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Research Article

Mass, Volume, Density and Elements in the Polystyrene: Experiments and Neural Networks

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Abstract

In this paper we study the volume, density and mass of five different sizes of the polystyrene polymer. We use acrylic shield to protect the mass balance to obtain steady mass of the polystyrene for the first time. The acrylic shield blocks the streamflow of the air to measure the steady mass. We use Energy Dispersive Spectroscopy (EDS) to obtain the percentage of carbon, oxygen and calcium in the polystyrene. We obtain the mass of the elements. We develop theoretical model, Data Driven Neural Network (DDNN) and Physics Informed from Theory in the Neural Network (PINN). In our neural network models, the training data are limited. These are the advantages of our neural networks. We use four training data sets. We predict the mass of the polystyrene for the fifth data, corresponding to the size of the polystyrene. The fifth data is the test set. We obtain 99% accuracy using both our neural networks. The computer time for training is 30s and for prediction are 0.17s in our simulations. Further, we train and predict the mass of the oxygen using both our neural networks. We provide the mass of carbon, oxygen and calcium for four training data sets only. We provide the mass of carbon and calcium for the prediction of the mass of oxygen. We obtain 98% accuracy using both our neural networks. The mass of the light weight polystyrene is small. The mass of the carbon, oxygen and calcium in the polystyrene are very small. Our data driven neural network and physics informed from theory in the neural network predicts the small values with 99% accuracy for the first time. Furthermore, our theoretical mass and density for the various sizes of the polystyrene matches the experiments. Our work can find applications in packaging industry, printing, sensors, storage, energy and automobiles.

Introduction

In the recent years, the study of polymers is important. They provide the elements in the polymer. The size study and its relation to the polymer properties are must. Predominant polymers are many. We study polystyrene. Polystyrene like polyethylene oxide also have carbon and oxygen. In our polystyrene we observe small traces of calcium. The size relates the chemical composition of the elements from their mass. The structure of the polystyrene is thus understood. The composition of the elements is obtained from energy dispersive spectroscopy [1]. The internal structure of the polystyrene, arrangement of the elements with the relation factor of the size, volume, mass and density are not sure other than the numerical values of their element's presence [2]. The understanding of the polystyrene will be complete with this finding. The surface roughness in relation to the chemical elements and size should be the scope for the future. The understanding of the polarization from the structures for polymers in the molecular origin is well known [3]. The study of polymers evolved to incorporate the valence contribution of atoms, electrons and ions from the first principles simulations [4-5]. Researchers have studied polystyrene from the ethylene and benzene hybridization fabrication methods [6]. Polystyrene are thermoplastics. They are opaque. The study of the vibrational mode provides the elements in the polystyrene [7]. Polystyrene is thermally stable below 200 °C. However small traces of carbon, oxygen and hydrogen are detected from the polystyrene in the air. The temporal change in the mass of the polystyrene needs further studies to understand the air plasma with polystyrene. The applications are many for polymers from printing to energy [8-11]. The nanoparticle preparation provides the size of the particle [12].

The change in the structure during the fabrication are yet to be studied.

The Machine Learning (ML) of polymers are studied. The machine learning provides new materials [13-16]. The availability of data and experiments for polymers are limited. The study of polymers is taken from the membranes, packaging and 3D printing. Machine learning methods use random forest regression, extreme gradient boost and support vector regression. Neural networks are used to study the density and weight of the polymers [17]. The design of the polymer to their property are studied [18]. The structure, elements, melting point and dynamic modulus are studied for different polymers. The glass transition temperature based on the structure are studied in details for polymers [19-20]. Convolutional neural networks are used to predict the temperature. Convolutional neural networks use multiple layers to optimize the weights. Convolutional networks use logarithm formula. hey find the maximum between 0 and positive value [21-22].

In this paper, we study the volume, mass and density of the polystyrene. We study the mass of the carbon, oxygen and calcium in the polystyrene. We study different sizes of the polystyrene. Here, we develop data driven neural network to predict the mass of the polystyrene with limited data sets. This is the novel contribution of our work. We develop physics informed from theory incorporated in the neural network. The physics informed from theory in the neural network predicts the mass of the polystyrene for size 5 given the mass of the polystyrene for four different sizes. The DDN, PINN simulations require training time 30s and prediction time 0.17s. Our model uses less computer power, energy and time to perform calculations to predict next results of experiments. The simulations are performed in the laptop. The rest of the paper is outlined as follows. Section 2 discusses the materials and methods. The theory for the polymers is given in Section 3. The neural networks simulations that include the data driven neural network and physics from theory in the neural network are given in section 4. A detailed discussion is provided in section 5. Finally, conclusions are presented in Section 6.

Materials and Methods

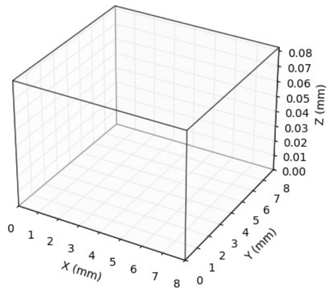
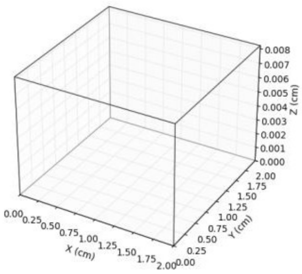
The materials are polystyrene purchased from Lakshmi Electrical and Hard wares, India. The mass balance is obtained from Kern, India. The maximum mass that is measured using the mass balance is 1200 grams. The display accuracy is 0.01 grams. The acrylic box is used during the mass measurement of the polystyrene. We obtain steady mass. The micrometre is obtained from Progressive Trading Corporation, India. The thickness of the polystyrene is 0.082 mm. The figure in the Table 1 shows the digital micro meter. The cutter is purchased from Nimi bind, India. The material cutter is used to cut the light weight polymers to many pieces of cuboid shapes. OM system camera is purchased from Kesari Scientific Chemicals, India. The camera has features for micron size imaging. The transparent plastic scale is used to measure 30 cm. The energy dispersive spectroscopy is used to obtain the percentage of the elements carbon, oxygen and calcium in the polystyrene, respectively. Table 1 shows seven equipment's in figures (Table 1,2).

Table 1: Equipment details.

Equipments	Images
Digital Micrometer	
Mass Balance	
Light Weight Material Cutter	

OM System Camera	
Energy Dispersive Spectroscopy	
Plastic Transparent Scale of 30 cm.	
Acrylic Box Having Doors	

Table 2: Parameters of the polystyrene.

Experiments	CAD model	Geometry
		L = 8 mm, B = 8 mm and H = 0.082 mm V = 5.25 $\times 10^{-9}$ m^3
		L = 2 cm, B= 2 cm and H = 0.082 mm V = 3.28 $\times 10^{-8}$ m^3

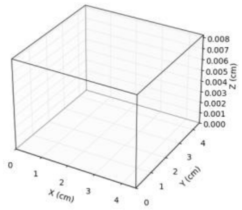
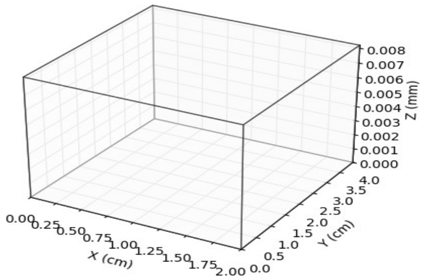
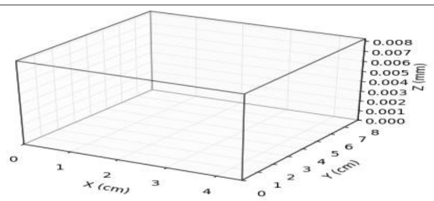
		L= 4.5 cm, B = 4.5 cm and H = 0.082 mm V = 1.67 × 10^{-7} m^3
		L = 4 cm, B = 2 cm and H = 0.082 mm V = 6.56 × 10^{-8} m^3
		L = 7.6 cm, B = 4.6 cm and H = 0.082 mm V = 2.87 × $10^{-7}m^3$

Table 2 shows the polystyrene of different sizes studied. We consider five sizes of the polystyrene. The first size studied have length L = 8 mm, width = 8 mm and thickness H =0.082 mm. The volume of the first size is V = 5.25 × 10^{-9} m^3. The second size have length 2 cm, width 2 cm and thickness 0.082 mm. The volume is 3.28 × 10^{-8} m^3. The third size have length 4.5 cm, width 4.5 cm and thickness 0.082 mm. The volume is 1.67 × 10^{-7} m^3. The fourth size have length 4 cm, width 2 cm and thickness 0.082 mm. The volume is 6.56 × 10^{-8} m^3. The fifth size have length 7.6 cm, width 4.6 cm and thickness 0.082 mm. The volume is 2.87 × 10^{-7} m^3. We develop Computer Aided Design (CAD) model of the polystyrene in python. We develop the model for various sizes of the polystyrene (Table 3).

Table 3: Mass measurement of different sizes of polystyrene. The mass balance is protected with acrylic shield.

Mass measurement set up	size
	L = 8 mm, B = 8 mm, H = 0.082 mm and V = 5.25 × 10^{-9} m^3
	L = 2 cm, B= 2 cm, H = 0.082 mm and V = 3.28 × 10^{-8} m^3

	L= 4.5 cm, B = 4.5 cm, H = 0.082 mm and V = 1.67 $\times 10^{-7}$ m^3
	L = 4 cm, B = 2 cm, H = 0.082 mm and V = 6.56 $\times 10^{-8}$ m^3
	L = 7.6 cm, B = 4.6 cm, H = 0.082 mm and V = 2.87 $\times 10^{-7}$ m^3

Table 3 shows the mass balance protected with acrylic shield. The acrylic shield is used to measure steady mass of the polystyrene. The stream flow of air is blocked using the acrylic shield. We measure the steady mass for various sizes of the polystyrene as shown in the Table 3. The dimensions of each of the polystyrene length, width, thickness and volume are given in Table 3. In the case of small sizes of the polystyrene we place the polystyrene in plastic box to measure the mass. The mass of the empty plastic box and the mass of the polystyrene in the box are measured. The mass of polystyrene for each size is thus obtained. We use the plastic box for four different sizes of the polystyrene as shown in the Table 3 (Table 4).

Table 4: With acrylic shield: mass of the polystyrene with repeats. We study various sizes. All experiments are done.

Polystyrene	Steady State Mass of the Polystyrene with Acrylic Shield			
	Trial 1 (mg)	Trial 2 (mg)	Trial 3 (mg)	Trial 4 (mg)
Size 1	10	5.5	6	10
Size 2	40	50	34	40
Size 3	160	140	161	150
Size 4	50	60	65	60
Size 5	278	260	280	260

Table 4 shows the mass of polystyrene for various sizes. The sizes are represented as size 1 to size 5. The size 1 to size 5 are following the same order having the volume as given in Table 3. We perform our experiments for four repeats. The experiment is performed for 60 seconds. The mass for size 1 used is 5.5 mg. The mass for size 2 used is 34 mg. The mass for size 3 used is 161 mg. The mass for size 4 used is 65 mg. The mass for size 5 used is 280 mg, respectively. The mass balance maximum mass measurable is 1200 grams. The precision is 0.01 g. The mass mentioned as used here and our polystyrene measured volume, gives the respective density for the polystyrene. The density measured for each size of the polystyrene matches the literature. The density in the literature ranges from 964 kg/m^3 to 1050 kg/m^3. We consider literature results as theory. Table 5 shows the considered five different sizes of the polystyrene. The experiment volume for each size is shown in Table 5. The experiment mass, the obtained density for each volume and their size are given in the Table 5.

Table 5: Size of the polystyrene, volume, mass and density from experiments.

Size	Experiment Volume (m^3)	Experiment Mass (kg)	Indirect Density (kg/m^3)
1	5.25×10^{-9}	5.50E-06	1048
2	3.28×10^{-8}	3.40E-05	1037
3	1.67×10^{-7}	1.61E-04	964
4	6.56×10^{-8}	6.50E-05	991
5	2.87×10^{-7}	2.80E-04	976

Composition of elements in the polystyrene

Table 6 shows the mass measured for different sizes of the polystyrene. Table 6 shows the percent of elements measured in the polystyrene. The type of elements are carbon, oxygen and calcium, respectively. The elements are measured in the polystyrene using Energy Dispersive Spectroscopy (EDS). The composition of the elements is also obtained. We obtain 96.9% carbon, 2.1% oxygen and 1% calcium, respectively. We consider the same percent composition of the elements for different sizes of the polystyrene. We measure from the mass of polystyrene, it's percent composition of carbon, oxygen, calcium, the mass of carbon, oxygen and calcium, respectively. Table 6 shows the mass of carbon, oxygen and calcium present in the polystyrene. We study for various sizes of the polystyrene (Table 6).

Table 6: Mass of the polystyrene and their elements mass. The elements are carbon, oxygen and calcium. We study different sizes of the polystyrene.

Size	Mass (kg)	Percent of Elements	Mass of Carbon (kg)	Mass of Oxygen (kg)	Mass of Calcium (kg)
1	5.50E-06	96.9% C, 2.1 % O and 1% Ca	5.33E-06	1.16E-07	5.50E-08
2	3.40E-05	96.9% C, 2.1 % O and 1% Ca	3.29E-05	7.14E-07	3.40E-07
3	1.61E-04	96.9% C, 2.1 % O and 1% Ca	1.56E-04	3.38E-06	1.61E-06
4	6.50E-05	96.9% C, 2.1 % O and 1% Ca	6.30E-05	1.37E-06	6.50E-07
5	2.80E-04	96.9% C, 2.1 % O and 1% Ca	2.71E-04	5.88E-06	2.80E-06

Theory

We consider five sizes of polystyrene to understand neural networks with limited number of data sets. Size 1 of the polystyrene. Table 1 shows the parameters. L = 2 cm, B = 2 cm and H= 0.082 mm. The volume is given in Eq. (1)

$$v = LBH \quad (1)$$

where v is the volume of the polystyrene.

1. We first calculate the Residuals (R). The residuals are obtained by calculating the absolute difference between the experiment result and the model. We avoid negative values in the answers because they are physical quantities.
2. We calculate the square of the residuals (R^2).
3. The mean square error is calculated for each of the size. We consider square of the residual.
4. The Root Mean Square Error (RMSE) is calculated from the mean square error for each of the size. We consider the residual as the root mean square error (Table 7).

Table 7 shows the theoretical density from the literature. We compare the experiment density that is obtained from the volume and measured mass to the theoretical density. We calculate the residual explained above. We calculate the square of the residual, and the values are shown in the Table 7.

We calculate theory mass from the volume and theory density using Eq (2).

$$m_{theory} = \rho_{theory / v} \quad (2)$$

Table 7: Comparison of the density of polystyrene for different sizes between theory and experiments.

Size	Experiment Density (kg/m³)	Theory (kg/m³)	Residual (R)	(R)²
1	1048	1050	2	4
2	1037	1050	13	169
3	964	964	0	0
4	991	1050	59	3481
5	976	976	0	0

where m_{theory} is the theoretical mass and ρ_{theory} is the theoretical density of the polystyrene.

Table 8 shows the comparison of the theoretical mass with the experiments. We consider different sizes of the polystyrene. Table 8 shows the volume of the polystyrene. The theoretical density to calculate the theoretical mass are given in the Table 8. The residual and the square of the residual are given in the Table 8. The square of the residual considered as the mean square error are very small. The value is 16e-12. The root mean square error is 4e-6 kg. The precise measurements are observed in our experiments.

Table 8: Comparison of the polystyrene mass between theory and experiments. The residuals are calculated.

Size	Volume (m³)	Theory Density (kg/m³)	Theory Mass (kg)	Experiment Mass (kg)	Residual (R)	(R)²
1	5.25×10^{-9}	1050	5.5e-6	5.5e-6	0	0
2	3.28×10^{-8}	1050	34e-6	34e-6	0	0
3	1.67×10^{-7}	964	161e-6	161e-6	0	0
4	6.56×10^{-8}	1050	69e-6	65e-6	4e-6	16e-12
5	2.87×10^{-7}	976	280e-6	280e-6	0	0

We calculate the theoretical mass of the elements carbon, oxygen and calcium in the polystyrene. We use the theoretical mass. The composition of the elements in the polystyrene is explained earlier. The elements percent are 96.9% carbon, 2.1% oxygen and 1% calcium, respectively. The theoretical mass of carbon is given in Eq. (3).

$$m_c = \frac{s_1}{100} \times m \quad (3)$$

The mass of the oxygen in theory is given in Eq. (4).

$$m_o = \frac{s_2}{100} \times m \quad (4)$$

The mass of the calcium in theory is given in Eq. (5).

$$m_{ca} = \frac{s_3}{100} \times m \quad (5)$$

where m_c is the theoretical mass of the carbon, S_1 is the percent for carbon, m_o is the theoretical mass of the oxygen, S_2 is the percent for oxygen, m_{ca} is the theoretical mass of the calcium, S_3 is the precent for calcium and m is the mass of the polystyrene, respectively (Table 9).

Table 9: Theoretical mass of the elements carbon, oxygen and calcium in the polystyrene. We consider different sizes of the polystyrene.

Size	Theory Mass (kg)	Percent of Elements	Theory Mass of Carbon (kg)	Theory Mass of Oxygen (kg)	Theory Mass of Calcium (kg)
1	5.50E-06	96.9% C, 2.1 % O and 1% Ca	5.33E-06	1.16E-07	5.50E-08
2	3.40E-05	96.9% C, 2.1 % O and 1% Ca	3.29E-05	7.14E-07	3.40E-07
3	1.61E-04	96.9% C, 2.1 % O and 1% Ca	1.56E-04	3.38E-06	1.61E-06

4	6.90E-05	96.9% C, 2.1 % O and 1% Ca	6.69E-05	1.45E-06	6.90E-07
5	2.80E-04	96.9% C, 2.1 % O and 1% Ca	2.71E-04	5.88E-06	2.80E-06

Table 9 shows the theoretical mass of the polystyrene for various sizes. Table 9 gives the precent of the elements of carbon, oxygen and calcium in the polystyrene. The theoretical mass of the carbon, oxygen and calcium are calculated using Eq. (3), Eq. (4) and Eq. (5), respectively. Table 9 gives the values of the theoretical mass of the elements. Table 10 shows the comparison of the experiment mass of carbon and theoretical mass of carbon in the polystyrene for different sizes. The residual is calculated. The mean square error is very small 1.5e-11. The root mean square error is 3.9E-06 kg. The small root mean square error confirms the small size polystyrene that are accurately measured using the mass balance (Table 10).

Table 10: Comparison of mass of carbon between theory and experiments.

Mass of Carbon (kg)	Theory Mass of Carbon (kg)	Residual (R)	$(R)^2$
5.33E-06	5.33E-06	0	0
3.29E-05	3.29E-05	0	0
1.56E-04	1.56E-04	0	0
6.30E-05	6.69E-05	0.39E-05	0.15E-10
2.71E-04	2.71E-04	0	0

Table 11 shows the comparison of the experiment mass of oxygen and theoretical mass of oxygen in the polystyrene. Table 11 shows the values for different sizes. The residual is calculated. The mean square error is 0.0064e-12. The root mean square error is 0.08E-06 kg.

Table 11: Comparison of mass of oxygen between theory and experiments.

Mass Of Oxygen (kg)	Theory Mass of Oxygen (kg)	Residual (R)	$(R)^2$
1.16E-07	1.16E-07	0	0
7.14E-07	7.14E-07	0	0
3.38E-06	3.38E-06	0	0
1.37E-06	1.45E-06	0.08E-06	0.0064E-12
5.88E-06	5.88E-06	0	0

Table 12 shows the comparison of the experiment mass of calcium and theoretical mass of calcium in the polystyrene. Table 12 shows the values for different sizes. The residual is calculated. The mean square error is zero. The root mean square error is 0.4E-07 kg. The residuals are small.

Table 12: Comparison of mass of calcium between theory and experiments.

Mass of Calcium (kg)	Theory Mass of Calcium (kg)	Residual (R)	$(R)^2$
5.50E-08	5.50E-08	0	0
3.40E-07	3.40E-07	0	0
1.61E-06	1.61E-06	0	0
6.50E-07	6.90E-07	0.4E-07	0
2.80E-06	2.80E-06	0	0

Data Driven Neural Network

In the data driven neural network the input are the training data sets. As discussed, we provide limited 4 training data sets. The training data variables are polystyrene volume, mass and density corresponding to size 1, size 2, size 3 and size 4 mentioned earlier. The neural network algorithm is given here. We use ReLU given in Eq (6) to obtain the maximum between the two numbers 0 and x_1.

$$F_1 = \max\left(0, x_1\right) \quad (6)$$

where $F1$ is the fit to the variable. x_1 is the mass. The formula to obtain weight is given in Eq

(7) and Eq (8), respectively.

$$x_1 = w_1 F_1 + x_0 + x_2 \quad (7)$$

$$w_1 = \frac{(x_1 - x_0 - x_2)}{F_1} \quad (8)$$

where x_0 and x_2 are the volume and density, respectively. w_1 is the weight for the training data set 1. The optimization of the weight w_1 is obtained by repeating x_1, x_0, x_2 in the codec. We use four repeats. The number of training data sets are 4. Hence, we obtain four weights from our training data set. The weights are represented as w_1, w_2, w_3 and w_4 for the training data sets 1, 2, 3 and 4, respectively. Each training data set have 4 repeats. Thus, we provide the training data set 1 in [3 × 4] array in csv file. We provide 4 training data set csv files. We use Adam optimizer to obtain w_1. We use the Adam optimizer to obtain w_2, w_3 and w_4, respectively. In our study, the output of the data driven neural network is the predict mass of the polystyrene for one data set. The data set are designated as test data set. The test data variables are polystyrene volume and density corresponding to the size 5. We denote x_{test1} is the predict test mass of the polystyrene for the size 5. We denote x_{test0} is the given volume and x_{test2} is the given density corresponding to the size 5 of the polystyrene. In order to correlate the weights w_1 to w_4 we use linear function in our code and relate them to

x_{test0}, x_{test1}, x_{test2}, respectively. We relate them to training data set 4 masses. Eq (9) is used to relate the variables.

$$x_{test1} = w_1 x_1 + w_2 y_1 + w_3 z_1 + w_4 t_1 + x_{test0} + x_{test2} \quad (9)$$

where x_1 is the mass of the training data set 1, y_1 is the mass of the training data set 2, z_1 is the mass of the training data set 3 and t_1 is the mass of the training data set 4, respectively. The test data are also provided 4 repeats. Thus, we provide the one test data set in [3×4] array in csv file. The column corresponding to the test mass of polystyrene of size 5 are given as zero.

Table 13 shows the training data. We provide the small number of data sets as training to our data driven neural network. This is the advantage in our model. The training data sets include the volume, mass and density for 4 sizes. We provide the test data corresponding to the size 5. We provide the test data volume and density as shown in the Table 13. We predict the test set mass of polystyrene. The light weight polymer is studied with limited data set using data driven neural network for the first time. The mass value for the sizes studied are small numbers.

Table 13: Parameters used to predict mass of the polystyrene in the data driven neural network.

Size	Experiment Volume of Polystyrene (m^3)	Experiment Mass of Polystyrene (kg)	Experiment Density of Polystyrene (kg)	Mass of Polystyrene (kg)
1	Given	Given	Given	
2	Given	Given	Given	
3	Given	Given	Given	
4	Given	Given	Given	
5	Given	Not Given	Given	Predict

Table 14 shows the mass of the polystyrene obtained in the experiments. We compare the experiment mass measured with the predicted mass. The predicted mass is obtained from the data driven neural network. We also obtain the predicted density from our model. The density matches the experiment. Table 14 shows four repeats of the data. The repeat numbers are equal to the training data. We have to ensure this in our data driven neural network for accuracy. The model provides match with the experiment mass of polystyrene for size 5 whose weight is small. The polymer polystyrene is light weight material.

We repeat our data driven neural network for problem 2. The problem 2 have training data variables mass of carbon, oxygen and calcium, respectively. We use limited 4 training data sets corresponding to the size of the polystyrene. The size 1 to size 4 parameters of the polystyrene are given as the training data sets.

The method to optimize the weight are same as above. We predict for one test data. The test data corresponds to the size 5 of the polystyrene. We predict only the mass of oxygen for size 5. The test data variables mass of carbon and calcium are given.

Table 14: Comparison of the mass of polystyrene for size 5 between experiments and data driven neural network. The density values are informed.

Test Mass from Experiments (kg)	Predict Mass from The Data Driven NN (kg)	Test Density (kg/m^3)	Predict Data Driven NN Density (kg/m^3)
2.80E-04	3.29e-03	976	976
2.80E-04	3.29e-04	976	976
2.80E-04	2.29e-03	976	976
2.80E-04	1.14e-03	976	976

Table 15 shows the mass of the carbon, oxygen and calcium for different size of the polystyrene. We use the mass of the carbon, oxygen and calcium for 4 sizes of the polystyrene as the training data. The element mass of the carbon, oxygen and calcium are measured using energy dispersive spectroscopy. We use the mass of carbon and calcium for size 5 of the polystyrene, respectively as the test data. We use data driven neural network. We predict the mass of oxygen for size 5 of the polystyrene. The mass of the elements that includes carbon, oxygen and calcium in the polymer polystyrene are very small. Table 16 shows the mass of the oxygen predicted. We compare them with the experiment mass. The data driven neural network predicts with high accuracy. The predict capability of element mass of oxygen in the polymer polystyrene using data driven neural network is the novelty of the work. The limited data set is the novel contribution of our work.

Table 15: Parameters used in the data driven neural network.

Size	Experiment Mass of Carbon and Calcium	Experiment Mass of Oxygen	Mass of oxygen
1	given	given	
2	given	given	
3	given	given	
4	given	given	
5	given	not given	predict

Table 16: Comparison of the mass of oxygen for size 5 between experiments and data driven neural network.

Test Mass of Oxygen from Experiments (kg)	Predict Mass of Oxygen from Data Driven NN (kg)
5.88E-06	1.16E-05
5.88E-06	3.12E-05
5.88E-06	3.55E-05
5.88E-06	5.15E-05

Physics Informed from Theory in the Neural Network (PINN)

The only different between the data driven neural network and the physics informed from theory in the neural network are that in the data driven neural network we provide experiment results as the data. Here in PINN, we provide theoretical data. The neural network algorithm remains the same as the data driven neural network. In physics informed from theory in the neural network we use limited 4 training data and one test data. We solve two problems. Firstly, we predict the mass of the polystyrene for size 5. We input the theoretical mass corresponding to size 1 to size 4. The training and test variables are same as data driven neural network for problem 1 to predict mass of the polystyrene. Secondly, we predict the mass of the oxygen in the polystyrene for size 5. We input the theoretical mass of carbon, oxygen and calcium corresponding to the size 1 to size 4. The training and test variables are same as data driven neural network for the problem 2 to predict mass of the oxygen for size 5.

Table 17 shows the training data. We provide the small number of data sets as training to our physics informed from theory in the neural network. This is the advantage in our model. The training data sets include the volume, mass and density for 4 sizes. We provide the test data corresponding to the size 5. We provide the test data volume and density as shown in the Table 17. Here, we provide the theoretical mass of the polystyrene for different sizes. We provide the theoretical density. The model uses the theory in this approach. We predict the test set mass of polystyrene. The light weight polymer is studied with limited data set using physics informed from the theory in the neural network for the first time. The mass value for the sizes studied are small numbers.

Table 17: Parameters used to predict mass of the polystyrene in the physics informed from theory included in the neural network.

Size	Volume of Polystyrene (m^3)	Theory Mass of Polystyrene (kg)	Theory Density of Polystyrene (kg)	Mass of Polystyrene (kg)
1	given	given	given	
2	given	given	given	
3	given	given	given	
4	given	given	given	
5	given	not given	given	Predict

Table 18 shows the mass of the polystyrene for size 5 obtained in the theory and experiments. We compare the experiment mass and theoretical mass with the predicted mass. The predicted mass from PINN has 99% accuracy. We also obtain the predicted density from our model. The density matches the theory. The repeat numbers are equal to the training data. We have to ensure this in the PINN to obtain 99% accuracy. The model provides good match with the theoretical mass and experiment mass of polystyrene for size 5 whose weight is small. The polymer polystyrene is light weight material.

Table 18: Comparison of the mass of polystyrene for size 5 between experiments, theory and physics informed neural network. The density values are informed.

Test Theory Mass (kg)	Predict Mass (kg)	Test Experiment Mass (kg)	Test Theory Density (kg/m^3)	Predict Density (kg/m^3)
2.80E-04	1.28e-4	2.80E-04	976	976
2.80E-04	1.86e-3	2.80E-04	976	976
2.80E-04	2.48e-4	2.80E-04	976	976
2.80E-04	1.74e-3	2.80E-04	976	976

Table 19 shows the element theoretical mass of the polystyrene. The calculations are given in the theory section. We use the theoretical mass of the carbon, oxygen and calcium for 4 sizes of the polystyrene as the training data. We use the theoretical mass of carbon and calcium for size 5 of the polystyrene, respectively as the test data. We use physics informed from theory in the neural network. We predict the mass of oxygen for size 5 of the polystyrene. The mass of the elements that includes carbon, oxygen and calcium in the polymer polystyrene are very small. We compare the predicted mass of the oxygen obtained using the physics from theory in the neural network to the theoretical mass of oxygen and experiment mass of oxygen for size 5 of the polystyrene.

Table 19: Parameters used in the physics informed from theory in the neural network.

Size	Theory Mass of Carbon and Calcium	Theory Mass of Oxygen	Mass of Oxygen
1	given	given	
2	given	given	
3	given	given	
4	given	given	
5	given	not given	predict

Table 20 shows the predicted mass of the oxygen for size 5 of the polystyrene from the PINN simulations. Table 20 shows the theoretical mass of oxygen for size 5 of the polystyrene. We provide the experiment mass of oxygen for size 5 of the polystyrene. The predicted mass of oxygen from PINN simulations has 98% accuracy. The predict capability of element mass of oxygen in the polymer polystyrene using PINN are the novelty of the work. The limited data set are the novel contribution of our work.

Table 20: Comparison of the mass of oxygen in the polystyrene between experiment, theory and PINN.

Test Mass of Oxygen from Experiments (kg)	Test Mass of Oxygen from Theory (kg)	Predict Mass of Oxygen from PINN (kg)
5.88E-06	5.88E-06	5.84E-05
5.88E-06	5.88E-06	5.73E-05
5.88E-06	5.88E-06	8.98E-05
5.88E-06	5.88E-06	3.35E-05

Results and Discussion

Figure 1 shows the experiment mass for the size 5 of the polystyrene. The volume of the polystyrene is 2.87×10^{-7} m^3. We used data driven neural network to predict the mass of the polystyrene for the same size. In this study we use 4 training data. Each training data corresponds to each size. We observe the light weight size 5 has mass in the order of 1e-5 kg that is predicted accurately by the data driven neural network. The use of data driven neural network for small size weights of polymers like polystyrene is done for the first time (Figure 1).

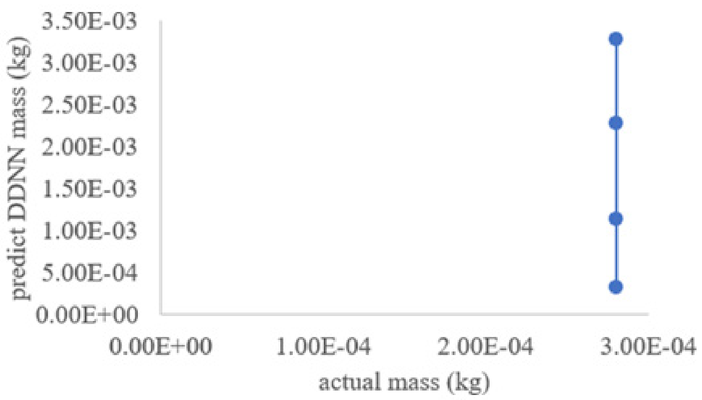


Figure 1: Comparison between the mass of the polystyrene for size 5 obtained from experiment and data driven neural network.

Figure 2 shows that we use 200 epochs. The loss for the convergence of the predict data is 1e-5. The lower the convergence the accuracy is high. We observe the loss is independent of the epochs. Figure 3 shows the run of the simulation in the Windows Power shell terminal to execute python script. The use of power prompt Windows Power shell for running neural networks are for the first time. Our data driven neural network predicts the test cases in less than a second for the first time. Figure 3 shows our simulation for predicting the test case using data driven neural network took 0.175 second. This is novel aspects of our work. Also, we use limited data set. We predict small sizes having very small weight.

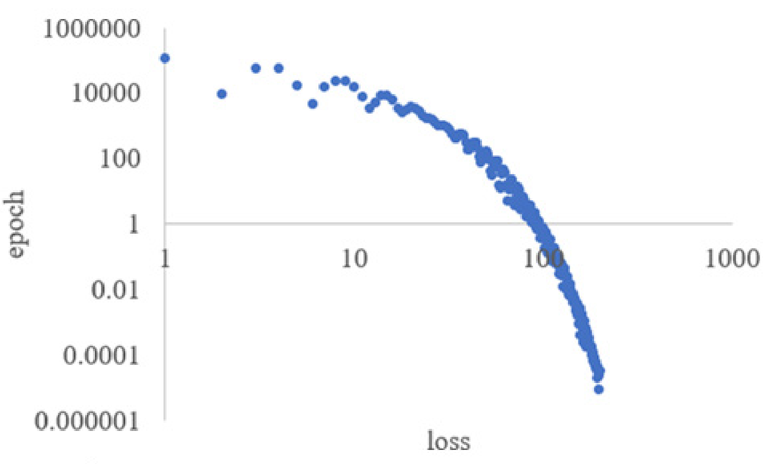


Figure 2: epoch vs loss.

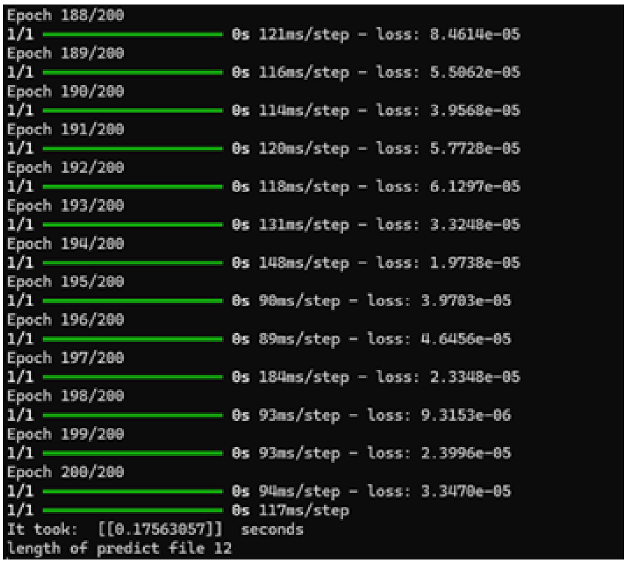


Figure 3: Running of the neural network in the Windows Power Shell terminal.

Figure 4 shows the experiment mass of oxygen for the size 5 of the polystyrene. The energy dispersive spectroscopy is used to measure the elements percent in the polystyrene. We used data driven neural network to predict the mass of the oxygen in the same size polystyrene. Figure 4 shows the mass of the oxygen is in the order of 5e-6 kg and that for the first time predicted using the data driven neural network with minimal data sets. The simulation to predict the test case took less than a second.

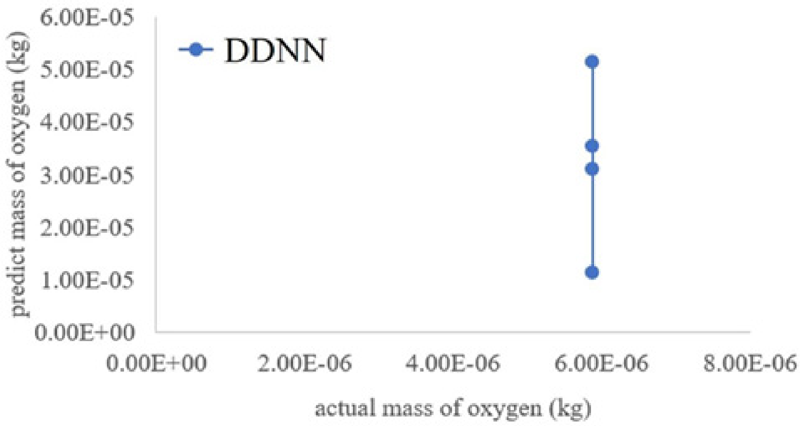


Figure 4: Comparison of mass of oxygen in the polystyrene for size 5 between experiments and data driven neural network.

Figure 5 shows the experiment mass for the size 5 of the polystyrene. The volume of the polystyrene is 2.87×10^{-7} m^3. We used physics from the theory in the neural network. The theoretical mass is obtained using Eq. (2). We obtain the mass for the same size using our model. Here, we use limited 4 training data. Each training data corresponds to each size. We observe the light weight size 5 has mass in the order of 1e-5 kg that is predicted accurately by the physics from the theory in the neural network. The prediction of the mass is shown in the Figure 5. The use of physics from theory in the neural network to obtain the mass for polystyrene having small weights are done for the first time.

Figure 6 shows the experiment mass of oxygen for the size 5 of the polystyrene. We used physics from the theory in the neural network to predict the mass of the oxygen for the same size. The mass of the oxygen is in the order of 5e-6 kg as shown in the Figure 6. The simulation to predict the test case took less than a second. Here, the prediction of mass of oxygen elements using our physics from theory in the neural network is the novelty of the work.

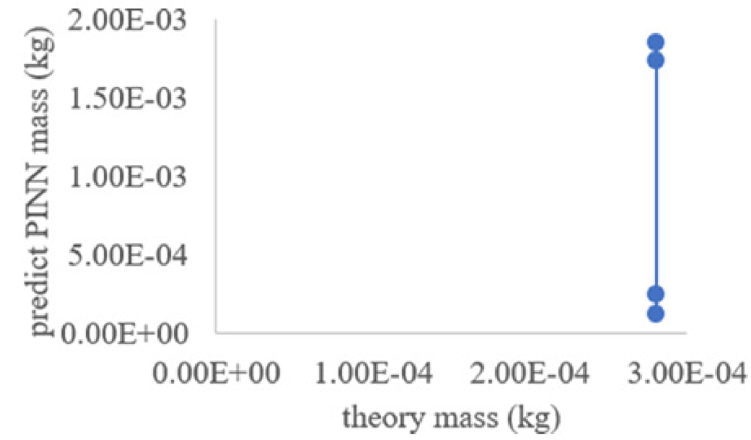


Figure 5: Comparison of mass of polystyrene for size 5 from theory and physics informed from theory to the neural network.

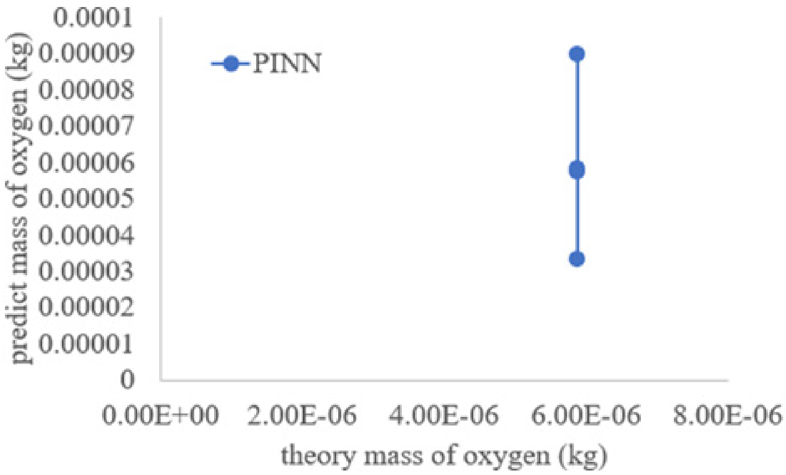


Figure 6: Comparison of mass of oxygen in the polystyrene for size 5 between theory and PINN.

Conclusions

To conclude, we study polystyrene polymer material their volume, mass, density and element mass that includes carbon, oxygen and calcium for different sizes. We provide theory to the density, mass and element mass for different sizes of the polystyrene polymer. The theory matches the experiments. In this paper, we develop two neural network models. First, data driven neural network model to predict the mass of the polystyrene. The predict mass matches the experiments with 99% accuracy. Our DDNN model predicts the mass of the oxygen matching experiments having 98% accuracy. The DDNN predicts density matching experiments having 99% accuracy. Second, we develop physics informed from theory in the neural network model to predict the mass of the polystyrene. PINN model predicts mass matches both the theory and experiments having 99% accuracy. Our PINN model predicts the mass of the oxygen matching the theory and experiments having 98% accuracy. The PINN model predicts density of the polystyrene matching the theory and experiments having 99% accuracy. Both DDNN and PINN model uses limited 5 number of data sets. The simulations are performed in the laptop. The simulations use less computer power and the computer time are 35 s.

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Author Contributions

Nandigana V. R. Vishal: Conceptualization, Data curation, Formal analysis, investigation, methodology, resources, software, supervision, validation, visualization, writing – original draft, writing – review and editing.

Conflicts of Interest

The authors declare no conflict of interest.

Data Availability

The data from the current study are available from the corresponding author upon reasonable request.

References

1. M A Abkowitz (1992) Electronic transport in polymers. Philosophical Magazine B 65(4): 817- 829.
2. A Babel, S A Jenekhe (2003) High Electron Mobility in Ladder Polymer Field-Effect Transistors. J Am Chem Society 125(45): 13656-13657.
3. K I Hong, A Kumar, A M Garcia, S Majumder, A R Carretero (2023) Electron spin polarization in supramolecular polymers with complex pathways. J Chem Phys 159: 114903.
4. A Landi, M Reisjalali, J D Elliott, M Matta, P Carbone, et al. (2023) Simulation of polymeric mixed ionic and electronic conductors with a combined classical and quantum mechanical model. J Mater Chem C 11(24): 8062-8073.
5. S Prodhan, A Troisi (2024) Effective Model Reduction Scheme for the Electronic Structure of Highly Doped Semiconducting Polymers. J Chem Theory Computation 20(22): 10147-10157.
6. J L Lenhart, D A Fischer, T L Chantawansri, J W Andzelm (2012) Surface Orientation of Polystyrene Based Polymers: Steric Effects from Pendant Groups on the Phenyl Ring. Langmuir 28(44): 15713-15724.
7. S A Hall, K C Jena, P A Covert, S Roy, T G Trudeau, et al. (2014) Molecular-Level Surface Structure from Nonlinear Vibrational Spectroscopy Combined with Simulations. J Phys Chem B 118: 5617-5636.
8. I M Ward, J Sweeney (2013) Mechanical Properties of Solid Polymers, Third Edition, John Wileyand Sons, Ltd.
9. G D Wignall, D G H Ballard, J Schelten (1976) Chain conformation in molten and solid polystyrene and polyethylene by low-angle neutron scattering, Journal of Macromolecular Science Part B 12(1): 75-98.
10. K Kik, B Bukowska, P Sicinska (2020) Polystyrene nanoparticles: Sources, occurrence in the environment, distribution in tissues, accumulation and toxicity to various organisms, Environmental Pollution 262: 1-9.
11. Y B Tatek, M Tsige (2011) Structural properties of atactic polystyrene adsorbed onto solid surfaces. J Chem Phys 135(17): 174708.
12. S Anguissola, D Garry, A Salvati, P J O Brien, K A Dawson (2014) High Content Analysis Provides Mechanistic Insights on the Pathways of Toxicity Induced by Amine-Modified Polystyrene Nanoparticles, Plos One 9(9): e108025.
13. T B Martin, D J Audus (2023) Emerging Trends in Machine Learning: A Polymer Perspective, ACS Polym Au 3(3): 239-258.
14. W Ge, R D Silva, Y Fan, S A Sisson, M H Stenzel (2025) Machine Learning in Polymer Research, Advanced Materials, 37(11): 2413695.
15. R S V D Hurk, B W J Pirok, T S Bos (2025) The role of artificial intelligence and machine learning in polymer characterization: emerging trends and perspectives. Chromatographia 88(5): 357- 363.
16. D C Struble, B G Lamb, B Ma (2024) A prospective on machine learning challenges, progress, and potential in polymer science. MRS Communications 14(6681): 1-19.
17. N K Roy, W D Potter, D P Landau (2006) Polymer Property Prediction and Optimization Using Neural Networks. IEEE Transactions on neural networks 17(4): 1001-1014.
18. N K Roy, D P Landau and W D Potter (2004) Designing polymer blends using neural networks, genetic algorithms and Markov chains. Appl Intell 20: 215-229.
19. L A Miccio, G A Schwartz (2020) From chemical structure to quantitative polymer properties prediction through convolutional neural networks Polymer 193: 1-7.
20. B E Mattioni, P C Jurs (2002) Prediction of glass transition temperatures from monomer and repeat unit structure using computational neural networks. J Chem Inf Comput Sci 42(2): 232-240.
21. A J Hopfinger, M G Koehler, R A Pearlstein, S K Tripathy (1988) Molecular modeling of polymers. IV Estimation of glass transition temperatures 26: 2007-2028.
22. D Boudouris, L Constantinou, C Panayiotou (2000) Prediction of volumetric behavior and glass transition temperature of polymers: a group contribution approach. Fluid Phase Equilibria 167: 1-19.