Understanding the mechanical and dynamic loading conditions of smart ceramic compounds

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Abstract

Dielectric and piezoelectric materials, e.g. barium titanate (BT) and hydroxyapatite (HA), have been extensively studied for the advancement of materials and devices for application to sensors/actuators, energy storage/harvesting, structural health monitoring and biomedical engineering scaffolds. Several studies examined how processing parameters influence the material properties. However few models exist that enable accurate prediction of the performance of these materials under both mechanical conditions specified by ASTM standards or less is known about the performance of piezoelectric structures undergoing non-traditional loading conditions and configurations. The goal of this project is to predict the mechanical, electrical, and electromechanical properties of these ceramic materials. Numerical models are being developed using COMSOL, a finite element modeling software, to compare empirical data from previous studies along with data from other publications. The models are configured by determining the proper mesh size in which the simulation is still accurate while not being too computationally overbearing or exhausting memory storage. Material properties are then defined and the ultimate compressive strength is measured.
GET UP Research Thrust:

- Devices and energy management systems for energy generation, conversion and storage.
- Nanotechnology and materials for energy storage and conversion

Methods

Configuring the model

Mesh size

A 2D model of a cylinder with dimensions 12mm x 6mm was designed in COMSOL. From the COMSOL material library, 100% poled BT was applied to the model and the density, Poisson's Ratio, and elastic modulus were defined: 5700 kg/m^3, .32, and 67 GPa respectively. Using the built in solid mechanics physics, boundary conditions were set and a load rate of 1 mm/min was placed at the top of the cylinder. A time-dependent study was conducted from 0 to 180 seconds with a time step of 0.01 seconds. Before computing, the mesh size for that study was chosen. The minimum and maximum values of the von MIses stress and 1st principal stress and strain were collected with 3D plot groups. The mesh sizes with the most similar results were chosen and the procedure was repeated for the 3D model and compared. The "Fine" mesh size was chosen for the remainder of the studies.

Time step

A time step of 0.01 seconds was used when studying the effect of mesh size on a model. Once the optimal mesh size was chosen, the next step was to determine whether the step size affected the model. With the control being 0.01, the simulations were run with a time step of 0.1 seconds and stress-strain curves were produced for the three points of observation (Figure 1).

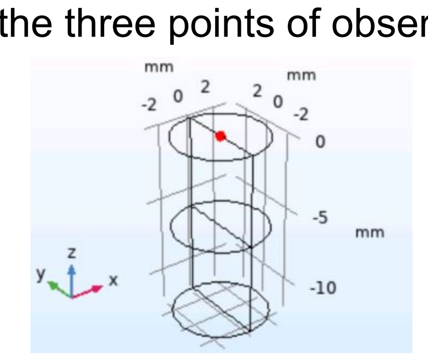

Figure 1a: Center of top of cylinder, data point for figure 2a

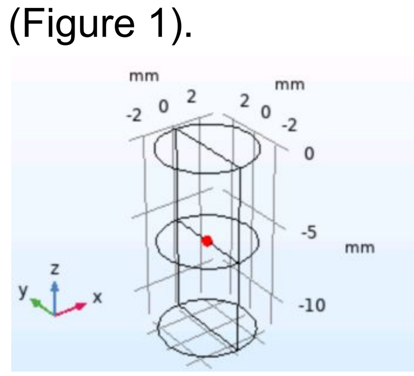

Figure 1b: Center of middle of cylinder, data point for figure 2b

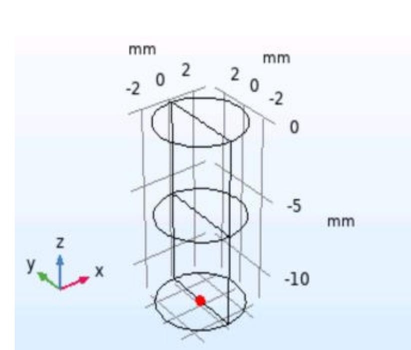

Figure 1c: Center of bottom of cylinder, data point for figure 2c

Methods (continued)

Material Properties

Testing material properties of the model

After configuring the simulation settings, the accuracy of the model needed to be determined by comparing the results produced from COMSOL to the empirical data collected last summer and to other publications. A 3D model emulating the specimens, particularly specimen BT_a, detailed in Trzepieciński et al. (Table 1) was produced.

Specimen properties			
Specimen name	BT_a	BT_b	BT_c
Height (mm)	13.5 mm		
Diameter (mm)	9 mm		
Load	2mm/min		
Poisson's ratio*	.32		
Density (kg/m^3)	5840	5850	5860
Elastic modulus (GPa)	115.5	118	116

**Poisson's ratio was not reported by* Trzepieciński et al., this was the value used in all BT models

Table 1: Properties used for Trzepieciński model

Calculating the properties for composite materials

Rule of mixtures was used to calculate the material properties of 40%, 50%, 60%, and 70% BT-HA composites (Table 2).

Pure and composite material properties			
	elastic modulus (GPa)	density (kg/m^3)	Poisson's Ratio
100% BT	67	5700	0.32
100% HA	114	3120	0.27
40% BT	95.2	4152	0.29
50% BT	90.5	4410	0.295
60% BT	85.8	4668	0.3
70% BT	81.1	4926	0.305

Table 2: Pure and composite material properties

Results

The 2D model was run with different mesh sizes (Table 3). Too large of a mesh size leads to inaccurate results and an extremely small mesh size may be impractical due to its run time. Mesh sizes that produce similar results allow for minimal tradeoff at which point the user must choose between accuracy and run time.

Min/Max Values for 2D 100% Poled BT model with time step of 0.01 from 0 to 180 seconds						
	von Mises stress (N/m^2)		1st Principal Strain		1st Principal Stress	
Mesh Size	Min (MPa)	Max (N/m^2)	Min	Max	MIn (N/m^2)	Max (N/m^2)
Coarse	9.17E+09	2.27E+10	3.12E-05	0.15	-8.15E+09	2.59E+09
Normal	9.13E+09	2.56E+10	6.11E-08	0.18	-8.31E+09	2.62E+09
Fine	9.13E+09	2.65E+10	1.21E-08	0.19	-8.83E+09	2.75E+09
Finer	9.13E+09	2.87E+10	7.78E-10	0.21	-9.75E+09	3.00E+09

Table 3: 2D mesh size comparison

Although the numerical values in Table 4 are not accurate, this study is not reliant on those values. The purpose of this study was to determine whether the mesh size chosen for a 2D model can be applied to a 3D model.

Min/Max Values for 3D 100% BT model with a time step 0.01 from 0 to 75.78 seconds							
		Von Mises		1st principal strain		1st principal stress	
Mesh Size	Number of elements	Min (MPa)	Max (MPa)	Min (mm/mm)	Max (mm/mm)	Min (MPa)	Max (MPa)
Normal	2916	2440	7160	8.23E-05	0.06	-4930	1770
Fine	5899	2430	7560	4.44E-05	0.07	-5000	2490

Table 4a: 3D mesh sizes values

Min/Max Values for 2D 100% BT model with time step 0.01 from 0 to 75.78 seconds							
		Von Mises		1st principal strain		1st principal stress	
Mesh Size	Number of elements	Min (MPa)	Max (MPa)	Min (mm/mm)	Max (mm/mm)	Min (MPa)	Max (MPa)
Normal	332	3840	10800	2.57E-08	0.07	-3500	1100
Fine	520	3840	11200	5.10E-09	0.08	-3720	1160

Table 4b: 2D mesh sizes values

Boxes highlighted in blue and yellow show the same result when switching between mesh sizes for both models. The number of elements in a model drives the precision of the calculations. In the 3D model, "Fine" having double the elements of "Normal" explains the difference in minimum von Mises stress, which is otherwise negligible when comparing boxes highlighted in green.

Results (continued)

The greatest obstacle encountered was exhausting the memory on a Rutgers DSV lab computer, a common occurrence for simulations with a 0.01 step—changing to a 0.1 step effectively eliminated that.

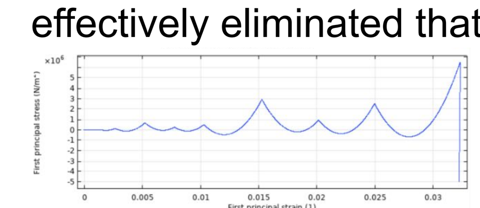

Figure 2a: Stress-strain curve for 0.01s and 0.1s time step of center of top of cylinder

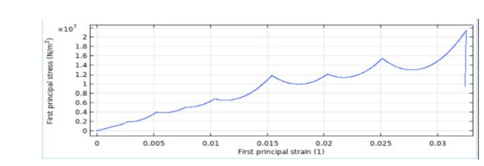

Figure 2b: Stress-strain curve for 0.01s and 0.1s time step of center of middle of cylinder

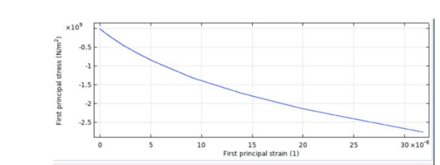

Figure 2c: Stress-strain curve for 0.01s and 0.1s time step of center of bottom of cylinder

Between all three points (Figure 1), the stress-strain curves are the same (Figure 2). A plethora of problems had surfaced after analyzing the results from the different models. Most importantly, the ultimate compressive strength was significantly higher than desired in all models. The expected compressive strength for the Trzepieciński model was 655.7 MPa, but the compressive strength from COMSOL was 235972.5 MPa. Another issue emerged when the Trzepieciński and HA models both would compute the full time range, i.e. 0 to t seconds, as did the 2D model. The 3D model would stop running at 75.78 seconds.

Conclusion

- Optimal mesh sizes do not change for the same model in different dimensions. Done properly, a 2D model can replace a 3D model. 2D models have shorter run times and demand less memory, greatly expediting the modeling process.
- The time step has no effect on calculations. This is extremely substantial as it presents multiple applications. A larger time step requires less memory and run time especially in complex models. If the user wishes to closely observe the simulation in between two steps e.g. from 1 to 2 seconds, the time range can be modified and the time step reduced.
- Built-in COMSOL materials are lacking properties required for an accurate model capable of replicating the results from other studies. The predefined material properties are useful for modeling elastic properties of a sample but need user defined properties to model plastic deformations.

Future Work

- Add the necessary material properties, reconfigure mesh sizes, continue working towards reproducing the results from empirical data
- Calculate the composite material properties for modeling
- Develop models for non-traditional loading

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Economic Models for Evaluation of Feasibility of Wave and Tidal Systems

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Introduction

The two forms of offshore renewable are Wind Turbines (WT) and Wave Energy Converters (WEC). Several case studies determine the economic feasibility of these renewable energies, by generating three values: Levelized Cost of Energy (LCOE), Internal Rate of Return (IRR), and Net Present Value (NPV). While different variables are included in the calculations, the definition of these three values is consistent between authors. In each study, one or several locations are observed for possible wind, wave, or hybrid farm sites. Wave farms may also provide coastal protection due to the dampening effects of the wave capturing technology.

GET UP Research Thrust:

- Devices and energy management systems for energy generation, conversion and storage.

Discussion

WT have longer periods of sustained energy production while WEC are more effective generators producing closer to their maximum output [3]. Several case studies examine similar regions, and a reoccuring location was the north of Spain and Portugal. The LCOE for the WT was 100.31 €/MWh and the best LCOE for a WEC was 316.90 €/MWh and 513.17 €/MWh [1] [2] [4]. The best LCOE for a WEC was achieved by the WaveDragon. With that in mind, the WaveDragon was profitable with a 400 €/MWh feed-in tariff for sites in Portugal and a 600 €/MWh in both Spain and Portugal [1] [4]. WT are more profitable than WEC, but that is subject to change as WEC gain better footing in the market and the technology advances. Joint wind-wave farms are needed to expedite development. European countries dominate when it comes to the most offshore wind farms and would be the best region to develop joint wind-wave farms. The biggest deterrent in the European market is that the amount of wind and wave resources is at its peak in the winter [3]. Latin American sites were determined to be the best option for joint wind-wave farms due to the slight changes in weather patterns [3].

Future Work

- The model presented in one study needs to be applied to the conditions of another study.
- Certain models need to be re-evaluated with updated data

References

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