Journal of Engineering and Applied Sciences 13 (Special Issue 10): 8244-8252, 2018
ISSN: 1816-949X

Prediction of Some Physical and Mechanical Properties of Bioceramics Through Using Genetic Algorithm Approach

Mohammed A. Ahmed Al-Dujaili, Shaker J. Adrees and Raghda Ibrahim Abdalwahad
Faculty of Materials Engineering, The University of Babylon, P.O. Box: 4, Hilla, Babylon, Iraq

Abstract: Bioceramics are crucial materials to be used in clinical, dental, load bearing and other biological applications that require good mechanical, physical and biological properties. In this research, physical properties such as (density and porosity) and mechanical properties such as (impact strength, tensile strength, elastic modulus, elongation at break and hardness) of biocomposite are predicted by developing model using Genetic Algorithm (GA) technique and regression equation on assumed values and compare it with the values gained from experimental work via. Get Data Graph Digitizer 2.26.

Key words: Physical properties, mechanical properties, Genetic algorithm method, biocomposite, values

INTRODUCTION

Ceramic materials are intermediate in mass properties like density and porosity between metals (higher than ceramics) and polymer (lower than ceramics) (The symbol is the Greek letter rho, ρ). $\rho = m/v$ where m is the mass, v is the volume. The common units used for density are usually (kg/m^3) and (g/cm^3). Porous materials used in different biomedical applications includes filters and implants for extracorporeal devices (i.e., heart-lungs machines) porosity may decrease the mechanical strength due to stress concentration and thus, it is unrequired in some applications such as bone plates. The porosity often expressed as; Porosity = $1-V_s$ where, V_s is solid volume fraction The mechanical properties consider as the most important for the materials used in medicine and dentistry (Park and Lakes, 2007).

Hardness defined as the ability of materials to resist penetration caused by sharp object, it is commonly occur by local deformation of the surface, over a region in micrometer in width and depth. At first, hardness quantified depending on the scratch as measured in mhos but later it measured by the size of indentation that became the standard method (Watchman *et al*., 2009).

Impact strength or impact resistance is the measurement of the absorbed energy when a significant object breaks under speed collision. In another word when two objects undergo colliding, damage occur on one or both objects the ability to resist the damage known as impact resistance (Anonymous, 2008).

Elasticity known as the reduction of the deformation (at least part of it) when the applied load is released from the body. Modulus of elasticity (Young's modulus E) measures the stiffness of the material; it also called the elasticity constant (Roman, 2013; Boch and Jean-Claude, 2007). The GA is one of the most successful techniques that can solve combinatorial optimization problems (Al-Dujaili *et al*., 2017a, b). Solution that generate by GA called chromosome (collection of chromosomes is population), these chromosomes go through process called fitness function that measures the solution stability. After that, the GA operator (selection, crossover and mutation) that replaces the old population employs a new population. Repeating this process gives the optimum solution (Hermawanto, 2013; Al-Dujaili *et al*., 2017a, b).

Literature review: Demirkiran *et al*. (2010) have added 45S5 bioglass to hydroxyapatite and sintered together when adding (1, 2.5 and 5 wt.%) of bioglass; it worked as sintering aid with β-TCP ($Ca_3(PO_4)_2$) being the minor phase which increases as increasing bioglass content. When (10 and 25 wt. %) of bioglass added; new phases formed which are calcium phosphate silicate ($Ca_5(PO_4)_2SiO_4$) and sodium calcium phosphate ($Na_3Ca_6(PO_4)_5$). Density and porosity were characterized, XRD used to determine phases and SEM used to illustrate the microstructure (Demirkiran *et al*., 2010).

Husin *et al*. (2011) have made HA reinforced HDPE composite with HA content up to 50 phr. The characteristics of HA/HDPE were examined using Scanning Electron Microscope (SEM), Differential Scanning Calorimetry (DSC), tensile testing. It was realized that tensile strength and modulus of elasticity increased with increasing HA content while elongation at breakage decreases (Husin *et al*., 2011).

Corresponding Author: Mohammed A. Ahmed Al-Dujaili, Faculty of Materials Engineering, The University of Babylon, P.O. Box: 4, Hilla, Babylon, Iraq

Zarifah *et al.* (2016) have studied the structural and physical of HA reinforced with different addition of 45S5 at different sintering temperature. The reinforced HA have synthesized and investigated in term of mechanical strength, density and crystalline phases. The crystalline phases were detected using XRD, density determined using the Archimede's method and micro hardness were obtained using AVK-C2 hardness tester (Zarifah *et al.*, 2016).

The objective of the current research is to build reliable models that predict the effect of adding BG or HA on the physical and mechanical properties of biocomposite using regression equation and genetic algorithm method and to define the best concentration to be used which gives the optimal values.

MATERIALS AND METHODS

The software GetData Graph Digitizer 2.26 which is a program for digitizing plots and graphs. It obtains original (X, Y) data. Data obtained by the following steps:

- Open the required graph
- Setting the scale
- Digitize
- Export the data to TXT, XLS, XML, DXF or EPS file

Then these data optimized using Genetic algorithm option from the optimization tool via. MATLAB Software. Then theoretical data also, optimized using the same procedure for the porosity, density, hardness, impact strength, tensile strength, elasticity of modulus and elongation of modulus. The regression function (fitness function) obtained using Minitab 17 (Fig. 1).

RESULTS AND DISCUSSION

Regression function of values obtained by GetData Software: In density prediction model, the density used as dependent variable and bioglass ratio used as independent variable.

$$\rho = 2.6521 - 0.01702BG$$

Where:

ρ = The density
BG = The bioglass content

The R^2 (36.10 %), R-adj (32.10 %). The prediction model of porosity made by taking the porosity as dependent variable and BG as independent variable.

$$\rho = 2.30 + 0.531BG$$

where, ρ is the porosity. The R^2 (51.73%), R-adj (48.72 %). The prediction model of impact strength, tensile strength, elastic modulus and elongation at break made by taking them as dependent variables and HA content as independent variable.

- Impact strength = 15.61-0.1436 HA, The R^2 (36.19%), R-adj (32.64 %)
- Tensile strength = 21.926 +0.1153HA, The R^2 (84.74%), R-adj (83.97%)
- Elastic modulus = 1.1439 +0.012815HA, The R^2 (96.92%), R-adj (96.77%)
- Elongation at breakage = 105.3 -2.516HA, The R^2 (56.90%), R-adj (54.63%)

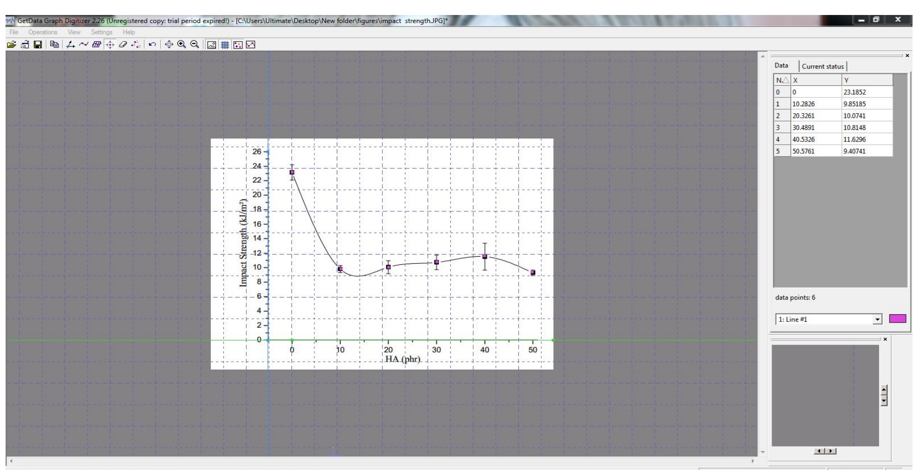


Fig.1: Illustrate the get data graph digitizer 2.26

Table 1: Regression equation analysis of density

Terms	Coef.	SE coef.	t-values	p-values	Vif
Constant	2.65210	0.06920	38.35	0.000	
Concentration	-0.01702	0.00566	-3.01	0.008	1.00

Table 2: Regression equation analysis of porosity

Terms	Coef.	SE coef.	t-values	p-values	Vif
Constant	2.30	1.730	1.33	0.203	
Concentration	0.531	0.128	4.14	0.001	1.00

Table 3: Regression equation analysis of impact strength

Terms	Coef.	SE coef.	k-values	k-values	Vif
Constant	15.610	1.2100	12.90	0.000	
Concentration	-0.1436	0.0449	-3.19	0.005	1.00

Table 4: Regression equation analysis of tensile strength

Terms	Coef.	SE coef.	t-values	p-values	Vif
Constant	21.926	0.316	69.36	0.000	
Concentration	0.1153	0.0109	10.54	0.000	1.00

Table 5: Regression equation analysis of elastic modulus

Terms	Coef.	SE coef.	t-values	p-values	Vif
Constant	1.143900	0.015400	74.18	0.000	
Concentration	0.012815	0.000511	25.09	0.000	1.00

Table 6: Regression equation analysis of elongation at break

Terms	Coef.	SE coef.	t-values	p-values	Vif
Constant	105.30	13.90	7.55	0.000	
Concentration	-2.516	0.502	-5.01	0.000	1.00

Table 7: Regression equation analysis of hardness

Terms	Coef.	SE coef.	t-values	p-values	Vif
Constant	1.449000	0.20400	7.09	0.000	
Concentration	-0.00335	0.00463	-0.72	0.479	1.00

And the prediction model made by taking the hardness as dependent variable and bioglass content as independent variable.

Hardness = 1.449 -0.00335BG, the R^2 (2.82%), R-adj (0.00%). Analysis the regression equation: (Table 1-7).

Genetic algorithm of values obtained by GetData: The generation versus fitness value shown in the Fig. 2:

Regression function of the assumed values: In density prediction model, the density used as dependent variable and bioglass ratio used as independent variable.

$$\rho = 2.7856 - 0.02236BG$$

Where:

ρ = The density

BG = The bioglass content

The R^2 (56.53%), R-adj (53.82 %). The prediction model of porosity made by taking the porosity as dependent variable and BG as independent variable p = 0.40+0.645BG, where p is the porosity. The R^2 (65.09%), R-adj (62.90%).

Table 8: Regression equation analysis of assumed density

Terms	Coef.	SE coef.	t-values	p-values	Vif
Constant	2.785600	0.07400	37.65	0.000	
Concentration	-0.02236	0.00490	-4.56	0.000	1.00

Table 9: Regression equation analysis of assumed porosity

Terms	Coef.	SE coef.	t-values	p-values	Vif
Constant	0.400	1.650	0.24	0.811	
Concentration	0.645	0.118	5.46	0.000	1.00

Table 10: Regression equation analysis of assumed impact strength

Terms	Coef.	SE coef.	t-values	p-values	Vif
Constant	15.6800	1.2200	12.83	0.000	
Concentration	-0.1575	0.0490	-3.22	0.005	1.00

Table 11: Regression equation analysis of assumed tensile strength

Terms	Coef.	SE coef.	t-values	p-values	Vif
Constant	21.9490	0.275	79.69	0.000	
Concentration	0.11409	0.00985	11.58	0.000	1.00

Table 12: Regression equation analysis of assumed elastic modulus

Terms	Coef.	SE coef.	t-values	p-values	Vif
Constant	1.141100	0.014000	81.48	0.000	
Concentration	0.012910	0.000485	26.62	0.000	1.00

Table 13: Regression equation analysis of assumed elongation at break

Terms	Coef.	SE coef.	t-values	p-values	Vif
Constant	109.20	13.40	8.18	0.000	
Concentration	-2.650	0.499	-5.31	0.000	1.00

Table 14: Regression equation analysis of assumed hardness

Terms	Coef.	SE coef.	t-values	p-values	Vif
Constant	1.5760	0.2360	6.67	0.000	
Concentration	-0.0194	0.0162	-1.20	0.246	1.00

The prediction model of impact strength, tensile strength, elastic modulus and elongation at break made by taking them as dependent variables and HA content as independent variable.

- Impact strength = 15.68-0.1575HA, The R^2 (36.49%), R-adj (32.97 %)
- Tensile strength = 21.949+0.11409HA, The R^2 (84.81%), R-adj (84.18%)
- Elastic modulus = 1.1411+0.012910HA, The R^2 (96.99%), R-adj (96.85%)
- Elongation at breakage = 109.2-2.650HA, The R^2 (58.50%), R-adj (56.42%)

And the prediction model made by taking the hardness as dependent variable and bioglass content as independent variable.

- Hardness = 1.576 -0.0194BG, The R^2 (7.41%), R-adj (2.26%) (Table 8-14)

Analysis the regression equation:

Genetic algorithm of theoretical assumed values: The generation versus fitness value shown in the Fig. 3 below: Comparison between experimental and theoretical (assumed) values using excel.

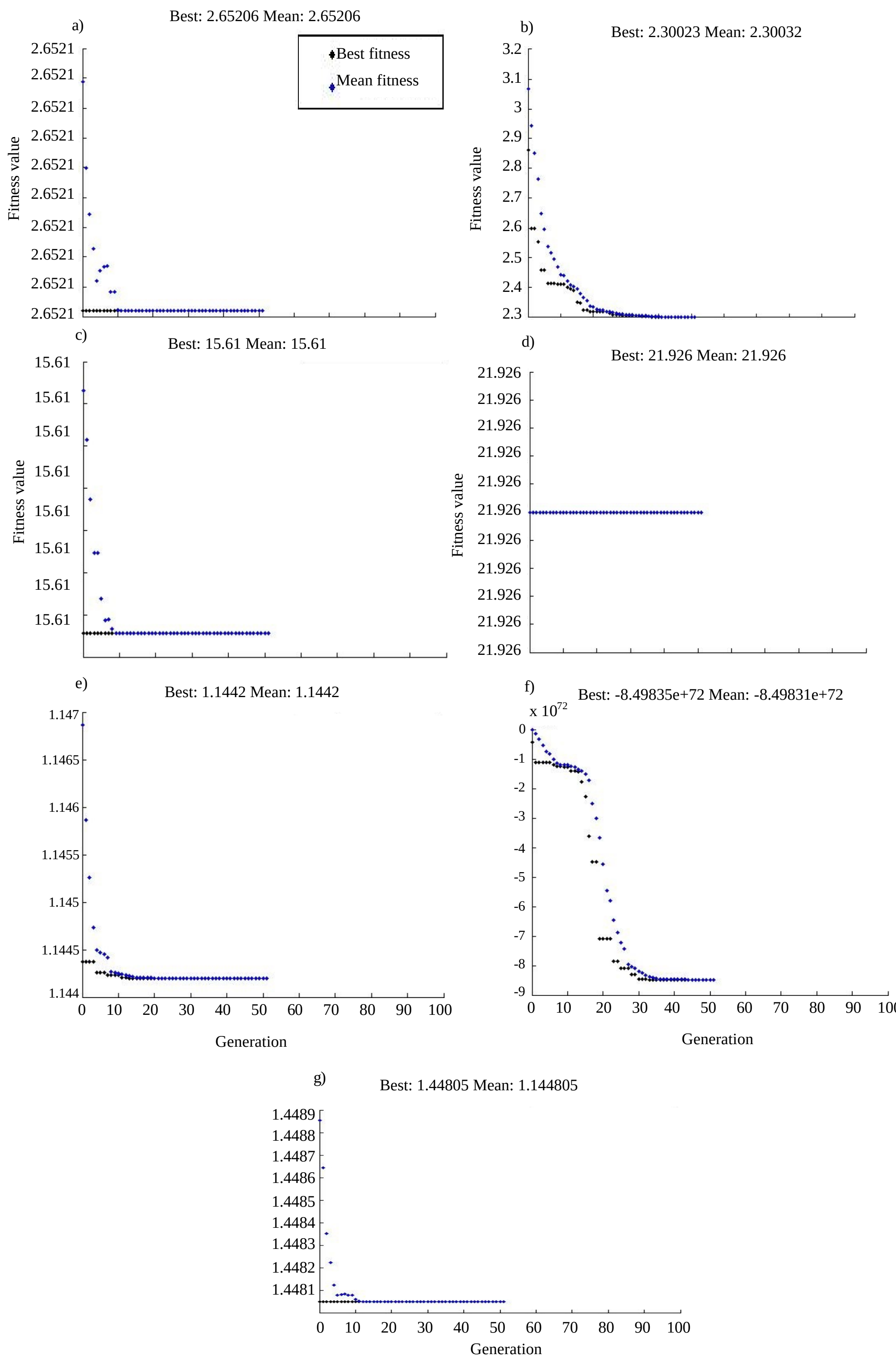


Fig.2: The regression versus the fitness value for; a) Density; b) Porosity; c) Impact strength; d) Tensile strength; e) Elastic modulus; f) Elongation at break and g) Hardness

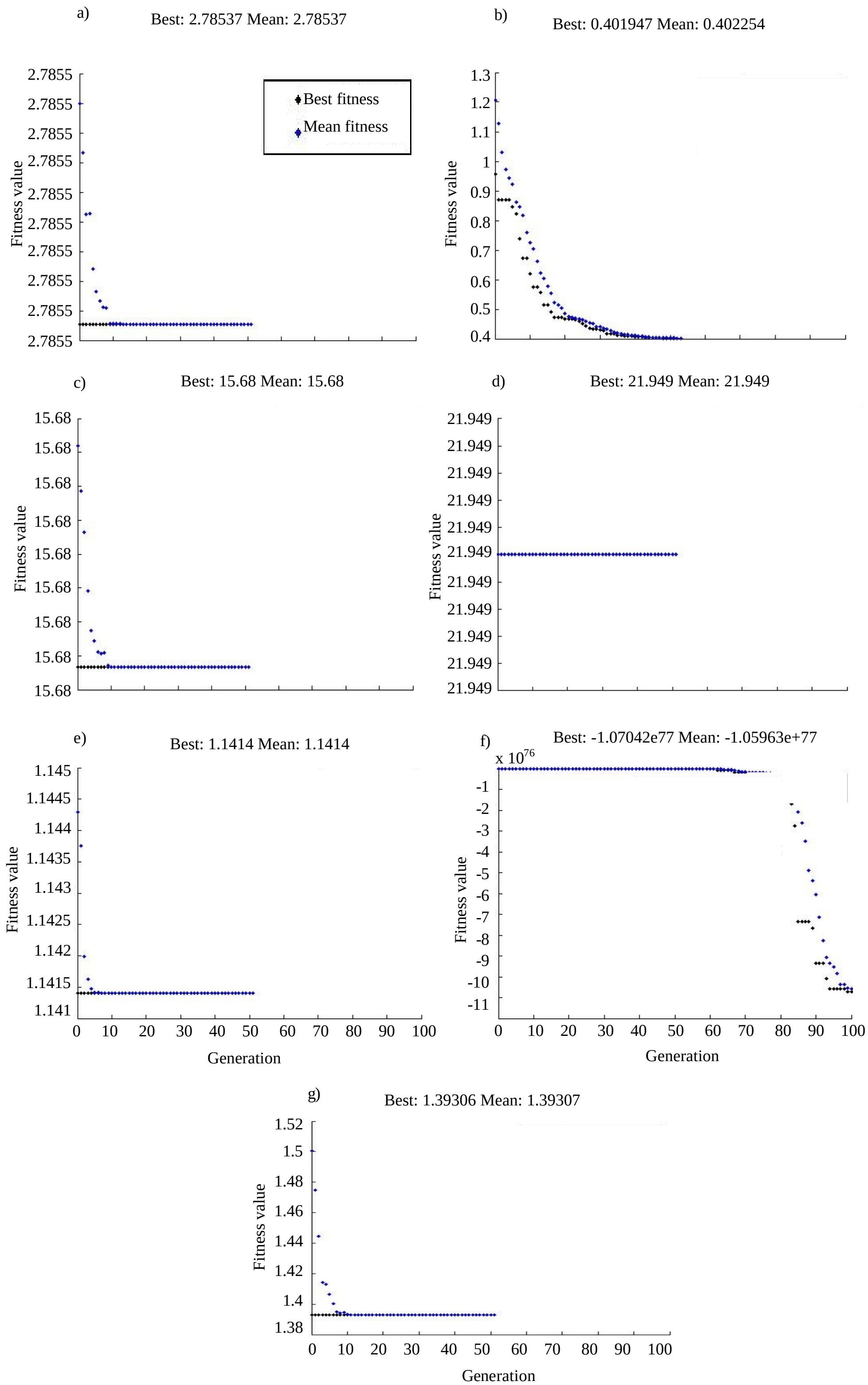


Fig.3: The regression versus the fitness value for; a) Density; b) Porosity; c) Impact strength; d) Tensile strength; e) Elastic modulus; f) Elongation at break and g) Hardness

Table 15: Density test

BG 1	Density 1	BG 2	Density 2
1	2.99219	0	2.99219
2	2.82478	0.53259	2.82478
4	2.66295	1.06518	2.82478
5	2.70201	1.69460	2.70201
7	2.72433	2.51769	2.72433
9	2.61830	3.63128	2.61830
10	2.50112	4.98696	2.50112
12	2.47321	5.56797	2.47321
13	2.36161	7.55307	2.36161
14	2.23884	9.44134	2.23884
15	2.20536	10.02235	2.20536
17	2.23884	11.42644	2.23884
18	2.27790	13.36313	2.27790
20	2.31138	15.25140	2.31138
21	2.35045	17.23650	2.35045
22	2.37835	19.12477	2.37835
23	2.45647	22.99814	2.45647
25	2.50112	24.98324	2.50112

Table 16: Porosity test

BG 1	Porosity 1	BG 2	Porosity 2
1	0.22779	0	0.22779
2	0.22779	1.78108	0.22779
4	0.11390	2.56030	0.11390
5	0.11390	4.00742	0.11396
6	0	5.00928	0
7	3.53075	6.23377	3.53075
9	8.08656	7.79221	8.08656
10	10.02278	8.46011	10.02278
11	12.64237	9.40631	12.64237
13	14.35080	9.96289	14.35080
14	14.12301	10.63080	14.12301
15	13.43964	12.96846	13.43964
17	13.09795	15.08349	13.09795
18	12.64237	17.36549	12.64237
20	12.07289	19.59184	12.07289
21	11.61731	21.81818	11.61731
22	11.16173	24.04453	11.16173
24	10.93394	25.04638	10.93394

Table 17: Impact strength test

HA 1	Impact 1	HA 2	Impact 2
0	23.185190	0	23.18519
2	20.740740	1.434780	20.74074
4	17.851850	3.228260	17.85185
5	15.777780	4.544348	15.77778
6	14.814810	5.260870	14.81481
8	11.851850	7.771740	11.85185
10	10..37037	9.326090	10.37037
13	9.777780	10.282610	9.77778
15	8.888890	14.228260	8.88889
17	9.777780	18.891300	9.77778
18	10.148150	20.326090	10.14815
21	10.518520	23.793480	10.51852
22	10.666670	28.456520	10.66667
25	10.814810	30.489130	10.81481
29	11.037040	33.239130	11.03704
33	11.555560	38.021740	11.55556
38	11.555560	40.652170	11.55556
41	11.333330	42.923910	11.33333
46	10.222220	47.706520	10.22222
50	9.333330	50.815220	9.33333

Microsoft excel used in order to compare the theoretical and experimental concentration and draw graphs illustrate the effect of changing the concentration on the properties (density, porosity, impact strength, tensile strength, elastic modulus, elongation at break and hardness) (Fig. 4) (Table 15-21).

Table 18: Tensile strength test

HA 1	Tensile 1	HA 2	Tensile 2
0	20.326810	0	20.32681
1	20.487310	0.60706	20.48730
12	21.371700	3.52097	21.61271
3	21.612710	5.46358	22.33609
5	22.336090	6.55629	22.73794
6	22.577100	10.19868	23.70090
7	22.737940	12.99117	24.26164
10	23.700900	15.17660	24.58120
12	24.261640	17.36203	24.82007
14	24.581200	20.51876	25.13821
15	24.518200	25.01104	25.53508
17	24.820070	26.83223	25.69379
21	25.138210	29.86755	25.93141
25	25.535080	30.47461	26.01121
27	25.693790	32.90287	26.08834
28	25.931410	34.60265	26.08584
30	26.011210	37.39514	26.24313
33	26.088340	39.45916	26.15941
35	26.085840	40.67329	26.23832
37	26.243130	44.31567	26.39436
40	26.158941	49.17219	26.71000
41	26.238320	50.99338	26.86871
43	26.234400	0	0
44	26.394360	0	0
49	26.710000	0	0
51	26.868710	0	0

Table 19: Elastic modulus test

HA 1	Elastic 1	HA 2	Etastic 2
0	1.05522	0	1.05522
2	1.13162	2.60146	1.13962
3	1.13962	4.17675	1.19027
4	1.19027	9.47950	1.25774
5	1.21603	9.14683	1.31941
7	1.25774	10.36029	1.33040
10	1.31941	13.87892	1.36908
11	1.33040	16.67077	1.37958
13	1.36908	18.73414	1.39030
17	1.37958	20.31219	1.39550
18	1.39030	23.46657	1.43429
21	1.39550	26.13529	1.47324
22	1.43429	28.56117	1.51226
26	1.47324	30.86599	1.54563
27	1.51226	33.29326	1.56193
30	1.54563	38.14779	1.59451
32	1.56193	41.06003	1.62202
39	1.59451	43.00060	1.65551
42	1.62202	45.79004	1.70578
43	1.65551	47.85065	1.76196
46	1.70578	49.42663	1.80125
48	1.76196	51.36548	1.86314
50	1.80125	0	0
51	1.86314	0	0

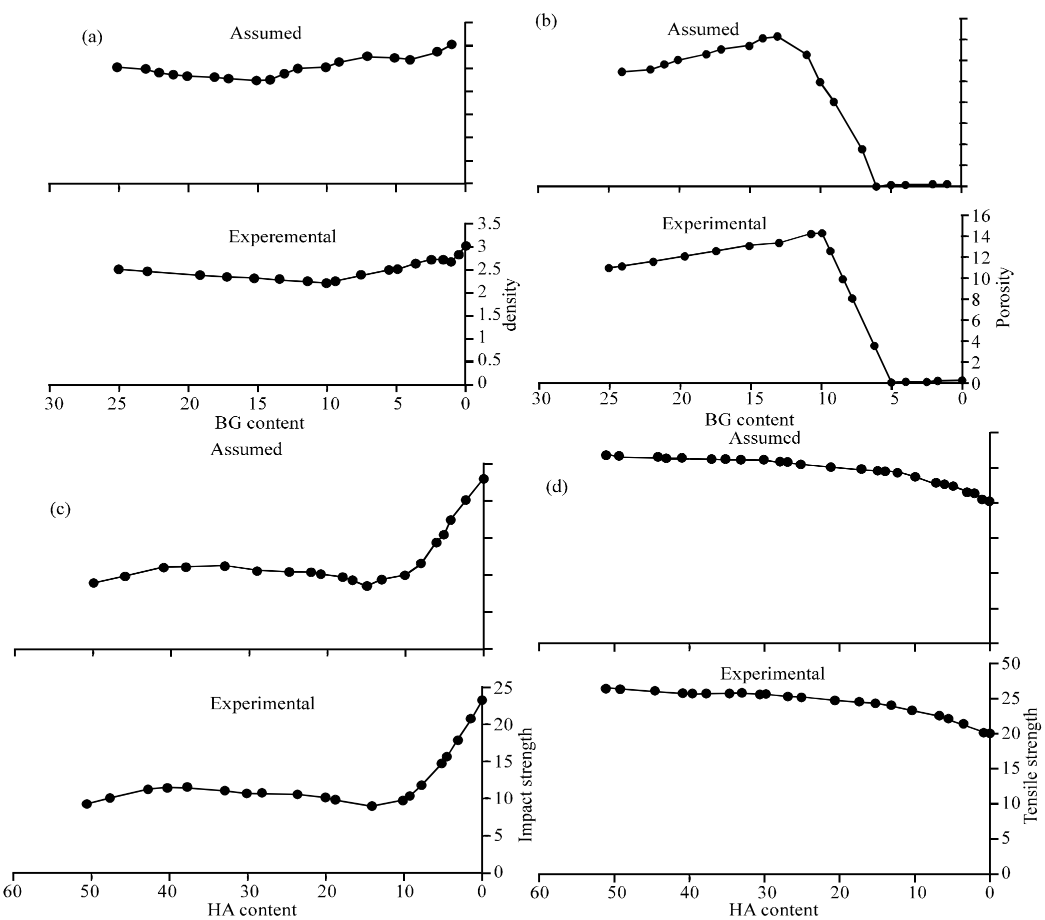
The best value of obtained density is (2.65206) compared with the range (2.20536-2.99219) and the assumed best density is (2.78537). For porosity in the range (0-14.3508), the obtained best value is (2.30023) while the assumed best porosity is (0.401947). For impact strength in the range of (9.33333-23.1852) the best impact value is (15.61) while the assumed best impact strength is (15.68) in tensile strength having the range (20.3268-26.8687) the best tensile strength value is (21.926) while the assumed best tensile strength is (21.949). For elastic modulus having the range (1.05522-1.86314) the best value is (1.1442) and the best-assumed value is (1.1414). For elongation at break with the range (10.6-182) the best value is (-8.49835e+72) and the best assumed value is (-1.07042e+77). Lastly, the hardness best value is (1.44805) while the assumed one is (1.39306) compared to the range (0.43085-2.56117).

Table 20: Elongation at break test

HA 1	Elongation 1	HA 2	Elongation 2
0	182	0	182
1	169	0.873	169
2	146.796	2.62	142
3	142	4.37	116
4	116	6.11	89.1
5	89.1	7.86	62.5
7	62.5	9.48	38.5
9	38.5	10.4	25.9
11	25.9	14.5	21.9
13	21.9	19.6	19.9
19	19.9	20.8	19.3
20	19.3	24.6	17.3
23	17.3	27.3	16
27	16	29.4	15.3
29	15.3	31.3	14
32	14	34.5	14
34	14	39.4	14
39	14	41.8	14
42	14	4404	14
44	13.3	49.4	12
48	12	52.1	10.6
52	10.6	0	0

Table 21: Hardness test

BG 1	Hardness 1	BG 2	Hardness 2
1	2.56117	0	2.56117
2	2.23404	3.43284	2.23404
4	1.90691	6.26866	1.90691
5	1.60372	9.25373	1.60372
6	1.27660	12.23881	1.27660
7	0.94947	15.07463	0.94947
9	0.63032	17.91045	0.63032
10	0.43085	20	0.43085
11	0.62234	24.77612	0.62234
12	0.86968	30.89552	0.86968
13	1.10106	36.86567	1.10106
14	1.22074	40.14925	1.22074
15	1.29255	42.68657	1.29255
17	1.40426	48.80597	1.40426
18	1.52394	54.92537	1.52394
20	1.61170	60.14925	1.61170
21	1.49202	66.86567	1.49202
22	1.34840	72.68657	1.34840
23	1.26064	78.65672	1.26064
25	1.22074	80	1.22074



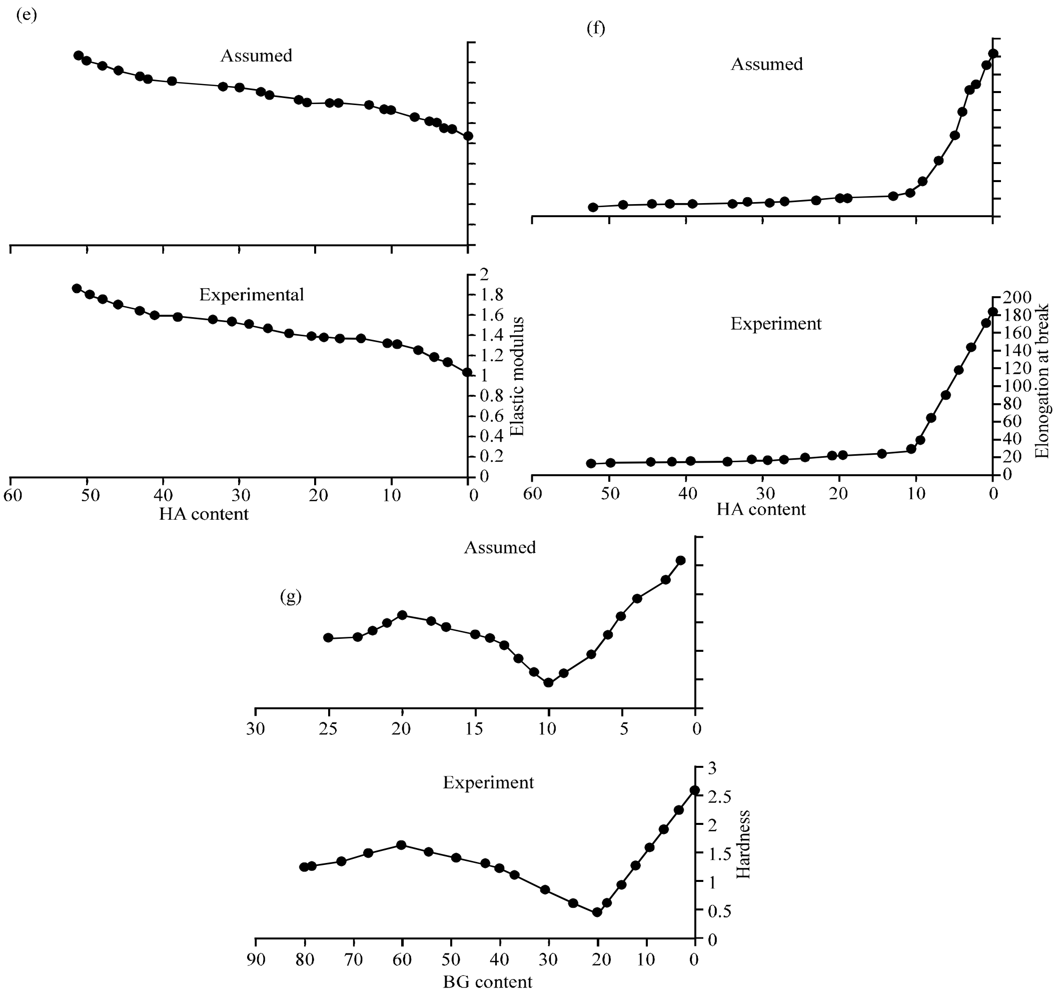


Fig. 4: Differences between assumed values and values obtained experimentally from get data for; a) Density; b) Porosity; c) Impact strengthp; d) Tensile strength; e) Elastic modulus; f) Elongation at break and g) Hardness

CONCLUSION

In the present study the Genetic Algorithm, allow us to determine the best concentration to be used in order to get the optimum value of a specific property. For example the best concentration to get the optimum value for density is (6.9) and so forth for porosity is (16.8), impact strength is (6.8), tensile strength is (3.7), elastic modulus is (3.9), elongation at break is (83.1) and for hardness is (4.8).

RECOMMENDATIONS

The study recommend to take the best concentration that obtained by assuming theoretical values as a reference, apply the same procedure on other properties and other materials whether biomedical or other engineering material and study the effect of other variables (besides concentration) such as sintering temperature, heating rate, particle size, pressing pressure and rate, etc.

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