



Original software publication

Pypiezo-GO: A software tool for processing electromechanical measurements of piezoelectric reduced graphene oxide-cement composites



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ABSTRACT

Self-diagnostic composites have become increasingly popular for structural health monitoring due to their ability to develop load-bearing strain sensors. Piezoelectric cement composites, in particular, represent an emerging area of research with vast potential for developing innovative self-powered or ultra-low power consumption sensors. In this context, this paper presents Pypiezo-GO, a software tool designed for the electromechanical characterization of reduced graphene oxide (rGO)-cement composites. The software tool, developed as an online cloud computing platform, accesses a database organized into DataFrame structures. The database contains the measurements from a set of experiments conducted on rGO-cement samples, including open circuit potential, cyclic voltammetry, and compressive testing. On this basis, Pypiezo-GO allows extracting the electrical properties of the samples, including their capacitance and piezoelectric factors. Furthermore, the platform enables the comparison of experimental time series with numerical predictions from a lumped circuit model implemented in MATLAB/Simulink, which is also included in this contribution. The presented software code is intended to represent a valuable tool for the development of new piezoelectric cement composites for strain self-sensing applications.

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Current code version	v1.0
Permanent link to code/repository used for this code version	https://github.com/ElsevierSoftwareX/SOFTX-D-23-00305
Permanent link to reproducible capsule	N.A.
Legal Code License	GPL
Code versioning system used	git
Software code languages, tools, and services used	Python 3.7
Compilation requirements, operating environments & dependencies	The file Medidas_GO.xlsx and the path files of impedance, voltammetry, open circuit potential, and compressive measurements
If available Link to developer documentation/manual	https://github.com/dantrica/cement-based-composites/blob/main/README.md
Support email for questions	dantrica@saber.uis.edu.co

1. Motivation and significance

Carbon-based additives, such as carbon nanotubes (CNTs), graphite, carbon fillers (CF), graphene oxide (GO), or reduced

graphene oxide (rGO), have been widely studied over the past decade to enhance the physicochemical properties of cementitious materials, such as stiffness, strength, or fracture toughness, and to improve hydration reactions and reduce carbonation contents [1–3]. More recently, researchers have found that these composites can also provide cement pastes with strain self-sensing capabilities, being possible to develop load-bearing sensors with high potential for structural health monitoring (SHM)

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	A	B	C	D	E	F	G	H	I	J	K	L	M	N	O	
	time	specimen	measure	serie	measurement_date	sample_fabrication_date	path	start_curing_date	end_curing_date	concentration	re	energy	solvent	electric	field	remarks
1	5/10/2022 22:18:00	p30	OCP	1	6/4/2022	20220406_e_MedidasOCP_p30_1.txt	2023/02/01	2023/02/01	0.2259 g / 80 g H2O-GO	Branson	Agua tipo 1	Ninguno	(febrero 20) por 2 horas (equipo Branson)			
2	5/10/2022 22:18:00	p40	OCP	1	6/4/2022	20220406_e_MedidasOCP_p40_1.txt	2023/02/01	2023/02/01	0.2259 g / 80 g H2O-GO	Branson	Agua tipo 1	Ninguno	(febrero 20) por 2 horas (equipo Branson)			
3	5/10/2022 22:18:00	p41	OCP	1	6/4/2022	20220406_e_MedidasOCP_p41_1.txt	2023/02/01	2023/02/01	0.2259 g / 80 g H2O-GO	Branson	Agua tipo 1	Ninguno	(febrero 20) por 2 horas (equipo Branson)			
4	5/10/2022 22:18:00	p42	OCP	1	6/4/2022	20220406_e_MedidasOCP_p42_1.txt	2023/02/01	2023/02/01	0.2259 g / 80 g H2O-GO	Branson	Agua tipo 1	Ninguno	(febrero 20) por 2 horas (equipo Branson)			
5	5/10/2022 22:18:00	p43	OCP	1	6/4/2022	20220406_e_MedidasOCP_p43_1.txt	2023/02/01	2023/02/01	0.2259 g / 80 g H2O-GO	Branson	Agua tipo 1	Ninguno	(febrero 20) por 2 horas (equipo Branson)			
6	5/10/2022 22:18:00	p44	OCP	1	6/4/2022	20220406_e_MedidasOCP_p44_1.txt	2023/02/01	2023/02/01	0.2259 g / 80 g H2O-GO	Branson	Agua tipo 1	Ninguno	(febrero 20) por 2 horas (equipo Branson)			
7	5/10/2022 22:18:00	p45	OCP	1	6/4/2022	20220406_e_MedidasOCP_p45_1.txt	2023/02/01	2023/02/01	0.2259 g / 80 g H2O-GO	Branson	Agua tipo 1	Ninguno	(febrero 20) por 2 horas (equipo Branson)			
8	5/10/2022 22:18:00	p46	OCP	1	6/4/2022	20220406_e_MedidasOCP_p46_1.txt	2023/02/01	2023/02/01	0.2259 g / 80 g H2O-GO	Branson	Agua tipo 1	Ninguno	(febrero 20) por 2 horas (equipo Branson)			
9	5/10/2022 22:18:00	p47	OCP	1	6/4/2022	20220406_e_MedidasOCP_p47_1.txt	2023/02/01	2023/02/01	0.2259 g / 80 g H2O-GO	Branson	Agua tipo 1	Ninguno	(febrero 20) por 2 horas (equipo Branson)			
10	5/10/2022 22:18:00	p48	OCP	1	6/4/2022	20220406_e_MedidasOCP_p48_1.txt	2023/02/01	2023/02/01	0.2259 g / 80 g H2O-GO	Branson	Agua tipo 1	Ninguno	(febrero 20) por 2 horas (equipo Branson)			
11	5/10/2022 22:18:00	p49	OCP	1	6/4/2022	20220406_e_MedidasOCP_p49_1.txt	2023/02/01	2023/02/01	0.2259 g / 80 g H2O-GO	Branson	Agua tipo 1	Ninguno	(febrero 20) por 2 horas (equipo Branson)			
12	5/10/2022 22:18:00	p50	OCP	1	6/4/2022	20220406_e_MedidasOCP_p50_1.txt	2023/02/01	2023/02/01	0.2259 g / 80 g H2O-GO	Branson	Agua tipo 1	Ninguno	(febrero 20) por 2 horas (equipo Branson)			
13		p30	f		6/4/2022	20220406_f_Medidasf_p30										
14		p40	f		6/4/2022	20220406_f_Medidasf_p40										
15		p41	f		6/4/2022	20220406_f_Medidasf_p41										
16		p42	f		6/4/2022	20220406_f_Medidasf_p42										
17		p43	f		6/4/2022	20220406_f_Medidasf_p43										
18		p44	f		6/4/2022	20220406_f_Medidasf_p44										
19		p45	f		6/4/2022	20220406_f_Medidasf_p45										
20		p46	f		6/4/2022	20220406_f_Medidasf_p46										
21		p47	f		6/4/2022	20220406_f_Medidasf_p47										
22		p48	f		6/4/2022	20220406_f_Medidasf_p48										
23		p49	f		6/4/2022	20220406_f_Medidasf_p49										
24		p50	f		6/4/2022	20220406_f_Medidasf_p50										
25		p30	CV	0kg_2	6/4/2022	20220406_e_MedidasCV_p30_0kg_2.txt										
26		p40	CV	50kg_2	6/4/2022	20220406_e_MedidasCV_p40_50kg_2.txt										
27		p50	CV	100kg_2	6/4/2022	20220406_e_MedidasCV_p50_100kg_2.txt										

Fig. 1. Excel spreadsheet that manages the measurements from the mechanic and electric tests.

applications [4]. Most studies have focused on their piezoresistive properties as the main strain self-sensing principle [5–7].

For instance, it is worth noting the work by Ding and co-authors [8] who reported the electromechanical characterization of CF-CNTs cement composites. By directly synthesizing 1.5 vol.% of CNTs on the CF, their results reported excellent increases in the mechanical properties as well as in the piezoresistive properties ($0.506\% \text{ MPa}^{-1}/221.6$). Nevertheless, while promising, piezoresistive sensors require an external electric power supply to conduct electrical resistivity measurements and to infer the strain condition, which represents a serious obstacle to their field implementation. Therefore, researchers are exploring emerging self-powered sensing technologies, such as piezoresistive materials combined with energy harvesting devices [9], piezothermal sensors [10], or piezoceramic composites [11]. In this light, Triana-Camacho et al. [12] reported the development of piezoelectric rGO-cement composites with self-powered strain sensing capabilities. These materials require a minimal power supply to record and transmit the electrical output data, making it possible to adopt ultra-low power consumption electronics for SHM field applications. The electromechanical characterization of these materials for strain sensing applications is challenging, since it involves a series of mechanical and electrical tests involving different measurement systems. This requires researchers to manually work on the data processing of the experimental data, with software tools such as Origin, Excel, or software available in potentiostats [13]. To facilitate this task, this manuscript presents a software tool called Pypiezo-GO for the processing of the electromechanical tests conducted for the rGO-cement samples reported in [12].

Pypiezo-GO comprises a sequence of methods developed in Python language and implemented on a Google Colaboratory notebook, which is suitable for efficient cloud computing and simplifies the cooperative work between the researchers. The experimental database is organized with a Data-Frame called *Medidas_GO.xlsx*. This Excel file includes the paths and metadata of the experimental measurement files with extensions .txt or .xlsx. In particular, the experimental database includes the measurement records extracted from cyclic voltammetry (CV), open circuit potential (OCP), and compressive testing (CT), as reported in Ref. [12]. On this basis, Pypiezo-GO synchronizes the mechanical and electrical records, calculates the effective capacitance and the piezoelectric parameters of voltage g_{33} and charge d_{33} , which represent the key features of these materials for their use as strain sensors. The code also includes the possibility of calibrating a lumped equivalent circuit developed in MATLAB/Simulink for signal processing applications.

2. Software description

The experimental database is organized in the Excel file *Medidas_GO.xlsx*, which contains the directories of all the measurement files (CT, CV, and OCP), as well as the metadata about the fabrication methodology of the rGO-cement specimens (Fig. 1), such as the start and end dates of the curing, the filler concentration, the dispersion energy, and the solvent agent. This information is loaded in code cell 1.1. in Pypiezo-GO (see Fig. 2), where the user has to choose one or more specimens to perform the analysis. Then, the experimental data are loaded in code cells 1.2. and 1.3., which include the electrical (voltage and current) and mechanical (force and deformation) time series. Such data are then synchronized in the code cell 1.4. by linear time interpolation using the method `interp`. Afterwards, the method `plot_electromechanical` in the code cell 1.5. is in charge of plotting the output graphs, and computing new electric (power, resistance, and fractional change in resistance (FCR)) and mechanic (strain and stress) data series. The code cells inside the module 2.0. contain the plotting options and the correlations between strain and other data series such as force, voltage, current, resistance, power, and FCR. Finally, the module 3.0. conducts the comparison between the numerical simulations of the equivalent lumped circuit described hereafter in Section 2.1 and the experimental curves in terms of FCR, electric power, and piezovoltage.

The module 4.0. (Analysis of voltammograms) allows getting the capacitance as a function of the applied force. To this aim, the capacitance of the samples is calculated by integrating the area under the CV curves for cyclical compression loads, including force values of 0, 500, 1000, 1500, 2000, and 2500 N. Note that, as indicated in Ref. [12], the integral of the voltammograms is related to the specimen's capacitance. The capacitance is a key magnitude to determine the piezoelectric charge parameter d_{33} together with estimating the correlation between the output piezovoltage and the applied force. Instead, the piezoelectric voltage parameter g_{33} depends only on the generated voltage, the applied force, and the geometry of the rGO-cement composites. Finally, the code cell 5.0. of Pypiezo-GO is dedicated to saving the electromechanical characterization parameters, the output plots, as well as their file paths into a new DataFrame saved with extension .xlsx.

2.1. Equivalent lumped circuit

An equivalent lumped circuit model implemented in MATLAB/Simulink environment to interpret and predict the experimental results is also included in Pypiezo-GO. For an in-depth discussion on the structure and accuracy of the equivalent circuit,

1.1. Selection of the specimen(s).

```
data = pd.read_excel('data/Medidas_GO_20220406.xlsx')
#path_list = data.path
#measure = ['OCP', 'f']

ss1 = input("Please select the specimens from (p39 - p50), for instance: p39 p44 ... : ")

def to_list(string):
    li = list(string.split(" "))
    return li
picked_samples = to_list(ss1)

print('Chose specimen(s) is/are: ', picked_samples)
```

Please select the specimens from (p39 - p50), for instance: p39 p44 ... : p39
Chose specimen(s) is/are: ['p39']

Fig. 2. Code cell to support the selection of the specimen for analysis.

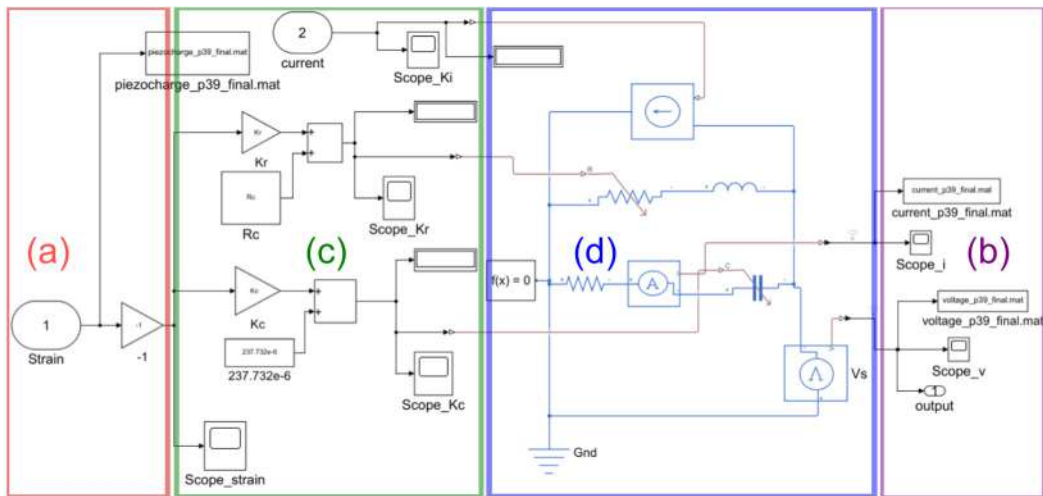


Fig. 3. Equivalent lumped circuit model implemented in Simulink. The model is organized into (a) input, (b) output, (c) electromechanical, and (d) circuit definition blocks.

readers may refer to the main work in [12]. The parameters of the circuit include the resistive λ_{R_m} and capacitive λ_{C_m} gauge factors, the cement matrix R_m and charge transfer R_{ct} electric resistances, as well as the inductance L and capacitance C_m of the composite. The Simulink model was designed with three major blocks: (i) inputs and outputs, which represent the applied strain on the rGO-cement composite as input, and the resulting electric current and voltage generated by the composite as outputs (see Figs. 3(a) and 3(b), respectively); (ii) electromechanical coupling blocks (Fig. 3(c)), which consist of transfer functions that establish the relationship between the parameters R_m and C_m and the applied strain; and (iii) the circuit model, composed of the piezoelectric (current source), piezocapacitive (charge transfer resistance and capacitance controlled by the applied mechanical strain), and piezoresistive branches (resonance inductor and resistance controlled by strain) (Fig. 3(d)).

The parameters of the model are estimated by inverse calibration using experimental data of generated voltage and mechanical strain. Specifically, the model calibration is defined as a minimization problem with a cost function involving the mean squared errors between the model predictions and the experimental data. The optimization problem is solved using the gradient descent optimization algorithm implemented in Simulink. To obtain physically meaningful solutions in the calibration, the

model parameters are constrained to realistic intervals. In particular, the gauge factors λ_{R_m} and λ_{C_m} are restricted to the intervals $(0, \infty)$ and $(-\infty, 0)$, respectively. With regard to the intervals of the passive components, the resistances are restricted to $(R_m > R_{ct})$, while the capacitance (C_m) and inductance (L) are forced to maintain positive values. In these analyses, given the suspicion about the applicability of linear piezoelectricity theory as reported in [12], the electrical current $i(t)$ is directly taken from the experimental data. Once calibrated, the simulation results are stored in the form of .txt files that are later processed in Pypiezo-GO for validation and comparison purposes.

2.2. Software architecture

Pypiezo-GO is not only a software that performs data processing of electromechanical testing data of piezoelectric cements; but it also represents a complete strategy to organize, analyze, process, and present dense databases in an efficient way as shown in Fig. 4.

To facilitate the use of Pypiezo-GO and share of sharing between users, Google Colaboratory was selected as the software framework because it offers an accessible environment that can interpret Python, HTML5, Markdown, and LaTeX codes, and all the computations are conducted entirely in the cloud

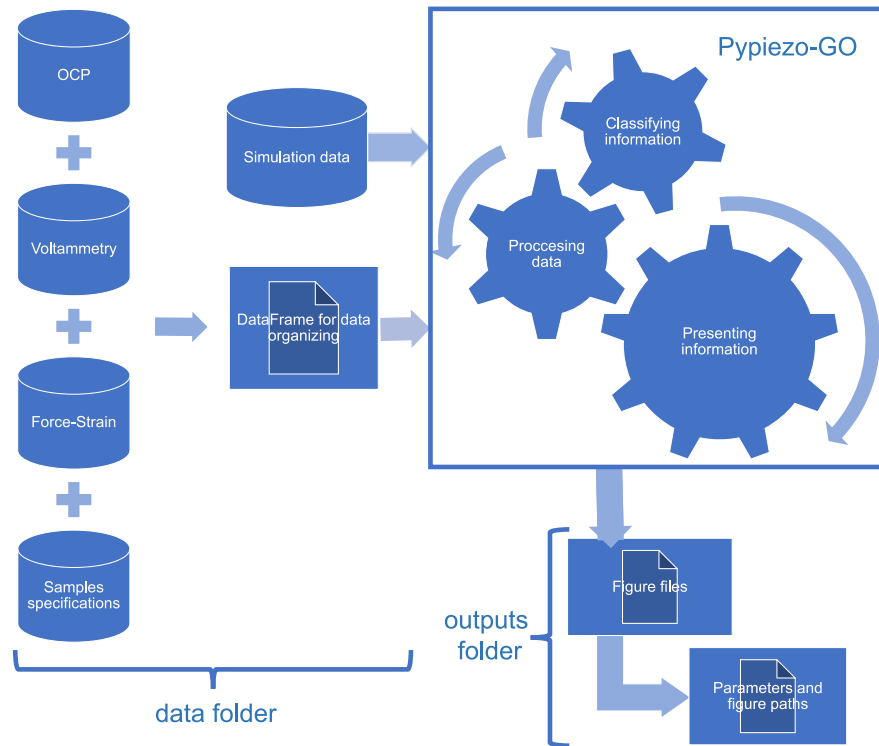


Fig. 4. Pypiezo-GO software architecture.

(Google Drive). To create a structure for manipulating the python scripts and the input and output data, three new folders called scripts, data and outputs are created inside the main folder. The data folder is intended to store the data from experiments organized into separate folders with names organized by the corresponding acquisition dates (year/month/day, for instance, 20190904). The data folder also contains the Excel sheet *Medidas_GO.xlsx*. Within these dated folders, the files are arranged with the measurement data denoted by: *measurement technique_sample name_measurement series*. For example, the first OCP measurement performed on the p49 sample has for name OCP_p49_1.

Once organized, the Pypiezo-GO script receives the information contained inside the DataFrame, and the data from the CS, CV, and OCP tests are classified according to the selected specimen(s) in separated DataFrames. Finally, the data series are processed to calculate the electromechanical characteristics of the samples. In this light, the tabular output data and graphs are respectively stored by means of DataFrames and figures in the outputs folder. Finally, the outputs of Pypiezo-GO in the shape of newly calculated data series, parameters are presented in graphical and tabular format in a log viewer, shown in Fig. 5.

2.3. Software functionalities

The primary functionalities of Pypiezo-GO (along with the Simulink model) are centered around the management, manipulation, modeling, and presentation of information from the electromechanical testing of piezoelectric cement composites, as elucidated in the following statements:

1. (Pypiezo-GO) Classify the information of the measurements (CT, OCP, CV) according to previously chosen specimen(s). It is essential to clarify that a specimen can be associated with different measurements or several series of the same test type.

2. (Pypiezo-GO) Synchronize data series from the mechanical (force) and electrical (voltage) experiments to obtain the piezoelectric voltage parameter g_{33} .
3. (Pypiezo-GO) Setting the combination options from data series of different measurements such as force, displacement, strain, voltage, and electric current or the new data series calculated by Pypiezo-GO as strain, electrical resistance, power, and FCR.
4. (Pypiezo-GO) Analyze the voltammograms at different constant compressive loads to determine the capacitance and the piezoelectric charge parameter d_{33} .
5. (Simulink model) Extract the parameters of the circuit model through the Parameter Estimator App. Subsequently, in Pypiezo-GO, the fitted outputs are compared with the experimental data series for validation and verification purposes.

3. Illustrative example

This section provides an illustrative example that shows the data manipulation and the result delivery using Pypiezo-GO. Specifically, this example demonstrates the determination of the piezoelectric properties of a rGO-cement specimen denoted as "p39". The process begins with the selection of the specimen(s), as illustrated in Fig. 2. Next, the code cell prompts the user to enter the sample's nomenclature. In this example, the specimen "p39" was entered. Afterwards, two new dictionaries (see code cells 1.2 and 1.3 of Pypiezo-GO in Figs. 6(a) and 6(b), respectively) are created to organize the data for the selected specimen. The second dictionary includes the mechanical and electrical data series.

In code cell 1.4., the method `interp` allows the user to specify the time interval in the interpolation used for the time synchronization of the electromechanical records. It also provides a warning when the minimum and maximum times specified full outside that interval. Then, `plot_electromechanical` in code

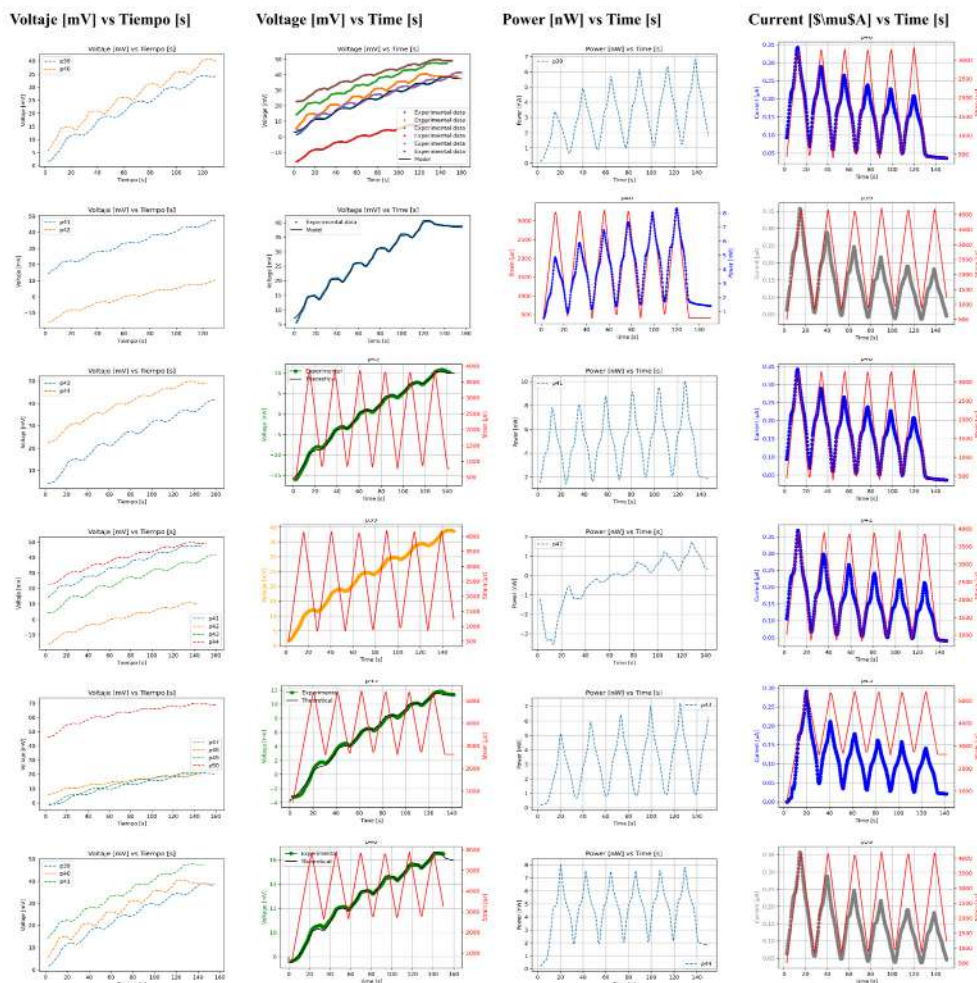


Fig. 5. Log viewer for presenting the new DataFrames created by Pypiezo-GO.

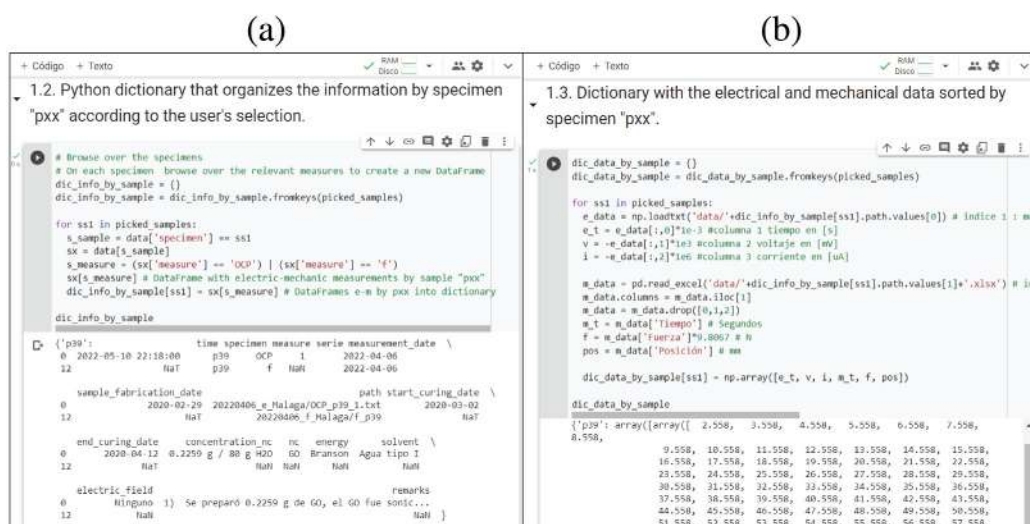


Fig. 6. Screenshots of cells 1.1. and 1.2. containing a programming structure based on dictionaries to organize the information by specimen according to the user's selection (a) and the dictionary with the electromechanical data (b).

cell 1.5. is responsible for configuring the plotting, labels, and analysis options shown in Fig. 7. The labels can be displayed in either Spanish or English.

Furthermore, in the code cell 2.1. Plotting options the previous methods are instantiated to present the figures and results.

In this example, the `interp` method was called by typing the following arguments: `t_min_max = [2.56, 13]` and `n=500`. In addition, the `plot_electromechanical` method was also instantiated in the following code line: `option = 7, marker = '--', etiqueta = '', label_axes = 'en', dpi = 100`. This

```

...
There are xx options (0 - XX) to choose the figure to be plotted,
according to set of specimens 'pxx'
option = 0 --- force vs time
option = 1 --- strain vs time
option = 2 --- force vs strain
option = 3 --- voltage vs time
option = 4 --- current vs time
option = 5 --- current vs voltage
option = 6 --- voltage vs strain
option = 7 --- voltage vs force
option = 8 --- current vs strain
option = 9 --- resistance vs strain
option = 10 --- resistance vs force
option = 11 --- potencia vs time
option = 12 --- resistance vs time
option = 13 --- Delta resistance / R vs strain
option = 14 --- Delta resistance / R vs time
option = 15 --- voltage / electrodes separation vs force / cross section
option = 16 --- nomalized strain vs time
option = 17 --- normalized current vs time
option = 18 --- power vs strain
...

```

Fig. 7. Plotting options in Pypiezo-G0.

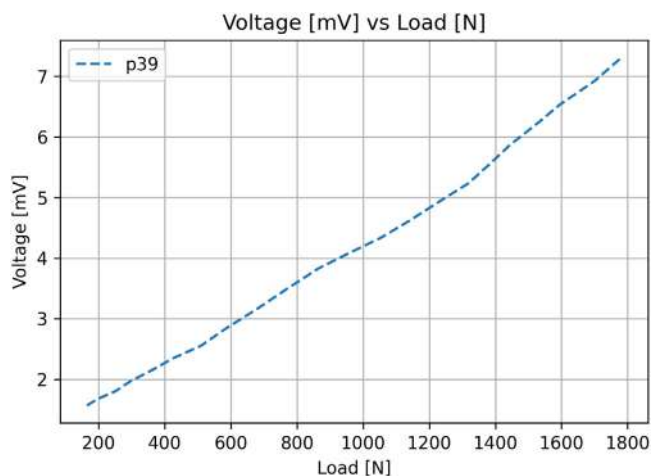


Fig. 8. Output voltage versus compressive load curve obtained for the specimen p39.

option is for constructing the voltage [mV] versus force [N] figure and calculating the piezoelectric parameter of voltage, which is presented in the output cell as $g_{33} = 12.19434782E-5$ mVm/N. Additionally, Fig. 8 is generated to visually represent the results.

4. Impact

Piezoelectric cement composites have enormous potential for solving the scalability issues of self-diagnostic materials for SHM of civil engineering structures, which are typically located in remote sites without access to the electrical grid. For their application, it is essential to identify their strain sensing properties through specific electromechanical characterization tests [14–16]. Of particular interest are the piezoelectric voltage g_{33} and charge d_{33} coefficients, which are determined in this work through the combination of CT, OCP and CV following the methodology presented in [12]. To enable the processing of the measurement files and characterize the piezoelectric coefficients, this study was presented Pypiezo-G0, an open-source software program

written in Python within the cloud platform Google Colab. Given the great potential of these composites, Pypiezo-G0 is envisaged to represent a valuable tool for the scientific community working on piezoelectric composites for SHM applications. Specifically, the main impacts of Pypiezo-G0 comprise:

- Enabling the analysis of large volume of data from electromechanical characterization campaigns with minimum computational time demands.
- Integrating the data obtained from different laboratory equipment.
- Representing a general methodology to organize the information from intensive experimental campaigns in a structured manner.

In addition, these impacts (i) can inspire future works investigating different types of nanomaterials to develop new smart cement composites, exploiting piezoelectricity as the main strain self-sensing principle and enabling the software tool (Pypiezo-G0) to analyze such properties. Besides, (ii) new experiments could be conducted to expand the presented database and so obtain a more representative characterization of the piezo properties of rGO-cement composites, including other volume fractions of rGO in the cement paste or inducing polarization during the curing stage. Finally, (iii) the presented lumped equivalent circuit can be enhanced to obtain more reliable predictions or it can be adapted to other smart composite materials. Increasing the size of the present database can be easily performed owing to the optimized architecture of the software, which allows organizing the data in an intuitive manner, even when different types of measurements have been carried out on each specimen. In addition, the user-friendly nature of Pypiezo-G0 is enhanced by the popularity of organizing information in a dataframe structure, which is similar to popular software tools like Excel, Google Sheets, and Open Office calculus sheets. With Pypiezo-G0, users do not require licensed software such as Origin or Maple to process information or need to combine different software tools to achieve the same result.

5. Conclusions

Pypiezo-G0 is a software tool designed to facilitate the organization, analysis, and processing of the measurements from

experiments conducted using a Potentiostat/Galvanostat and a Universal Testing Machine for the electromechanical characterization of piezoelectric rGO-cement composites. The testing sequence include measurements of open circuit potential, cyclic voltammetry, and compressive tests, each of which comprises distinct data series, including time, voltage, current, force, displacement, among others. On this basis, Pypiezo-GO has been designed to integrate these data series in an intuitive manner and through cloud computing, enabling the estimation of the effective piezoelectric voltage g_{33} and charge d_{33} coefficients, which are fundamental for self-powered strain self-sensing applications. The presented open-source software also represents an ideal environment for constructing new equivalent circuit models for enhancing the understanding of rGO-cement composites, as well as to interpret experimental data and conduct signal processing applications.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Data availability

Data will be made available on request

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