JOURNAL OF ENERGY SYSTEMS

2021, 5(1)

2602-2052

DOI: 10.30521/jes.847237

Research Article

Evaluation through finite element and numerical simulation of triboelectric polymer pairs in vertical contact mode

Shimna Shafeek
University of Bolton, United Arab Emirates, s.shafeek @bolton.ac.uk
Sibgatulla Sharieef
University of Bolton, United Arab Emirates, ss21ocd@bolton.ac.uk

Submitted: 26.12.2020
Accepted: 21.03.2021
Published: 31.03.2021

Abstract: Triboelectric nanogenerators are shown a recent development in the energy field in various applications powering sensors to biomedical applications. The research development of tribogenerators is trending in the renewable energy area as it can harness waste mechanical energy due to the friction. Studies have shown various mathematical modeling done on the triboelectric principle based on Gauss electric field principle. Triboelectricity generation due to contact electrification depends on various factors that include the surface charge density, materials, the geometrical features of the tribo pairs, the mode of operation in terms of velocity etc. The significance of nanomaterials in the generation of triboelectricity is a research area where polymers have shown good results. In this study, a detailed computational and numerical simulation is done on selected pairs of triboelectric material combination chosen from the triboelectric series. Computational simulation is performed using Comsol Multiphysics to evaluate the output performance in terms of V_{oc} and Q_{sc}. Numerical simulation is performed using MatLab to evaluate the output performance current, power, voltage with respect to time for selected input parameters. The numerical performance of the device is validated by the experiments. The numerical method adopted will be a useful tool for determining the output characteristics of any triboelectric pairs.

Keywords: *Computational, Energy harnessing, Numerical, Simulation, Triboelectric generator*

Cite this paper as: Shafeek, S., & Sharieef S. Evaluation through finite element and numerical simulation of triboelectric polymer pairs in Vertical Contact mode. *Journal of Energy Systems* 2021, *5*(1), 35-45, DOI: 10.30521/jes.847237

1. INTRODUCTION

In the era of harnessing energy from various sources that lead to the production of waste, energy has been trending in the research field. Due to the depletion of fossil fuels and an increase in the demand of it, the replacement of fossil fuels by the renewable energy source attracted the world at a high level [1]. There will be a drastic increase in the demand of renewable energies due to increase in population in developed and developing countries by 2050, new methods of harnessing energy are of growing stage [2]. The world is moving towards artificial intelligence (AI) and internet of things (IoTs), where the demand for a huge number of the energy source is required [3]. The limited lifetime, maintainability, cost, continuous monitoring of the performance of the devices are some of the key drawbacks of the batteries. The idea of powering devices from its mechanism leads to the emerging sustainable solution of systems to work as self-powered [4]. This sustainable energy solution made the industry to think about the sensors to work as a self-powered using an active autonomous power source.

Various energy harnessing mechanical methods are adopted during the years which includes electromagnetic generator, electret generators and piezoelectric generators for exploiting the ambient environment by harvesting mechanical energy and providing self-powered devices [5]. The requirement of heavy permanent magnets in electromagnetic generators, the necessity of pre-charging and low electrical power in electret generators and the low output and toxicity in piezoelectric generators are considered as the drawback and thereby commenced on researching on the new energy source triboelectric generators as a cheap and efficient energy source for low powered systems [6-7]. From the time of the invention of Triboelectricity and Triboelectric Generators (TEG) by Wang (2012), the studies are going on powering the low power devices like sensors, its power management circuits and optimal output performance behavior.

Triboelectric generators work on the principle of contact electrification and electrostatic charge generation where two materials having varying electron affinities come in contact will generate the charges thereby developing an electric potential between them. If the system is assumed as a closed-circuit electron flow takes place thereby, electricity generation happens. The contact between the materials made by small movements, vibrations, environmental changes thereby charges produced by friction [8]. The material pairs used in the TENG are termed as tribo pairs where the materials with a maximum difference in electron affinity are chosen. With the development of four modes of operation of triboelectric generators to generate electric potential, vertical contact mode where tribo materials are vertically moved apart; sliding mode where the tribo materials are slide apart, single electrode mode and free-standing mode the TENGs are used in various applications as energy recovery and regeneration system. Considering the mechanical wear of the materials in contact, vertical contact mode is of high significance in the research area for its improvement [9]. Studies have shown the efficiency of the TENG depends on the material aspects in terms of the morphology, geometry and properties. Triboelectric materials are arranged in a triboelectric series based on the electron affinities. Dielectric polymer tribomaterials are showing good usage in the industry for TENG [10]. There are various analytical methods generated theoretically to find the output performance of TENG.

In this study, the dielectrics as tribopairs will be analyzed in theoretical and numerical basis, the computational simulation will be performed on different recently used tribopairs in applications thereby finding the optimal pair for a set of input parameters.

1.1. Polymers as Triboelectric Pair

Triboelectric generators work, when a pair of material rub against each other. Thereby there will be a tendency of one material to donate electrons, while the other to accept electrons. When these materials are having a chance to mechanically separate each other, it will create an air gap which results in dipole moment on the charges generated. To equalize the electric potential generated, a small current will flow when an electric load is connected between the contacting surfaces. If continuously the materials are in contact and separated by a distance, it will provide small amount of an alternating current (AC) [11]. For the material selection as tribopairs, a high difference in electron affinities considered as highly good as a choice for good performance. Metals like Al, Cu, and Au are good electron donors to act as a tribo positive pair, but due to the oxidation and highly reactive tendency of these materials to form an oxide layer made to select polymers as tribo positive layer [12]. Among the polymers, studies shown PA6/Polyamide6 as a good tribo positive layer due to its excellent donor characteristics whereas polymers like PTFE, FEP, PDMS, KAPTON, and PVDF are tribo negative layers due to negatively charged characteristics. Polymers superpower of charge transfer and capturing capacity when the tribomaterials come into contact thereby generating friction enabled it to use for a wide range of applications in the triboelectric field [13]. Though a huge number of tribo combinations made with an enormous number of materials, not all combinations will be able to provide good results. The various properties, which determine the output characteristics of TEG pairs, include the surface charge density, dielectric constant of materials, work function, frictional coefficient, the geometry of material combinations etc. Studies have shown that the surface charge density depends on the chemical potential difference between the tribo pairs [14], and given by,

$$\sigma = \frac{[(W - E_0)e]\left(1 + \frac{t}{\varepsilon z}\right)}{{}^{t}/_{\varepsilon\varepsilon_0} + (1\sqrt{N_s(E)e^2})(1 + {}^{t}/_{\varepsilon z})} \tag{1}$$

where W is the work function of the metal, E_0 is the charge-neutrality level of the surface states, e, t, ε, ε_0 and z are the charge of an electron, distance of space, relative permittivity of dielectric, vacuum permittivity of free space and thickness of the dielectric film and $N_s(E)$ is the density of surface states. Based on this since the work function between tribo material contacts increases, surface charge density increases thereby increase in output performance. In addition to work function, the dielectric constant is an important parameter, based on which the TEG performance vary. The mathematical expression for effective surface charge density which can be transferred (σ') in terms of the initial material surface charge density (σ_0) is given by Eq.(2) [15].

$$\sigma' = \frac{-\sigma_0 d_{gap}}{d_{gap} + {}^{d_1}/_{\varepsilon_1}} \tag{2}$$

where d_{gap} is the gap distance, d_1, ε_1 are the thickness and dielectric constant of tribo material pair. The equation shows the effective surface charge density increases with the increase in dielectric constant.

2. THEORETICAL OUTPUT CHARACTERISTICS OF TEG IN VERTICAL CONTACT MODE

The output characteristics (i.e. voltage, current and power) are derived based on Gauss electric field equation where the internal electric field of each part of TENG is calculated first. Since the size of the dielectric is much larger than the air gap and the thickness of the electrode, it can assume that the electric field is like an infinite electric plate. The triboelectric vertical contact mode includes two polymer pair of different electron affinities with the electrodes attached to it as shown in Fig. 1. The equations are derived from considering three dielectric areas, of which two are dielectric pair of ε_{r1} and ε_{r2} as the dielectric constants, d_1 and d_2 their thickness.

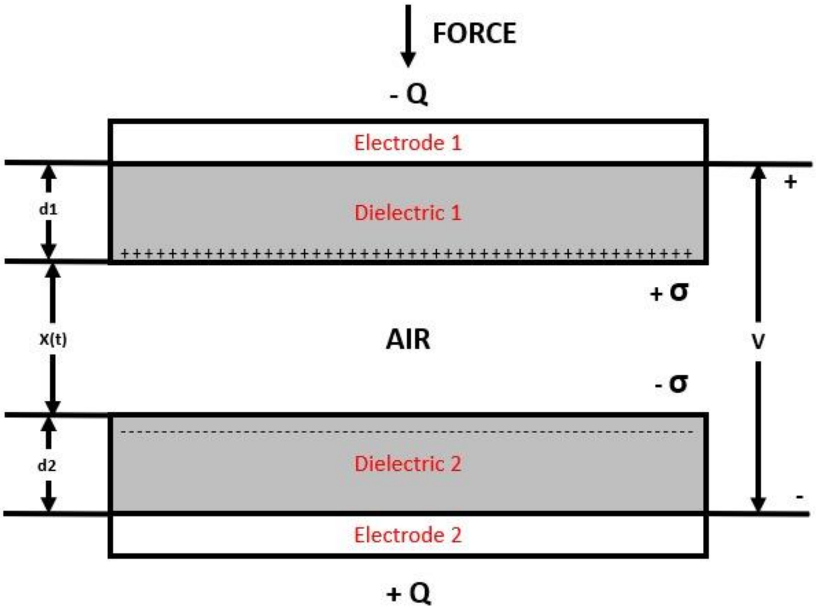


Figure 1. TEG in vertical contact mode.

$$E_{di-electric1} = \frac{Q}{A\varepsilon_0\varepsilon_{r1}} \tag{3}$$

$$E_{di-electric2} = \frac{Q}{A\varepsilon_0\varepsilon_{r2}} \tag{4}$$

$$E_{air-gap} = \frac{1}{\varepsilon_0}\left(\frac{Q}{A} - \sigma\right) \tag{5}$$

where Q is the charge generated by material in coulomb per meter square, A is the contact surface area of the dielectric material, ε_0 is the relative permittivity of vacuum [16,17]. For a separation distance of $x(t)$, of surface charge density σ, the electrical potential generated across the electrode given by Eq. (6),

$$V(t) = -\frac{Q}{A\varepsilon_0}\left(\frac{d_1}{\varepsilon_{r1}} + \frac{d_2}{\varepsilon_{r2}} + x(t)\right) + \frac{\sigma}{\varepsilon_0}x(t) \tag{6}$$

Assuming for open circuit (Q=0) and short circuit (V=0);

$$Voc = \sigma\varepsilon_0/x(t) \tag{7}$$

$$Qsc = A\sigma x(t)/(d_0 + x(t)) \tag{8}$$

Equating in Ohms law, $V = RdQ/dt$, where assuming the motion to be linear with velocity v, maximum distance as x_{max} [18,19,20]. Assuming time taken to reach x_{max} as t_{max}, where $t_{max} = x_{max}/v$, and using the displacement velocity concept condition below, $x(t) = v\ t$ ($t \leq t_{max}$) and $x(t) = x_{max}$ ($t \geq t_{max}$) charge generation with respect to time as follows:

$$Q(t) = \frac{\sigma v_0}{R\epsilon_0}e^{-(At+Bt^2)} \times \left[\frac{e^{At+Bt^2}}{2B} - M\ Erfi\left(\sqrt{Bt} + \frac{A}{2\sqrt{B}}\right) + M\ Erfi\left(\frac{A}{2\sqrt{B}}\right) - \frac{1}{2B}\right] \tag{9}$$

The error function,

$$Erfi(x) = \int \frac{2e^{x^2}}{\sqrt{\pi}}\, dx \tag{10}$$

Constant *A*,

$$A = \frac{d_0}{RA\varepsilon_0} \tag{11}$$

Constant *B*,

$$B = \frac{v_0}{2RA\varepsilon_0} \tag{12}$$

Constant *M*,

$$M = \frac{A\sqrt{\pi}}{4B\sqrt{B}} e^{\frac{A^2}{4B}} \tag{13}$$

Stands in Eq. 9. From *Q*, instantaneous current, voltage and power equated by the following expressions:

Instantaneous current,

$$I(t) = \frac{dQ(t)}{dt} \tag{14}$$

Instantaneous voltage,

$$V(t) = R\ I(t) \tag{15}$$

Instantaneous power,

$$P(t) = V(t)\ I(t) \tag{16}$$

3. SIMULATIVE EVALUATION

From the above discussions, the performance of triboelectric generators is influenced greatly by the material properties and thereby the type of material used for the implementation. Usually, materials used for the tribogenerators are nanomaterial, which can give good surface contact and hence the necessity of the right choice of materials required because of its cost. Though a vast range of materials from polymer itself there which can give output, the right combination can be found from numeric and computational analysis and evaluation. For the validation of the simulation tools, Comsol and MatLab with the theoretical concept of TEG done initially for a pair of tribo materials in the first phase. With the same methodology, five pair of TEG chosen with PA6 as the positive tribo pair, the other polymers PVDF, PDMS, PTFE, FEP, and Kapton as tribo negative pair to find the optimal pair showing the good output characteristics.

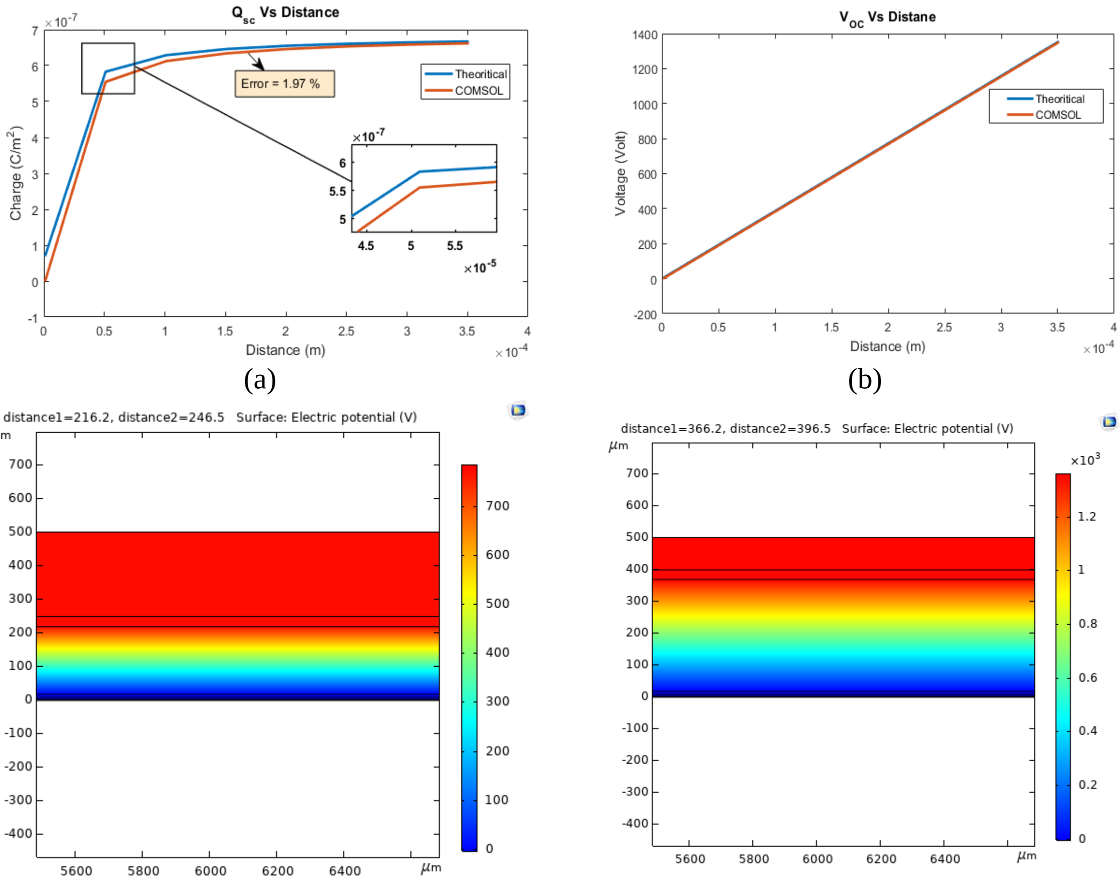
3.1. Phase study I: Validation of simulation tools

For the phase I study, a set of input data as shown in Table 1 is used to perform the numerical and computational analysis of open circuit voltage short circuit discharge based on the theoretical data from Eqs. (7,8).

Table 1. The Input data for phase I

Serial no	Material	Dielectric Thickness	Constant(m)
1	Tribomaterial1PVDF	$\varepsilon_{r1} = 7.4$	d1 $=0.1 \times 10^{-4}$
2	Tribomaterial2 PA6	$\varepsilon_{r2} = 4$	d2 $=0.3 \times 10^{-4}$
3	Contactarea A,m^2	4×10^{-4}	
4	Maximum distance(x)m	4×10^{-3}	

The other assumption taken for the model is the surface charge density of 34.2μC/m^2 for the study.



(a) (b)

(c) (d)

Figure 2. Numerical and computational study: (a) Q_{sc} vs distance (b)V_{oc} vs distance (c)V_{oc} distance 246.5μm spacer gap (d) V_{oc} distance 396.5μm spacer gap

The results show a good agreement between the numerical and Comsol results. The V_{oc} and Q_{sc} value for both the analysis results are shown in Figs. 2(a,b). The average error of numerical results with the Comsol is 1.97%, which is in good agreement with the theoretical data. The theoretical value matches with the Comsol values, which show the Comsol and MatLab simulation in agreement with the theoretical concept of TEG.

3.2. Phase study II: Simulation study of polymer tribopairs

Numerical study on tribopairs of five sets of polymers is done in Matlab. The input data chosen for the study is based on the material properties and polymer characteristics fit for the tribo device especially in the case of mechanical properties wear and tear of the materials. The assumptions taken for the study includes the surface charge density as 20 μC/m^2 and all the combination is subjected to a resistive load of 100Mohm. The contact area A is taken as 50x10^{-4}m^2, dielectric thickness 1 and 2 taken as 0.1x10^{-3}m. All the combinations are subjected to vertical contact mode for a maximum spacer distance of 5mm, the velocity of 0.1m/s for a time period of 20ms. PA6 is taken as tribo positive pair for all other materials in Table 2.

Table 2. The Input data for phase II

Item no	Material	Relative Permittivity
1	PA6	4
2	PVDF	7.4
3	PDMS	2.75
4	PTFE	2
5	FEP	2.1
6	KAPTON	3.34

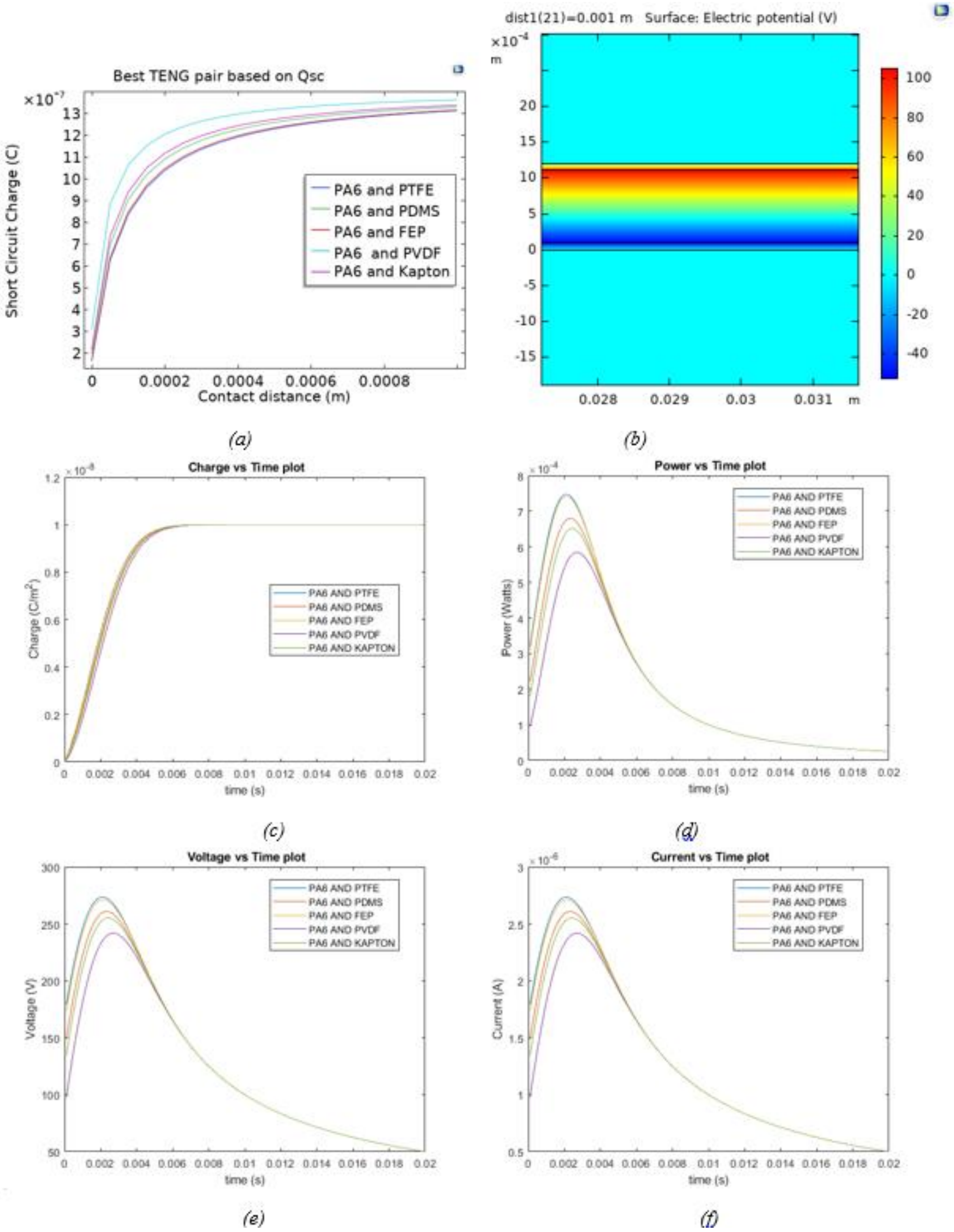


Figure 3. Numerical and computational simulation for polymer tribo pairs: (a) Q_{sc} vs x, (b) Q_{sc} vs x from Comsol simulation, *(c) Q vs t, (d) P vs t, (e) V vs t, (f) I vs t.*

The simulation is performed based on the theoretical Eqs. (9-16). From Figs. 3(a-f), PA6 and PTFE combinations show good output performance characteristics in terms of output current, voltage and power. PA6 and FEP combinations also show a similar performance to that of PTFE pair. Due to the presence of strong C-F bond and hence its high electronegativity results in the strong pull of electrons during the material contact, the PA6 PTFE simulation shows maximum power flux 0.75 mW/m^2 with the assumed surface charge density of 20 μC/m^2, when a load of 100 Mohm is connected in the circuit. More power can be expected by improving the material morphology and properties thereby improving the surface charge density [21].

A further study of the materials pairs evaluated by varying the load resistance from zero to infinity for all the material combinations as shown in Fig. 4. The results show that PA6 PTFE and PA6 FEP combination pair produce maximum power around 100 Momh resistance. Such high resistances have also been encountered in the piezoelectric specimens according to the literature, too [22].

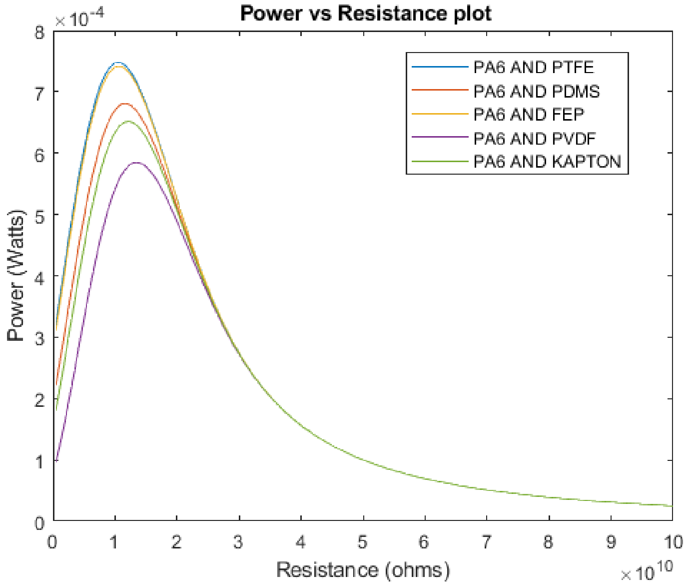


Figure 4. Power vs Resistance for tribo material pairs.

A study on varying the surface charge densities shows an increase in power with squares of the surface charge density, which is in agreement with the power formula as shown in Fig. 5.

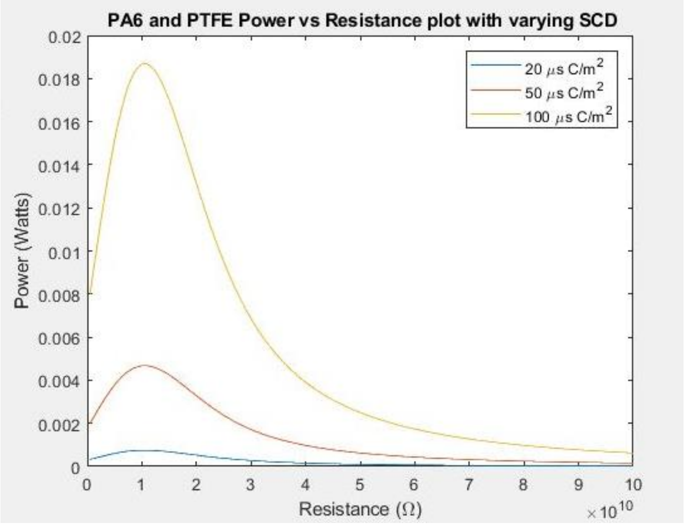
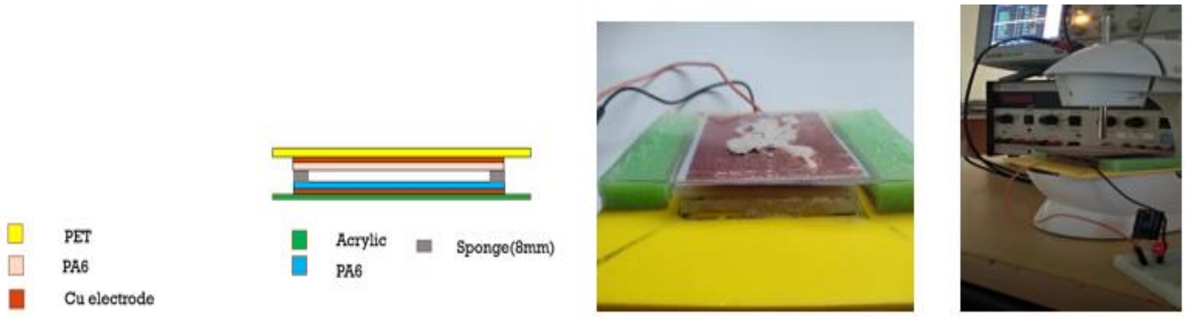


Figure 5. Power vs resistance by varying the surface charge densities for PA6 PTFE pair.

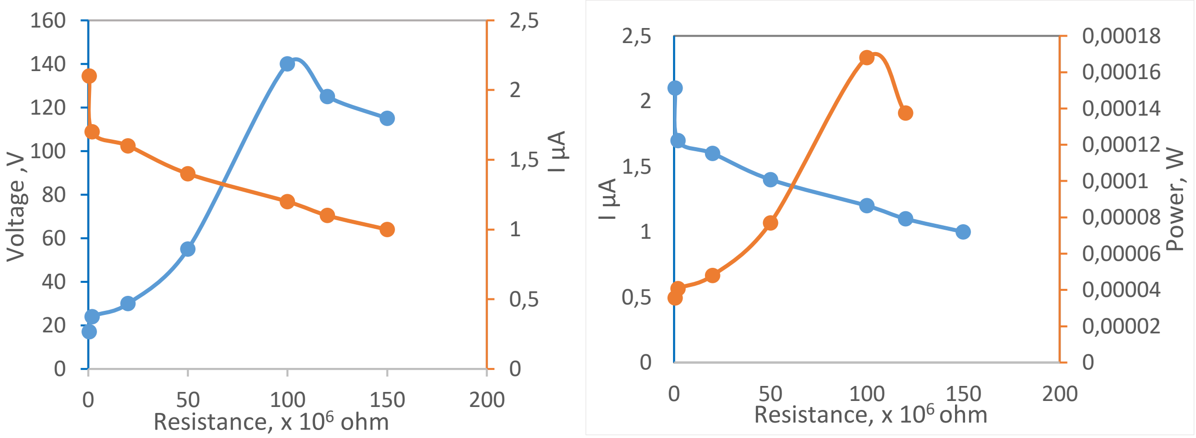
Since high surface charge density produces high output power, by patterning the tribo pairs at the contact surface can improve the contact area, ionized air injection can also enhance the tribo pair output power performance [23]. For the accuracy of the study, a polymer pair experiment is done based on vertical contact mode for validation. A TENG device is made of PTFE PA6 polymer pairs. PA6 used is AM303010 Polyamide - Nylon 6 Sheet of thickness 1mm and PTFE FP303050 Polytetrafluoroethylene Sheet of thickness 1mm. The materials are purchased from Goodfellow Cambridge Ltd., UK. The material combination PTFE PA6 is taken of which both are of size 5cm x 5cm x 1mm. For performing the experiment, PTFE is attached to the Cu electrode that is then supported with PET sheet of 2mm thickness and of size 7cm x 5cm.For the positive pair PTFE is attached to the acrylic substrate through Cu conductive electrode. The experiment is conducted for a gap of 8mm that is maintained by using a sponge of 2.5cm x 5cm.In the experiment triboelectric pair is fixed in a vertical moving shaft of electric sewing machine as shown in Fig. 6.



(a) *(b)* *(c)*

Figure 6. Experiment of vertical contact mode polymer tribo pair: (a) PTFE PA6 TENG, (b) device for experiment, (c) TEG in loading device powering red LED in glowing and a capacitor in charging stage.

The experiment is evaluated on the TEG device by varying resistors from 100 Kohms to 150 Mohms range. The voltage and current output characteristics are measured using HM 8012 multimeter, micro ammeter and GW INSTEK - GDS-2062 - Oscilloscope, DSO, 2 CHANNEL, 60MHZ. TEG will have high output impedance thereby the load resistor resistance will be high [24]. To match the impedance with TEG and to get accurate measurement, 2KV 250MHz P4250 100X BNC Oscilloscope High-voltage Probe is used for measurements. The results showed in agreement with the Comsol and MatLab numerical result as shown in Fig. 7(a,b). The maximum power output is shown 0.00016 Watts at 100 Mohm and an optimal power of 0.0001 W at 70 Mohm as shown in Fig. 7(b).



(a) *(b)*

Figure 7.Output performance of TEG: (a) Output voltage and current versus resistance, (b) Output current and power versus resistance.

Assuming a mechanical force of 1N applied through a distance of 8mm with 40-rpm motor speed, the input mechanical power is calculated around 0.00055 Watts, thereby calculated energy efficiency of the TENG system as 28.6%. The power generated from the vertical motion of the device is tested on powering a red LED and charging a capacitor of 100µF by replacing the load resistors as shown in Fig. 6 (c). The device measurement has shown 155V of open circuit voltage V_{oc} and the maximum output voltage, current and power is coming near to a resistance value of 100Mohms thereby showing the results in agreement with the numerical methods.

4. CONCLUSION

Triboelectricity has been a promising solution for the harnessing waste mechanical energy. The study to enhance the output performance of the device is an emerging area in research. The flexibility of choosing a variety of materials from organic to inorganic and to polymers, composite as tribo material pairs made the technology cheap and reliable. The polymer pairs as tribo materials are giving good performance characteristics compared to all other material combinations. Efficient tribo material combination by simulative evaluation show fluoropolymers PTFE, FEP with PA6 good output performance. Further studies done by evaluating the output power with the varying load resistance for all the tribo polymer combinations, numerically and experimentally. The validated simulation generated in the current study can be universally accepted and extended further to evaluate the output performance of any tribo material pair before the experiment and hardware implementation. The study shows how effectively power can be generated from low cost materials by simple construction and easy fabrication when compared to piezoelectric generators using high cost materials.

Acknowledgment

This research is supported by the Expo Live Innovation Impact Grant Programme 2020 who granted the University of Bolton RAK Academic Centre AED 50000 for winning the research and innovation university summit of Expo 2020. We would also like to show our gratitude to Jikui Luo, Research Supervisor, University Of Bolton, Bolton, BL3 5AB, United Kingdom, for sharing and mentoring the pearls of wisdom with us during this research.

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