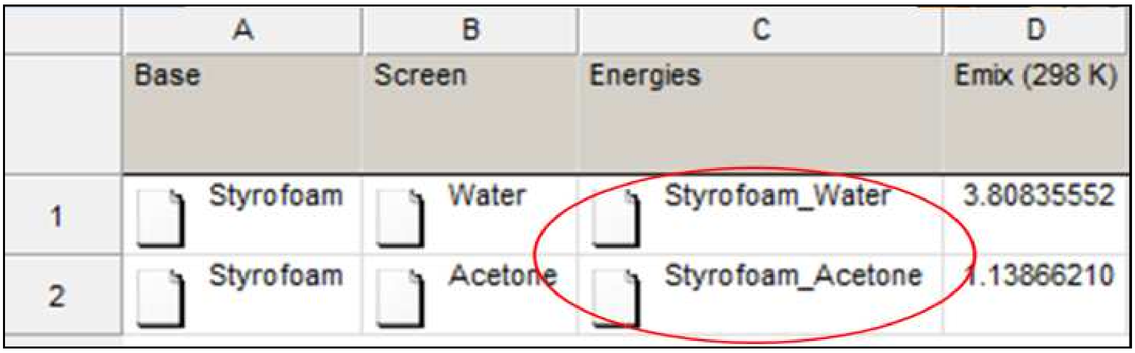


Figure 3: Conventional Miscibility Test

Therefore, Simulation method should be used to overcome the time and cost limitations; in simulation method the structures of test materials are tested by software known as Material studio. The test of *Styrofoam + water system* and *Styrofoam + Acetone system* was simulated to analyses the test results to justify which system is miscible and which is immiscible by comparing their energy graphs (Figure 5).



	A	B	C	D
	Base	Screen	Energies	Emix (298 K)
1	Styrofoam	Water	Styrofoam_Water	3.80835552
2	Styrofoam	Acetone	Styrofoam_Acetone	1.13866210

Figure 4: Software Simulation Result

It has to be noted here, that the both tests are conducted simultaneously and can be extended up to 100 solvents test on miscibility. And the concern here from previous discussion lead us a conclusion of: how much time can be saved by using a simulation method to test miscibility.

MISCIBILITY STUDIES ON STYROFOAM-SOLVENT SYSTEM

There are three important steps in simulation method to follow; Material structures are created in model generation (Figure 6), then these structures are modified in optimization step to obtain a stable form of structures and finally these stable structures are further simulated for calculation in miscibility test by Binding Energy and Mixing Energy graphs.

By comparing different energies in tables and studying closeness of curves in the energy graphs, comparing the closer miscible regions of the system can justify easily which test products are best miscible systems. Possibly, same methodology can be used to not only test the miscibility of systems but also other chemical properties and reactions of different products.

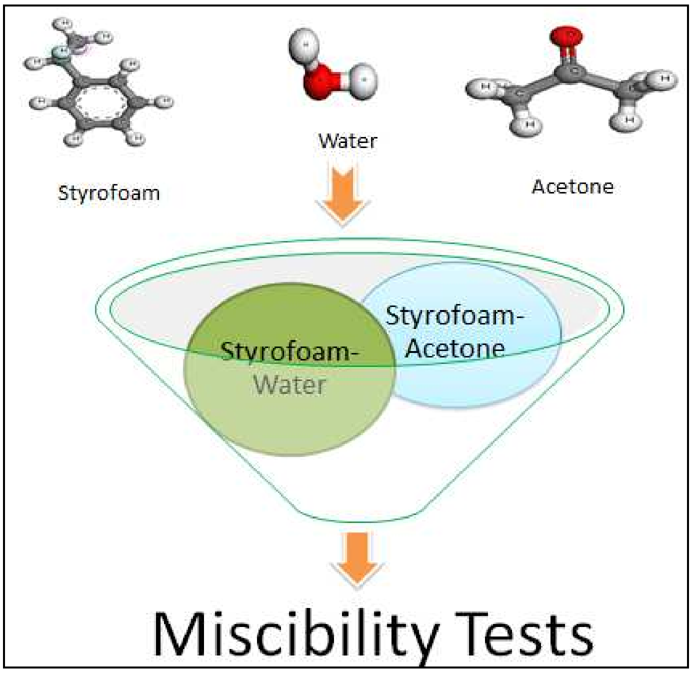


Figure 5: Model Generation of Structures

Method 1: Binding Energy

The Binding energy graphs achieved by Styrofoam-Water System and Styrofoam-Acetone System are illustrated in Figure 7.

In order to get the final conclusion from the binding energy graph concept, two things to look into: 1) Curve matching, i.e. how close the two curves of a mixture system is related and: 2) Study the intersection of curves (point intersection or regional intersection), i.e. how many overlapping section are between the curves. And the results of Styrofoam-Water system demonstrates that there is a very poor curve matching along with only one point intersection as compared to Styrofoam-Acetone system whereby Styrofoam-Acetone system curves are much better in shape with many curve matching areas and there is one point intersection and 2 regional intersection: Hence the Styrofoam-Acetone system demonstrates a good miscible system.

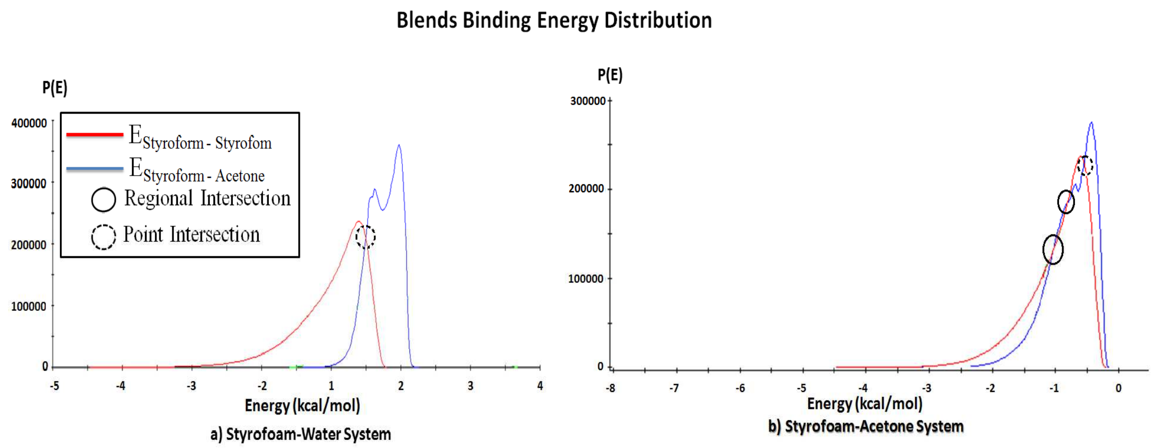


Figure 6: Binding Energy Graphs

Method 2: Mixing Energy

The second simulation test to justify the miscibility of system is done by mixing energy method. The temperature range to study mixing energy of both systems is from (0-56) ^{o} C. And Styrofoam-Water and Styrofoam-Acetone mixing energy graph is obtained in Figure 8.

The mixing energy graph here is presented with X-axis of temperature scale in kelvins and Y-axis with a scale of mixing energy in (kcal/mol). The green dotted line on the graph represents the range of miscible system i.e. from -1.5 to +1.5 for this system only. Any regions of energy falls within the miscible range on the graph is known as miscible system whereas any system energy on graphs falls out of the range lines, is known as immiscible system.

By looking at the Blue-mixing energy line of Styrofoam-Water system it is concluded that, its mixing energy is falling out of the miscible system region range (the green dotted line) and therefore, it is an immiscible system where as the Styrofoam-Acetone mixing energy line is falling in the range of miscible region, therefore it is miscible system. And if we observe the temperature scale, we can see that at all temperature Styrofoam-Water is an immiscible system whereas Styrofoam-Acetone is a miscible system. Hence, by mixing energy method also proved miscibility of two systems.

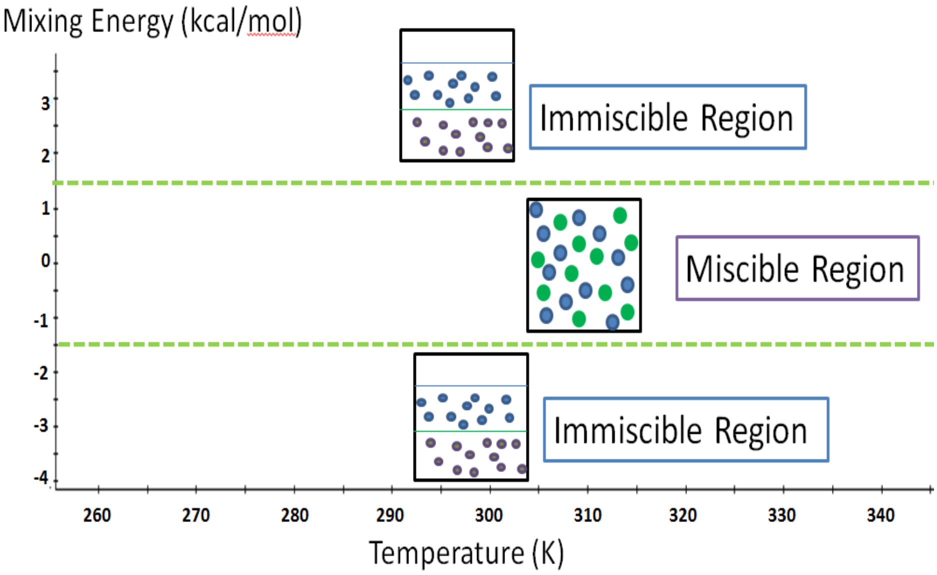


Figure 7: Mixing Energy Graph

RESULTS AND DISCUSSION

Forbore to our decomposition problem with Styrofoam, this problem is solved and has been proved to develop a sustainable method to conduct a chemical test virtually in environmental friendly method by using Modelling and Simulation Software.

Two miscibility tests: blending energy and mixing energy, were conducted on the optimized structures. In blending test, acetone was proven as a better solvent to dissolve the Styrofoam cup as compared to water. The temperature range of (0 - 56) ^{o}C was used in the mixing energy analysis. Results showed that the miscibility of the Styrofoam-acetone system was higher than the Styrofoam-water system at all temperatures. Besides, both systems also showed improvement of miscibility at elevated temperature.

Blending energy and mixing energy are good indicators to determine the miscibility of a system. The miscibility of Styrofoam cup in acetone (organic solvent) and water (inorganic solvent) has been proven by using modelling and simulation method and Styrofoam is more miscible in acetone as compared to water. The simulation results are as accurate as the experimental results

FUTURE RECOMMENDATION

Modelling and simulation method can be used widely to determine the miscibility of a solid object in any selected solvent in the future. Modelling and simulation method can be used to verify the experimental results and even replace it in certain researches to provide a sustainable method towards society.

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