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“Solubility of Polystyrene&Polyethylene Terephthalate in Diesel”

A Dissertation Submitted in Partial Fulfillment of the Requirement of the Award of the Degree of

“BACHELOR OF TECHNOLOGY in CHEMICAL ENGINEERING”

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CERTIFICATE

This is to certify that the work is being presented in the major project entitled, "*Solubility of Polystyrene& Polyethylene Terephthalate in Diesel*". In partial fulfillment of the needs for the award of degree of "Bachelor on Technology in Chemical Engineering "submitted in school of Chemical Engineering of Galgotias University, Greater Noida, is an authentic record of my work carried out under the supervision of Dr. Gagnesh Sharma.

This is to certify that the above statement made by the candidates is correct and true to the simplest of my understanding.

Dr. Gagnesh Sharma

(Head of the Department)

ACKNOWLEDGEMENT

The completion of this undertaking could not have been possible without the assistance and participation of so many people. I take the opportunity to manifest my deep sense of gratefulness and indebtedness to my esteemed supervisor **Dr. Gagnesh Sharma** Professor, who helped enormously and always inspired me by her indispensable guidance and encouragement during the whole long dissertation work. Her meticulous and valuable views, Constructive criticism, and tireless review of the manuscript have immensely helped me to improve the work, I am extremely thankful to her for her dedicated academics.

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The whole credit of my achievements goes to my parents who are always there for me in difficulties. It is their unshakable faith in me that always helped me to proceed further. Words fall inadequate to convey my indebtedness to my friends for their constant support and encouragement I wish to extend a warm thank to all those who could not find a separate name but have helped directly or indirectly.

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PREFACE

The field of theory, provides only the fundamental stone for the guidance of practice but practice examines the element of truth lying in the theory therefore stand coordination between theories and practice is very essential to make a B. Tech project perfect.

Each & every activity is started for the accomplishment of goals & for this purpose realistic approach is required. A project is a systematic and scientific study of a problem with application of experimental skill and concepts.

I was assigned a project on “Solubility of Polystyrene& Polyethylene Terephthalate in Diesel” in the field of " Plastics and Polymers industry"

Secondary is to share the practical knowledge and real experience in world of the Polymer industry. I hope the report will be special interest to the students who are on look for such real-life situation beyond their class room study.

Chapters:

Chapter 1 includes a brief introduction of plastics and polymers and an overview of polymer industry and its background.

In, Chapter 2, we gave a literature review which also includes some of the environmental challenges.

Chapter 3 includes of brief about experiments and process steps of experimentations

Chapter 4, is about result and discussion in which experimental results obtained is included.

Chapter 5 includes concluded discussions by the experimental data.

TABLE OF CONTENTS

LIST OF SYMBOLS

∂_d	Dispersion
∂_p	Polarity
∂_h	Hydrogen Bonding
ρ	Density
∂_t^2	Total Hildebrand parameter
∂_d^2	Dispersion component
∂_p^2	Polar component
∂_h^2	Hydrogen bonding component
R	Interaction radius
∂_x **s**	Hansen component-parameter for solvent
∂_x **p**	Hansen component-parameter for polymer

CHAPTER 1

INTRODUCTION

1.1 Background Study

The plastic waste produced by the world population is growing by the hour. And the problems caused by that waste produced are massive. Problems like air pollution, water pollution, land pollution, and many more. With ever-increasing waste, and too little waste management and investment in reducing the waste and recycling that waste, it is the need of the hour that we take this seriously and find ways to utilize our waste and reduce it.

There are mainly two methods practiced worldwide for managing waste. The First one is the use of landfills and the other is incineration.

A new study, which was the first universal scrutiny on the amount of plastic that has been fabricated till now. "Of the 8.3 billion tons of plastic produced since the 1950s, about 6.3 billion tons of plastic is plastic waste." Only nine percent of the waste plastic has been reprocessed and 12 percent incinerated. The rest of 79 percent is lying in the landfills from where it goes to the world's largest sink, that is the oceans. [1]

The numbers of plastic waste fabricated are alarming, and we are doing too little in contrast to reduce those numbers. So, to utilize the plastic waste produced, we will be investigating the idea of plastic dissolved fuels.

We have chosen polystyrene& polyethylene terephthalate, as the waste plastic, and the fuel is diesel. Polystyrene products (such as Styrofoam, food trays, and packaging materials) take up a lot of space while weighing very little. Which makes transporting waste plastic expensive. And Polyethylene terephthalate is largely used in the bottling beverages by blow molding. Pyrolysis, which entails the processing of plastic to fuel, takes energy and is costly. An easy method may be used to minimize waste plastic volume and recycle resources from waste polystyrene and polyethylene terephthalate, i.e., obtaining fuel with polystyrene and polyethylene terephthalate dissolved in diesel at lower energy consumption is suggested in this report.

1.2 Why are we calculating the density?

The density of the diesel fuel is important since it influences the volume of fuel which can be compressed and burnt within the combustion chamber. As the diesel fuel ignites by compression inside the diesel engine, the density of the diesel fuel becomes an important factor. When a denser fuel is used, the engine produces more particulate matter and smoke, while when a low-density fuel is used, the engine produces lower output power [2]. Density is a vital fuel property that affects the performance of the engine due to system calibration by volume, i.e., the volume of fuel injected changes if density changes, also it influences other properties of diesel like for example, cetane number and heating value [3].

1.3 Solubility Parameters

The solubility parameters have been used for several years to select solvent in the application of coating materials usually polymers. The term solubility parameter was first introduced by Hildebrand and Scott in their work on "non-electrolyte solubility". [4]. The overall van der Waal's force is expressed in simple solubility value by the Hildebrand Solubility Parameter.

The Hildebrand's theory, on the other hand, can only be used in the mixing of non-polar components and fails in cases of polar compounds, which are more common in solvents and polymers. Prediction for choosing a solvent for solute becomes more consistent if the three polar forces (hydrogen bonding, polar forces, and dispersion forces) are to be regarded simultaneously. This method generates three values for each solvent and predicts solubility if all three are the same. This is the basic concept for the Hansen Solubility Parameters.

Charles M. Hansen formed the most well-known and generally recognized method for estimating solubility in 1966. The total Hildebrand value was split into three sections by Hansen solubility parameters: a dispersion force component, a hydrogen bonding component, and a polar component. The soluble components will have similar values. The Hansen solubility parameters are therefore additive:

$$\partial_t^2 = \partial_d^2 + \partial_p^2 + \partial_h^2$$

where, ∂_t^2 Total Hildebrand parameter, ∂_d^2 is dispersion component, ∂_p^2 is polar component and ∂_h^2 is hydrogen bonding component [5].

A three-dimensional model for mapping polymer solubility was also developed by Charles Hansen. He found that by doubling the dispersion parameter axis, any polymer could have an average spherical solubility (solute) volume. The three-component parameters identify the centre of the solubility sphere, and the radius, known as the *interaction radius* (R).

A polymer would more likely be soluble in a solvent if the solvent's Hansen solubility parameters falls within the interaction radius of the polymer. For determining this, and building a model, it should be determined if the distance from the radius of interaction for the polymer is greater than the distance of the center of the polymer solubility sphere. Which is given by [5]:

$$R_a = [4(\partial_d\,s - \partial_d\,p)^2 + (\partial_p\,s - \partial_p\,p)^2 + (\partial_h\,s - \partial_h\,p)^2]^{1/2}$$

where R_a is the length between center of polymer solubility sphere and solvent, ∂_x s is Hansen component parameter for solvent and, ∂_x p is Hansen component parameter for polymer [5]. Even if, Hansen solubility parameters use three parameters for predicting the solubility, it is still just an approximation.

Another approach of Hansen solubility parameters without building a model can also be used by calculating the relative energy distance (RED). The interaction radius (R) of the polymer can be used for the material being dissolved to determine if the conditions for the polymer and solvent are inside an appropriate range. RED is the ratio of the length between center of polymer solubility sphere and solvent (R_a) and the interaction radius (R) [5].

$RED = R_a / R$

The RED value for better solvents is less than 1.0, whereas the RED value for bad solvents ought to be greater than 1.0 [5].

The values of Hansen solubility parameters of different polymers and solvents and the interaction radius are calculated using the HSPiP (Hansen solubility parameters in practice) software.

1.4 Previous Studies

Bio-diesel is produced by the transesterification reaction of vegetable oil or animal fats using a catalyst usually potassium hydroxide or sodium hydroxide, is commonly used in a blend with diesel [6]. B5 blend which is 5% bio-diesel and 95% diesel is the most common blend in use as it requires no modification to the diesel engine for its application. Using bio-diesel results in decreased engine emission like carbon monoxide, sulfur oxides, and also particulate matter [7]. But using bio-diesel has some drawbacks too, as the application of biodiesel fuel blends has been shown to have increased nitrogen oxides emission when compared to regular petro-diesel, moreover lower calorific value and power output are other disadvantages of using the bio-diesel blended fuels [8]. So to overcome the shortcoming of bio-diesel and its blends, studies have been done on dissolving the expanded polystyrene in bio-diesel and diesel blends. The large amount of air-filled in the expanded polystyrene due to its spongy structure provides a suitable condition for rapid flame spread. Also, the auto-ignition temperature of the polystyrene is 490 ^{o}C while the flash point is 350 ^{o}C [9], which makes it a suitable choice for the fuel additive.

Polystyrene and low-density polyethylene could dissolve in biodiesel, according to a physicochemical report. They concluded that the dissolved polymer in bio-diesel can be used as a fuel after studying the properties of the solution of polymer and bio-diesel [10]. Another team investigated the impact of exhaust gas recirculation and injection timing on engine power and carbon monoxide, nitrogen oxides, and soot emissions at high speed and full load operating conditions. They came to the conclusion that a polystyrene concentration of less than 5% resulted in greater engine efficiency, as well as higher values of emissions corresponding to the polystyrene concentration [11].

Research was done on expanded polystyrene with 25 g, 50 g, and 75 g concentration in bio-diesel forming B5 blend (expanded polystyrene-biodiesel-diesel) while also comparing with the control samples (diesel and conventional B5). The tests were conducted on a 4.244 DI diesel engine. The findings showed that incorporating expanded polystyrene into diesel and biodiesel blend fuels would reduce all emissions (carbon monoxide, nitrogen oxides, and soot) while improving engine performance, with a marginal reduction in brake power and a rise in brake thermal efficiency at peak rated power. They found out that 50 g of expanded polystyrene mixed with 1 L of bio-diesel can be a sweet spot for achieving a reduced emission while increased engine performance [12]. In another study, also done with 25 g, 50 g, and 75 g of polystyrene mixed in B5 blend fuel, and found similar result that 50 g polystyrene in 1 L of bio-diesel is the most desirable concentration for its application as a fuel [13]. Another study concluded that 5 g of expanded polystyrene mixed with Petro diesel fuel blended with 5% bio-diesel (B5) gave the best result when the fuel was evaluated on the basis of the engine performance and emission. Thus, the expanded polystyrene mixed fuel can be used as a replacement as it will result in the decrease in environmental pollutions, also providing a viable approach for recycling the expanded polystyrene in a way that is environmentally friendly and highly profitable [14].

A study involving polystyrene solubility in bio-diesel found that the methyl oleate, a key component in bio-diesel, selectively dissolves polystyrene. It was concluded that the kinematic viscosity of biodiesel derived from soybean cooking oil increased, while the cetane number decreased with an increase in the concentration of polystyrene. In addition, as compared to pure bio-diesel, polystyrene dissolved bio-diesel had smaller cycle-to-cycle variations in combustion pressure and ignition timing [15].

Investigation on the performance as well as emissions of a diesel engine which is powered by expanded polystyrene dissolved bio-diesel diesel blends, with added acetone, which will act as a fuel stabilizing additive, concluded that expanded polystyrene dissolved B50 with acetone showed the best brake thermal efficiency and also concluded that expanded polystyrene dissolved B50 with or without acetone had much fewer emissions of nitrogen oxides as well as carbon monoxide than pure diesel [16].

Polyethylene terephthalate has shown to have moderate to low solubility or volume swell in diesel, dimethyl ether, or its blends [17]. While in other research polyethylene terephthalate has shown to have negligible volume change when exposed to diesel [18]. In another research performed in Universiti Teknologi PETRONAS, in Malaysia [19], concluded that polyethylene terephthalate is insoluble in diesel treated with 11% hydrogen peroxide, which was added to avoid damaging the molecular structure of polyethylene terephthalate.

The research on the solubility of polymers has another importance, which is to check the compatibility of fuels and blended fuels with the components that it will be in contact with when used in a vehicle. Better compatibility will mean that the polymer is completely insoluble in the fuel. Research to find the compatibility of bio-oil, diesel and its blend with various infrastructure plastics used in the fuel system which also included polyethylene terephthalate concluded that polyethylene terephthalate experienced only a subtle increase in its volume, which would have been occurred due to added porosity during the drying process or due to physical changes in the polymer chains which could also have resulted due to the drying process done during the experimentation. Polyethylene terephthalate showed very low volume swelling when exposed to the bio-oil and was compatible for use with bio-oil as a fuel [20].

CHAPTER 2

LITERATURE REVIEW

The first research article "*Production, use, and fate of all plastics ever manufactured*" was written during the study of polymers and environmental waste and it covers the condition and impact of plastic debris in the maritime environment. This 2017 Global Survey builds history by providing the first global analysis of all mass-produced plastics produced so far. According to research authors Roland Geyer, Jenna R. Jambeck, and Kara Lavender Law, most of the 8.3 billion tonnes of plastic produced so far have reached our environment.

Meanwhile, "Measuring the Density and Viscosity of Biodiesel and Diesel Fuel Mixtures" by Ertan Alptekin and Mustafa Canakci describes a readily available mixture of two derivative diesel fuels. From 6 types of vegetable oils (sunflower, rapeseed, soybeans, cottonseed, corn oil, used palm oil). Blends of B2, B5, B10, B20, B50, and B75 were created based on volume.

The primary fuel characteristics of the blends, such as density and viscosity, were determined using ASTM test techniques. The blends' densities and viscosities were predicted using generalised equations, and the mixing equation—first proposed by Arrhenius and later defined by Grunberg and Nissan—was used to predict the blends' viscosities.

Koji Yamane and Kiyoshi Kawasaki's study, "A Study of Polystyrene Solubility in Biodiesel," describes the possibility for polystyrene to dissolve in fatty acid methyl esters utilising Hansen solubility parameters.

Additionally, it would be beneficial to utilise a straightforward procedure to recover the energy from recycling waste polystyrene and reduce the volume of waste plastic.

This chapter suggests a straightforward method for dissolving polystyrene in biodiesel to produce liquid fuel at lower energy costs.

Powered by citing Jorge Calder, Murari Mohon Roy, Wilson Wang's article "Biodiesel-powered Diesel Engine Performance and Emissions-Diesel Blend with Recycled Foamed Polystyrene and Fuel Stabilizing Additives" Examine the performance and emissions of diesel engines. Biodiesel-diesel mixture using EPS and acetone as fuel stabilizers. Compare different blends of EPS-dissolved biodiesel with or without the stabilizing component acetone to diesel in terms of performance and emission results. Test results show that EPS improves the heating properties of biodiesel dissolved in EPS.

The viscosity and cloud point of the blends were reduced with the stabilizing ingredient acetone. In general, smoke, CO, and NOx were reduced when biodiesel was dissolved in EPS, whether with or without acetone.

" Development of Solvent-Based Recycling Technique for Polyethylene Terephthalate from Waste Plastic" by Nor Sharizat Arieff bin Kamaruzamal cover the development of solvent-based recycling technique of polyethylene terephthalate (PET) taken from post-consumer drinks containers. It clearly explains about that the bottle containers are further processed to be made as small pellet with sizing of less than 2 mm (length) x 2 mm (width). This sample will then be treated with selected solvent in order to dissolve it from solid PET to liquid PET. Later on, this liquefied PET will be recovered through a dissolution/re-precipitation technique to make it as a pure PET polymer. This polymer is then will be tested with various chemical analysis methods in order to identify its purity so that the success of this project can be justified.

CHAPTER 3

EXPERIMENTS

3.1 Methodology

Experiments are performed separately for polystyrene and polyethylene terephthalate, but the methods used are similar for both. The general term plastic will be used for polystyrene and polyethylene terephthalate in the procedure given below.

Equipment used are thermometer, 200 mL flask, a beaker, testing tube, hotplate magnetic stirrer, oven, digital weighing machine, fume hood, and Whatman filter paper.

The procedure involved during this part of the experiment are as follows:

1. First of all, collect the sample plastic to test, which should be cleaned if was separated from waste plastic.
2. Break the plastic sample into small pieces for better solubility results.
3. Weigh the plastic sample's weight and record the mass in grams.
4. Clean the measuring flask to measure 200 mL of diesel and pour in a beaker and also check the temperature of the diesel.
5. Put the plastic pieces in the 200 mL diesel that was collected in the beaker and put the beaker on the hotplate magnetic stirrer.
6. Put the setup inside a fume hood for achieving a closed system.
7. Note down at what time and how much plastic is being in the diesel.
8. Remove the beaker from the hot plate and leave the solution to cool down.
9. Filter the diesel using the Whatman filter paper.
10. The collected sample of plastic from the diesel is put inside the oven for drying the sample and then measure the mass of the remaining plastic sample collected from the diesel.
11. Measure the mass of the solution using a digital weighing machine at different volumes to get at least four iterations for more accurate results and note down those readings.

3.2 Solubility Parameter Determination

Table 1 shows the Hansen solubility parameters values for polystyrene, polyethylene terephthalate, and diesel. Table 2 shows the RED, interaction radius, and the distance between solvent and polymer solubility sphere for polystyrene and polyethylene terephthalate.

Table 1. Values of Hansen solubility parameters [5].

Components	Dispersion, ∂_d ($MPa^{1/2}$)	Polarity, ∂_p ($MPa^{1/2}$)	Hydrogen Bonding, ∂_h ($MPa^{1/2}$)
Polystyrene	18.5	4.5	2.9
Polyethylene terephthalate	18	2	2
Diesel	17	2	2

Table 2. RED Numbers, Interaction Radius and Distance [5].

Components	Interaction Radius, R ($MPa^{1/2}$)	Distance, R_a ($MPa^{1/2}$)	RED
Polystyrene	5.3	4.0075	0.7561
Polyethylene terephthalate	2.8	6.2674	2.2384

CHAPTER 4

RESULT AND DISCUSSION

We will analyze our findings which were acquired by performing experiments and also the theoretical approach for our problem, which was done by Hansen solubility parameters.

1. The result for testing the solubility of polystyrene in diesel is:

Mass of polystyrene taken = 0.234 g

Volume of diesel taken = 200 mL

Density of pure diesel = 0.820 g/mL [21]

At 50°C and after 80 minutes, only 0.234 g of 0.234 g polystyrene had been dissolved in diesel.

Table 3. Density of Polystyrene and Diesel solution calculated at 15 °C.

Volume of Diesel (mL)	Mass of Diesel (g)	Density (g/mL)
68	56.23	0.826
90	74.99	0.833
134	110.7	0.826
197	163.7	0.830
	Average Density	0.829

Table 4. Amount of Polystyrene dissolved at different times.

Time (minutes)	Amount of Polystyrene dissolved (g)
5	0.117
15	0.195
30	0.214
80	0.234

The results show that the polystyrene is completely soluble in diesel and the density of diesel has increased due to that.

2. The result for testing the solubility of polyethylene terephthalate in diesel is:

Mass of polyethylene terephthalate taken = 0.226 g

Volume of diesel taken = 200 mL

Density of pure diesel = 0.820 g/mL [21]

At 76°C and after 120 minutes, only 0.012 g of 0.226 g polyethylene terephthalate had been dissolved in diesel.

Table 5. Density of Polyethylene terephthalate and Diesel solution calculated at 35 ^{o}C.

Volume of Diesel (mL)	Mass of Diesel (g)	Density (g/mL)
70	57.278	0.8182
120	96.764	0.8063
161	132.034	0.8200
189	153.095	0.8100
	Average Density	0.8136

Table 6. Amount of Polyethylene terephthalate dissolved at different times.

Time (minutes)	Amount of Polyethylene terephthalate dissolved (g)
45	0.001
60	0.002
90	0.008
120	0.012

The results show that polyethylene terephthalate is not soluble in diesel even after two hours of heating, the mass of polyethylene terephthalate which seems to be reduced may have been due to swelling or due to temperature or might have been an inaccuracy during the experiment. Also, the density of diesel hasn't changed due to polyethylene terephthalate not being soluble.

The Hansen model that can be created from the calculations are given below, for polystyrene and polyethylene terephthalate respectively.

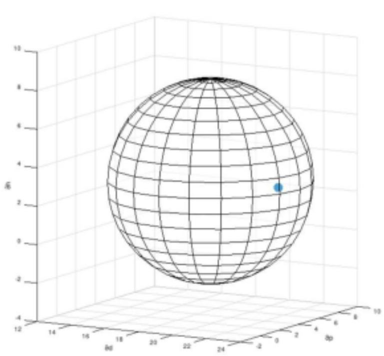

Fig. 1. Hansen Model for Polystyrene []

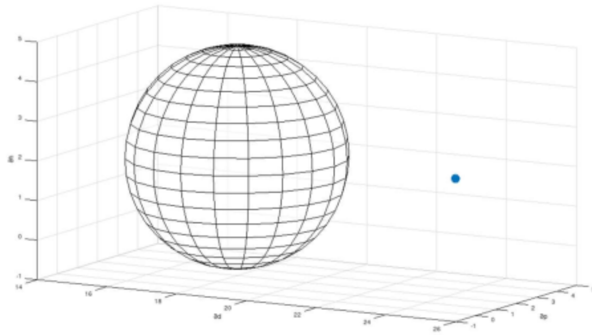

Fig. 2. Hansen Model for Polyethylene terephthalate []

In the Hansen model for polystyrene, the point plotted for the diesel lies inside the polystyrene solubility sphere which confirms our findings that the polystyrene is in fact soluble in the diesel. Also RED for polystyrene, i.e., 0.756 is well below 1. But on the other hand, in the Hansen model for polyethylene terephthalate, the point plotted for the diesel is well beyond the polyethylene terephthalate solubility sphere and also the RED for polyethylene terephthalate, i.e., 2.2384 is well above 1, which confirms our findings for polyethylene terephthalate, that polyethylene terephthalate is insoluble in diesel.

Table 7. Final Result.

Polymer	Solubility of polymer in Diesel
Polystyrene	Soluble
Polyethylene terephthalate	Insoluble

CHAPTER 5

CONCLUSION

The potential for dissolution of polystyrene and polyethylene terephthalate in diesel was estimated by laboratory experiments and confirmed by using the Hansen solubility parameters, theoretical approach. The results conclude that the diesel has the capability of dissolving the polystyrene. The dissolved polystyrene accounted for about 1.33% of the total mass of the solution.

On the other hand, the potential for dissolution of polyethylene terephthalate in diesel was estimated by laboratory experiments and confirmed by using the Hansen solubility parameters. The results conclude that polyethylene terephthalate is insoluble in diesel. The mass of polyethylene terephthalate which was seen to be reduced might have been due to the temperature fluctuations or inaccuracies but also the amount which seems to have been dissolved, happens to dissolve over a very long period of time.

In the case of polystyrene, the density seems to have slightly increased. The performance of the polystyrene dissolved diesel and how all of the properties of diesel are being affected could be checked by employing further research. If this research is a success, then we will have one more way of dealing with our plastic problem. There might have been inaccuracies either due to the inaccuracy of the equipment used or due to human errors.

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