Piezoelectric mathematical modeling; technological feasibility in the generation and storage of electric charge

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Abstract. Emerging technologies are efficient alternatives for satisfying the growing demand for sustainable and cheap energy sources. Piezoelectrics are one of the most promising energy sources derived from emerging technologies. These materials are capable of converting mechanical energy into electricity or vice versa. Piezoelectrics have been used for almost a hundred years to generate electrical and sound pulses. However, the use of piezoelectrics for power generation is constrained by the cost associated with equipment and infrastructure. This problem has been addressed through mathematical models that relate the physical and electrical properties of the piezoelectric material with the voltage generated. Although these models have high performance, they do not incorporate voltage rectification and electrical charge storage stages. This work presents a mathematical model that describes the relationship of the physical and electromechanical properties of a system employing a piezoelectric for energy generation. The voltage of the system and the charge stored in a capacitor are calculated through this model. Also, contour diagrams are presented as a tool for facilitating the efficiency of energy generation.

1. Introduction
Electronics, the direct application of electrodynamics, is fundamental to the current development of technology [1]. Electromechanics, the study of electrical conduction as a driving factor in the movement of bodies, is an important research area in the search for new sustainable technologies. One of the most promising research areas within electromechanics is the study of piezoelectrics. These materials are capable of generating electrical energy through passive vibrations and vice versa [2].

Piezoelectrics have a symmetric crystalline structure that is characterized by having a polar axis [3]. If an external force is applied to the endpoints of the polar axis, it induces a change in the polarization field of the crystal. The polarization change induces the displacement of electric charges towards the surface of the piezoelectric [4]. The intensity of the electric current is proportional to the piezoelectric cross-sectional area and the pressure gradient [5]. Subsequently, if the piezoelectric is connected to a rectifier, the induced alternating current can be converted to a direct current and be stored at a capacitor’s plates [1].

Piezoelectric materials have wide medical and acoustic applications due to their ability to generate movement, such as vibrations, from electrical pulses [6]. However, the process through
which passive vibrations generate electrical pulses remains poorly studied. This, along with the lack of an adequate description on the cost-energy benefit relation, has caused that piezoelectric materials have not managed to thrive in the energy generation sector [6].

The relationship between vibration frequency and the voltage of a piezoelectric is described by the mathematical model proposed by Roundy and Wright in [7]. This model gives an approximate representation of the vibration mode of the vibrating piezoelectric as a harmonic oscillator [3]. Still, it does not provide a qualitative, or quantitative, description of the relationship of the piezoelectric characteristics and the induced voltage not the magnitude of the charge that can be stored into a capacitor connected to the piezoelectric through a voltage rectifier [8].

This work shows the derivation of a mathematical model, coded in the open-source software “Octave”, to describe the relationship of the physical and electromechanical properties of the piezoelectric, concerning the vibratory system, gives the voltage and charge of the capacitor as output variables. Also, we present graphical and analytical expressions capable of estimating the efficiency of the system under study.

2. Methodology

In general, piezoelectric equations describe how the motion of a mechanical element can be associated to an electric field. Hassenzahl in [9] explain if an external force is applied to the piezoelectric, it can induce a mechanical deformation ($S_1$). The magnitude of the deformation can be calculated as the sum of the applied stress ($T_1$) multiplied by the elastic constant ($s_{11}$) plus the electric field ($E_3$) multiplied by the piezoelectric coefficient of the material ($d_{31}$). This relationship is shows in Equation (1).

$$S_1 = s_{11}^E T_1 + d_{31} E_3.$$  

(1)

Whereas, Equation (2) allows to calculate the electric displacement vector ($D_3$) as the sum of the stress, multiplied by the piezoelectric coefficient, and the electric field ($\varepsilon_3^T$), multiplied by the electric permittivity:

$$D_3 = d_{31} T_1 + \varepsilon_3^T \varepsilon_3.$$  

(2)

A simple description of the mechanical and electrical components of a piezoelectric system, in which an electric field is produced as a consequence of the mechanical deformation of a moving beam [3], is shown below.

2.1. Mechanical components

The piezoelectric system is based on a beam submitted to a bending stress and trough its movement is able to produce an electric field. Roundy and Wright in [7] shows the inertia moment of the beam is calculated by Equation (3).

$$I = 2 \left[ \frac{b \cdot h_p^3}{12} + b \cdot h_p^2 \cdot h_{ps} \right] + \frac{\eta_s h_s^3}{12},$$  

(3)

where $I$ is the second moment of inertia of the beam (measured in $m^4$), $b$ is the width of the beam, $h_p$ and $h_s$ are the thickness of the piezoelectric and metallic layers, $h_{ps}$ is the distance
between the neutral axis of the beam and the central plane. Whereas, $\eta_s$, Equation (4), corresponds to Young’s module between the piezoelectric and metallic materials:

$$\eta_s = \frac{E_{sh}}{E_p},$$

with $E_p$ is the Young’s modulus of the piezoelectric material (measured in Pa) and $E_{sh} = 2\times10^9$ Pa. The physical size of the piezoelectric is important for the calculation of the torsional force. The coefficient $k_1$, shown in Equation (5), represents a constant of proportionality in conjunction with the bending moment with the second moment or “moment of inertia”.

$$k_1 = \frac{h_p(4l_b + 3l_m)}{4I},$$

where $l_b$ and $l_m$ correspond to the free length of the beam and the length of the mass element. Whereas, the coefficient $k_2$, Equation (6), describes the constant of proportionality in the geometry of the piezoelectric.

$$k_2 = \frac{l_b(l_c + l_b)}{3b},$$

with $l_c$ representing the embedement length. In turn, $E_p$ divided by the product of the constants $k_1$ and $k_2$ express the amount of force required to move the spring through a fixed distance.

2.2. Electrical components
The coefficient of mechanical coupling ($k_{31}$) describes the connection between the piezoelectric coefficient and the resulting electric flux when the electric flux as show the Equation (7).

$$k_{31} = \sqrt{\frac{d_{31}^2 E_p}{\varepsilon}},$$

going from zero, when the system is not vibrating, to one, when the product of the piezoelectric coefficient and the electric field equal the permittivity constant ($\varepsilon$) of the piezoelectric. Regarding the storage of the electrical energy generated; the capacitance of the piezoelectric correspond to the Equation (8).

$$C_b = \frac{a^2 \varepsilon \ast b \ast l_c}{2h_p},$$

where the value of $a$ defines if the configuration of the system corresponds to a serial connection ($a = 1$) or to a connection in parallel ($a = 2$). The Equation (9), is the voltage in the frequency domain, unifies the contribution of the mechanical and electrical components of the system. This equation gives the amplitude of the voltage that passes through the rectifier as a function of the electric resistance of the system ($R$), its capacitance and the system’s vibrational frequency ($\omega$) and the acceleration amplitude ($A_{in}$).
\[ V(\omega) = \left\{ j\omega \frac{2E_p d_{31} h_p A_{mn}}{a + \varepsilon} \frac{k_2}{k_1} \right\} \]
\[ \times \left\{ \omega_n^2 \left( \frac{1}{R + C_b} + \frac{2\varepsilon \omega_n}{R + C_b} \right) - j\omega \left[ \omega_n^2 \left( 1 + \frac{k_2^2}{31} \right) + \frac{2\varepsilon \omega_n}{R + C_b} - \omega^2 \right] \right\}^{-1}, \quad (9) \]

where \( j \) is the imaginary unit, \( \omega_n \) is the maximum frequency of oscillation (measured in Hz) shows as Equation (10).

\[ \omega_n = \sqrt{\frac{E_p}{k_1 k_2 M}}, \quad (10) \]

and \( M \) corresponds to the inertia mass (measured in kg). Equation (11) shows the proportionality relation between the voltage produced by the alternating current and the one that the system acquires when this current pass trough the rectifier and its transformed into direct current [10].

\[ V_{cd} = 0.636 \times |V(\omega)|. \quad (11) \]

Finally, the charge Equation (12) relates the final charge, obtained by passive vibrations, to the piezoelectric capacitance and voltage [1].

\[ Q = C_b \times V_{cd} \quad (12) \]

3. Results
We started from the one-degree of freedom mathematical model proposed by Rondy [7] and coded the equations that make up the passive vibrational system conformed by the piezoelectric, the rectifier, and the capacitor. We used the data shown at the website of two international suppliers of piezoelectric materials to select the kind that could be fit the available resources and specifications of this study (Steiner & Martins Inc. in [11] and PICERAMIC in [12]). Table 1 and Table 2 shows the physical and electric properties of three piezoelectric plates which represent, respectively, the most economic option, one with an average cost and the most expensive one.

Table 1. Physical specifications of two piezoelectric plates obtained from Steiner & Martins Inc. in [11] and one from PIECERAMIC’s in [12].

| Model           | Price (USD) | Length (mm) | Width (mm) | Deep (mm) | Free length (mm) | Young module (Pa) |
|-----------------|-------------|-------------|------------|-----------|------------------|------------------|
| SMPL25W25T35411R | 69.80       | 25          | 25.0       | 3.50      | 22               | 54               |
| SMPL25W5T30311  | 139.94      | 25          | 5.0        | 0.30      | 22               | 53               |
| PL112           | 358.00      | 18          | 9.6        | 0.65      | 12               | 63               |
Table 2. Electrical specifications of two piezoelectric plates obtained from Steiner & Martins Inc. in [11] and one from PIECERAMIC’s in [12].

| Model                | Capacitance (F) | K31 (mm) | d31 (mm) | E_r (mm) | C_b (mm) | Natural Frequency (Hz) |
|----------------------|-----------------|----------|----------|----------|----------|------------------------|
| SMPL25W25T35411R     | 69.80           | 25       | 25.0     | 3.50     | 22       | 54                     |
| SMPL25W5T30311       | 139.94          | 25       | 5.0      | 0.30     | 22       | 53                     |
| PL112                | 358.00          | 18       | 9.6      | 0.65     | 12       | 63                     |

With the physical and electrical properties from the Table 1 and Table 2 of each piezoelectric plate, Equations (3) to Equation (11) were used to calculate the factorial regression Equation (13) and Equation (13). These equations give the rectified voltage and capacitor charge as a function of the system’s resistance and acceleration amplitude:

\[ y = a + b \cdot x_1 + c \cdot x_2 + d \cdot x_1 \cdot x_2 \]
\[ y = e + f \cdot x_1 + g \cdot x_2 + h \cdot x_1 \cdot x_2, \]  

where \( x_1, x_2 \) correspond, on each case, to the system’s resistance and acceleration amplitude (Equation (13)) or to the acceleration amplitude and oscillation frequency (Equation (13)). The values of each of the coefficients for the factorial regression are shown in Table 3.

Table 3. Coefficients of the factorial regression equation for each piezoelectric obtain from the authors.

| Model                | a    | b    | c    | d    | e    | f    | g    | h    |
|----------------------|------|------|------|------|------|------|------|------|
| SMPL25W25T35411R     | 0.1098 | 0    | 0.0295 | 0   | -0.2693 | 0.3180 | -0.2693 | -0.0033 |
| SMPL25W5T30311       | 4.6028 | 0    | 0.2373 | 0   | -0.2693 | 0.0273 | 0.0280 | -0.0003 |
| PL112                | 1.0498 | 0    | 0.0715 | 0   | -0.2693 | 0.0846 | 0.0028 | -0.0009 |

Graphically, these analytical expressions are described through the contour diagrams shown in Figure 1. The first three diagrams relate the effect of the resistance and acceleration amplitude on the resulting voltage while the last three show the magnitude of the final charge as a response to the acceleration amplitude and vibrational frequency of the system.

Figure 1(a), shows it is possible to obtain a voltage that can be used in home electrical systems since the operating range goes from 0 to 90 Volts (V). Specifically, to obtain a low voltage value (less than or equal to 10 V) the resistance can have relatively any value. However, the acceleration amplitude must be low. By increasing the acceleration amplitude, the voltage will be greater and what will limit the spectrum that the voltage can occupy will be the value of the resistance where, if it is less (100 KΩ), the voltage will remain low, while if it is higher (1 MΩ) when moving the acceleration amplitude upwards there is a wide voltage spectrum that can reach 110 V.

Figure 1(b) shows a significant increment on the voltage range (reaching almost to 2500 V) and, in particular; the broadest region corresponds to the smallest voltage response (around 500 V), which could indicate stability in the piezoelectric since for many combinations of resistance and acceleration amplitude it remains within this range. The other regions of the contour diagram have a similar width to their analogs in Figure 1(a). In Figure 1(c) shows that the last piezoelectric produces a intermediate range for the voltage response (around 600 V).
The contour diagrams of the panels in Figure 1(d), Figure 1(e) and Figure 1(f) describe the relation of acceleration amplitude with frequency of the system to obtain the electric charge, it is observed that: The curves that divide each load spectrum have a positive slope, in addition to the fact that the spectrum with the lowest load predominates, where it can be seen that, for high values of frequency and acceleration amplitude, the load will have small values compared to when there are low values. frequency and the acceleration amplitude is varied. However, the loading capacity has a significant variation with a maximum magnitude of $2.5 \times 10^3 \text{ C}$, $0.025 \text{ C}$ and $6.25 \times 10^{-3} \text{ C}$; values that can be used in various health, technology and energy sectors.

![Contour diagrams](image)

Figure 1. Contour diagrams that relate the effect of resistance and amplitude obtaining the voltage as a response (a), (b), and (c); contour diagrams that relate the final electric charge as a response to the system’s vibrational frequency and acceleration amplitude (d), (e), and (f).

4. Conclusions
This work describes the usage of free access software (Octave), to define, based on the requirements of an electrical circuit, the physical characteristics and mechanical and electrical properties of a piezoelectric coupled to a passive vibrational system. The mathematical model of Roundy and Wrigth was coupled to the equations for the rectification voltage and charge of the system. The resulting two factorial regression equations allow to define the specifications of a piezoelectric to evaluate the technical and economic feasibility of its implementation. As a future work, it is planned to expand the present equations to include the relevant thermodynamic properties for the system.

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