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Modeling of Gelcast Ceramics using GP and Multi Objective Optimization using NSGA-II

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Abstract

This proposed work introduces a novel integrated evolutionary approach and its applications for modeling and optimization of important manufacturing process namely gelcasting. Genetic programming (GP) is an evolutionary algorithm which uses principle similar to Genetic algorithms (GA) to model highly non-linear and complex processes resulting in accurate and reliable models. For developing models, GP method makes use of experimental data generated from the process. For gelcasting process input variables are solid loading, monomer content and ratio of monomers and performance measures are flexural strength and porosity. As the chosen performance measures are opposite in nature, there cannot be a single optimization solution. Hence the problem under consideration is to be formulated as multi objective optimization problem and solved using NSGA-II algorithm to retrieve the Pareto optimal front. Pareto set of process parameters in a gelcasting process in multi objective optimization of flexural strength porosity are obtained by executing these novel algorithms in a single run.

Keywords: gelcasting; flexural strength; porosity; solid loading; genetic programming; non-dominated sorting genetic algorithms-II.

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1. Introduction

Gelcasting is a new ceramic forming process developed by the Oak Ridge National Laboratory (ORNL) in 1990s. The manufacturing of complex shaped, high-quality ceramic parts are prepared by this process. The most important factor of the gelcasting technology is the use of an organic monomer solution that can be polymerized to form a strong, cross-linked solvent gel. The gelcasting process consists of the preparation of aqueous slurry of ceramic powder containing gel initiators, monomer, cross-linker, sintering aids, catalysts and other additives. Gelcasting consists of the dispersion of a kind of ceramic powder in an aqueous solution containing a gelation substance to form a stable suspension which is subsequently solidified in the mold. After sintering, material with uniform microstructure can be obtained [1-7]. In gelcasting, higher solid content of ceramic suspension can provide much more possibility to get higher density of the final ceramic products. Also the solid loading can be controlled at a desired level.

Nomenclature

Si_3N_4	Silicon Nitride
GP	Genetic programming
NSGA-II	Non-dominated sorting genetic algorithms II
MAM	Methacrylamide
MBAM	N, N^1-methylenebisacrylamide
APS	Ammonium persulfate
TEMED	Tetramethylethylenediamine
Al_2O_3	Alumina
Y_2O_3	Yttrium oxide
x_1	Solid loading
x_2	Ratio of monomers
x_3	Monomer content
FS	Flexural strength
P	Porosity

Genetic Algorithms (GAs) are evolutionary programs that manipulate a population of individuals represented by fixed-format strings of information. An initial population of individuals (solutions) is generated for the problem domain and these then undergo evolution by means of reproduction, crossover and mutation of individuals until an acceptable solution is found [8]. Genetic algorithms, although very useful for simple problems, can restrict complex problems due to its inability to represent individuals other than fixed-format character strings. Genetic Programming (GP) is a generalization of genetic algorithms devised by Koza [Koza, 1992]. Genetic Programming is a method to evolve computer programs. Genetic Programming, one of a number of evolutionary algorithms, follows Darwin's theory of evolution often paraphrased as "survival of the fittest". There is a population of computer programs (individuals) that reproduce with each other. Over time, the best individuals will survive and eventually evolve to do well in the given environment [9].

Almost every real-world problem involves simultaneous optimization of several incommensurable and often competing objectives. While in single-objective optimization the optimal solution is usually clearly defined, this does not hold for multi objective optimization problems. Instead of a single optimum, there is rather a set of alternative trade-offs, generally known as Pareto-optimal solutions. These solutions are optimal in the wider sense that no other solutions in the search space are superior to them when all objectives are considered. Multi objective optimization problems (MOPs) are common.

2. Experimental Details

2.1 *Preparation of gelcasting Si_3N_4 ceramics*

Fig. 1 shows the detailed flowchart of the gelcasting process.

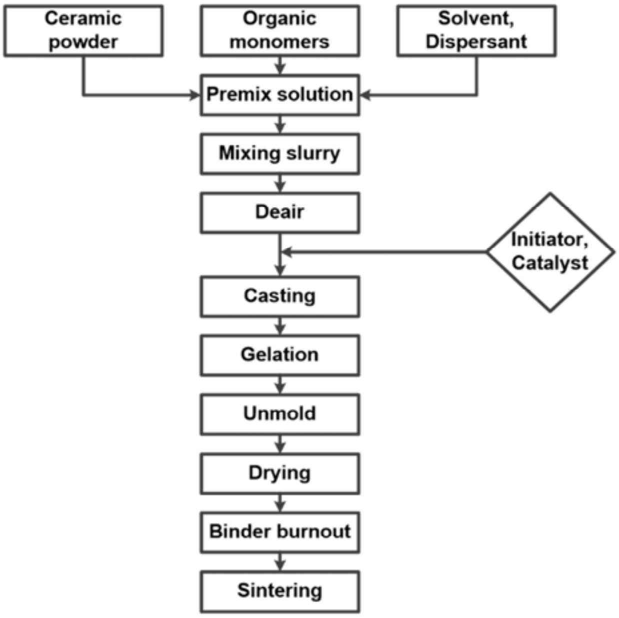


Fig. 1. Flow chart of gelcasting process

During the gelcasting preparation of porous Si_3N_4 ceramics, in the first step, dispersant (Dolapix A88, 1 wt%, based on silicon nitride) and monomers (MAM and MBAM) were completely dissolved in distilled water by magnetic stirring, and the premix solution was served as a dispersing media for the ceramic powders. The next step was to add silicon nitride powder and suitable sintering additives (2 wt%, Al_2O_3; 1 wt%, Y_2O_3) into the premix solution, and the slurry was degassed for 15–20 min. After that APS and TEMED are added to the premix slurry which acts as initiator and the catalyst. The slurry was cast into a nonporous rectangular glass mold. The slurry was kept at 50–60 ^{0}C for 30–40 minutes to polymerize to form gelled body after casting and then the gelled part was removed from the mold and dried to remove the solvent system. In order to avoid the occurrence of crack and warpage caused by rapid drying, the samples were dried in a commercial dryer at 25 ^{0}C of drying temperature and 98% of relative humidity. Finally, sintering was performed at a heating rate of 2 ^{0}C/min at 550 ^{0}C for binder burn out and heating rate 10 ^{0}C/min and 1 hour holding time at 1700 ^{0}C under nitrogen atmosphere, and then porous Si_3N_4 ceramics were achieved. The 27 runs full factorial method is chosen since the method provides a wider covering region of parameter space and good consideration of variables interaction in the model. The ranges of manufacturing parameters used were in Table 1.

Table 1. Factors and levels

S. No	Factors	Levels		
1	Solid loading (vol %)	30	40	50
2	Ratio of monomer to cross linking agent (MAM:MBAM)	3:1	6:1	9:1
3	Monomers content (Wt %)	5	10	15

The dispersant, TEMED and APS are kept constant. The materials and compositions are shown in Table 2.

Table 2. Materials kept constant

S. No	Material	Quantity
1	Al_2O_3(Aluminum Oxide)	2 wt% of solid loading
2	Y_2O_3(Yttrium Oxide)	1 wt% of solid loading
3	Dispersant	1 wt% of solid loading
4	APS	0.8 wt% of monomers
5	TEMED	0.5 wt% of monomers

The measured values of flexural strength and porosity for 27 experiments conducted as per full factorial for training data set. The 27 ceramic samples are shown in the Fig 2.

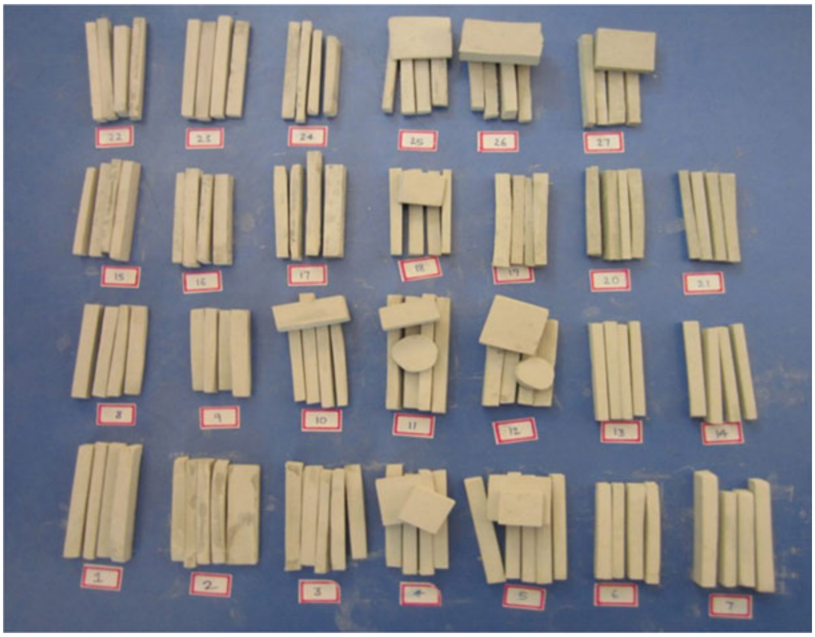


Fig. 2. Ceramic samples

3. Modeling using GP

Each individual in a genetic program is a computer program. However, this definition is a little vague since there is no general structure for all computer programs. Computer programs in GP are viewed as free-format trees, consisting of leaves (variables and constants) and non-terminal nodes (functions).The functions in the function set may include Arithmetic operations (+, -, *, etc.), Mathematical functions (such as sin, cos, exp, and log), Boolean operations (such as AND, OR, NOT), Conditional operators (such as If-Then-Else), Functions causing iteration (such as Do-Until). Crossover was categorized as the primary genetic operator for modifying program structures. Generally, after two programs (parents) are selected from the population, standard crossover randomly selects a node in each program tree except the root of the tree. It then exchanges the two sub trees rooted by the selected nodes (also called crossover points) between the two parent program trees to generate two new programs (off springs). Mutation was categorized as the secondary genetic operator for modifying program structures. For mutation, only one parent program is selected from the population. The new program is then inserted into the next population. Reproduction is where a selected individual copies itself into the new population. It is effectively the same as one individual surviving into the next generation. Execution of the previous mentioned three genetic operators constitutes one generation and the procedure is repeated until a termination criterion is met. The single individual with the best value of fitness over all the generations is designated as the result of a run. The termination criterion can be either a fixed number of generations or specified quality of the solution.

3.1. Description of NSGA-II

NSGA-II follows the same steps as classical GAs. First, it initializes a random population of N individuals, then it produces children/offspring by recombination and mutation, evaluates the individuals, and finally selects the fittest ones. Several aspects of NSGA-II are however very specific to this algorithm:

- The parental population is chosen through a tournament selection. This selection process enables to select a parent based on both convergence and spreading, while maintaining a reasonable diversity amongst the population.
- The genetic operators used inside NSGA-II are generally (although not necessarily) the Simulated Binary Crossover and the Polynomial mutation. These operators use a stochastic approach to determine children genes, based on the genes of their parents. They are extremely efficient when real variables are used.
- The selection process is computed at each generation on an intermediate population combining both parents and offspring. Therefore, no valuable solution can be lost, which makes NSGA-II elitist.
- For the selection, NSGA-II uses a non-dominated-and-crowding sorting and selection [10-12].

4. Results and Discussion

4.1 . Implementation of GP

The training data set for implementation of GP constitutes Table 3. GP, being a stochastic search technique, makes no prior assumptions about the actual model form. The structure and complexity of the model evolve automatically. The terminal set T and the function set F were defined as: T= $\{x_1, x_2, x_3\}$ and F= {+, -, *, /}. The genetic programming run is controlled by many parameters of which the two major numerical parameters are the population size and the maximum number of evolutionary generations. Evolutionary algorithms are generally robust to variations of control parameters and some guidelines are provided (Koza 1992) for choosing the control parameters of standard GP. The control parameters for GP are given in the Table 4.

Table 3. Training data set

S. No	Solid loading (vol %)(x_1)	Ratio of monomers (x_2)	Monomer content (wt%)(x_3)	Flexural strength (MPa)	Porosity (%)
1	30	3:1	5	116.93	43.01
2	30	3:1	10	110.07	44.03
3	30	3:1	15	102.03	46.5
4	30	6:1	5	110.69	45.7
5	30	6:1	10	98.69	48.1
6	30	6:1	15	85.03	51.76
7	30	9:1	5	108.98	46.0
8	30	9:1	10	88.229	51.01
9	30	9:1	15	68.64	53.0
10	40	3:1	5	190.76	33.36
11	40	3:1	10	182.21	35.08
12	40	3:1	15	173.32	38.04
13	40	6:1	5	180.46	36.1
14	40	6:1	10	180.9	36.7
15	40	6:1	15	149.81	39.2
16	40	9:1	5	175.32	37.4
17	40	9:1	10	157.88	40.7
18	40	9:1	15	120.73	42.23
19	50	3:1	5	290.50	25.01
20	50	3:1	10	285.52	26.5
21	50	3:1	15	273.05	27.0
22	50	6:1	5	270.9	27.3
23	50	6:1	10	260.3	28.0
24	50	6:1	15	250.26	29.7
25	50	9:1	5	250.51	30.5
26	50	9:1	10	248.23	31.1
27	50	9:1	15	229.07	32.5

Table 4. GP Control Parameters

Terminal set	{x1, x2, x3}
Functional set	{+, -, *, / }
Population size	500
Number of generations	100
Crossover probability (%)	85
Mutation Probability (%)	10
Elitism Probability (%)	05
Selection method	Tournament selection
Fitness measure	Minimum Error(10^{-4})

By investigation of various alternative models, the following expressions for flexural strength and porosity were found to have the best fitness value.

GP model for flexural strength (FS) (MPa)

$$FS = 3.428x_1 + 13.49x_2 + 6.856x_3 - 0.4056x_1x_2 - 0.2432\,x_1x_3 - 0.6585x_2x_3 - 0.002587x_1x_3^2 + 0.002587x_1^2x_3 + 0.08001x_1^2 + 0.003187x_3^2 - 0.0003491x_1x_2x_3^2 + 0.0003491x_1^2x_2x_3 - 66.14 \quad (1)$$

GP model for porosity (P) (%)

$$P = 4.42x_2 - 0.5689x_1 + 0.6357x_3 + 0.0001208x_1^2x_2^2 - 0.09356x_1x_2 - 0.01269x_1x_3 + 0.07347x_2x_3 - 0.0001208x_1^2x_2 - 0.1871x_2^2 - 0.0001208x_1x_2^2x_3 + 0.0001208x_1x_2x_3 + 53.33 \quad (2)$$

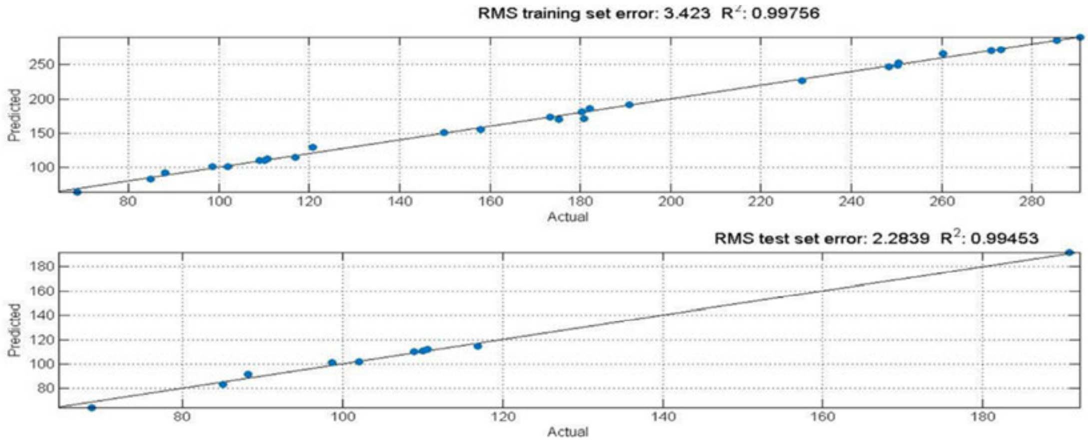


Fig.3. Predicted vs Actual values of flexural strength

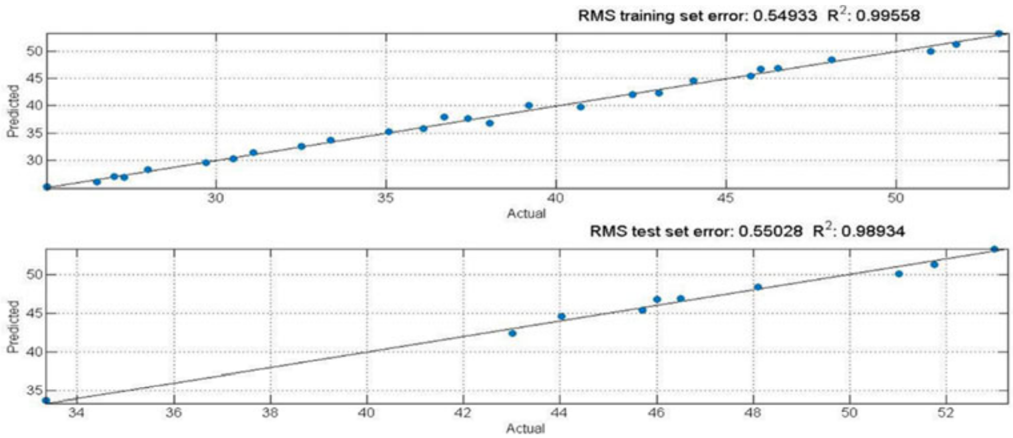


Fig.4. Predicted vs Actual values of porosity

A comparison of the predicted models and the experimental values for the validation datasets of flexural strength and porosity are shown in Fig. 3 and Fig. 4 respectively. GP predicts the response high values of correlation coefficient (R^2) for flexural strength and porosity are obtained and found to be 0.9945 and 0.9893 respectively. These indicate that the developed models satisfactorily represent the outputs.

4.2 Effect of manufacturing parameters on the responses

Surface plots have been drawn using MINITAB for the convenience of understanding the surface effects and selecting the best combinations of manufacturing parameters. The Flexural strength and porosity variation for different combinations of manufacturing parameters are shown in Fig. 5 and Fig. 6.

4.3 Flexural strength

Fig. 5 (a) shows the dependence of flexural on ratio of monomers (x_2) and monomer content (x_3) when the solid loading (x_1) is kept constant at 40 vol%. It can be seen that even though both factors have influence on the flexural strength ratio of monomers is a more dominant factor. The combination of low value of ratio of monomers and monomer content provide the highest flexural strength. The influence of solid loading (x_1) and monomer content (x_3) for the constant ratio of monomers (x_2) of 6:1 is shown in Fig. 5 (b). Both the factors show similar intensity of influence on flexural strength. The flexural strength increases if solid loading increases. Monomer content has the opposite effect, that is, flexural strength decreases if monomer content increases. Fig. 5 (c) shows how the flexural strength depends on the solid loading (x_1) and ratio of monomers (x_2) in the case when the monomer content (x_3) of 10 wt% is kept constant.

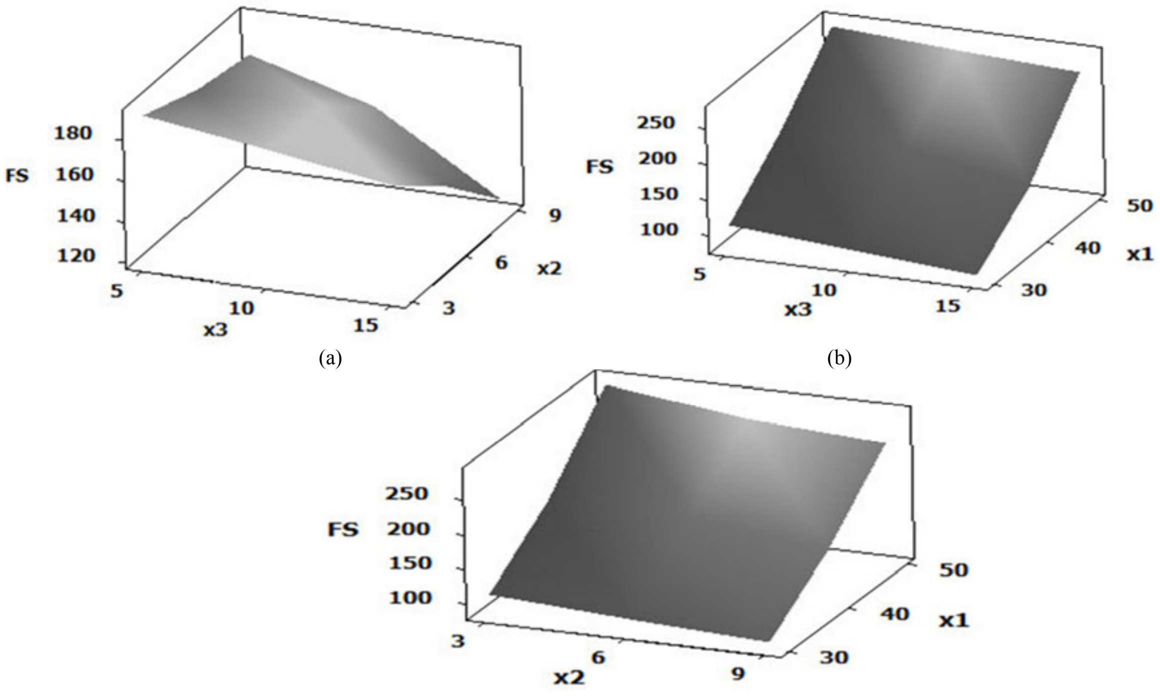


Fig.5. Surface plots of effect of solid loading, ratio of monomers and monomer content on flexural strength

4.4 Porosity

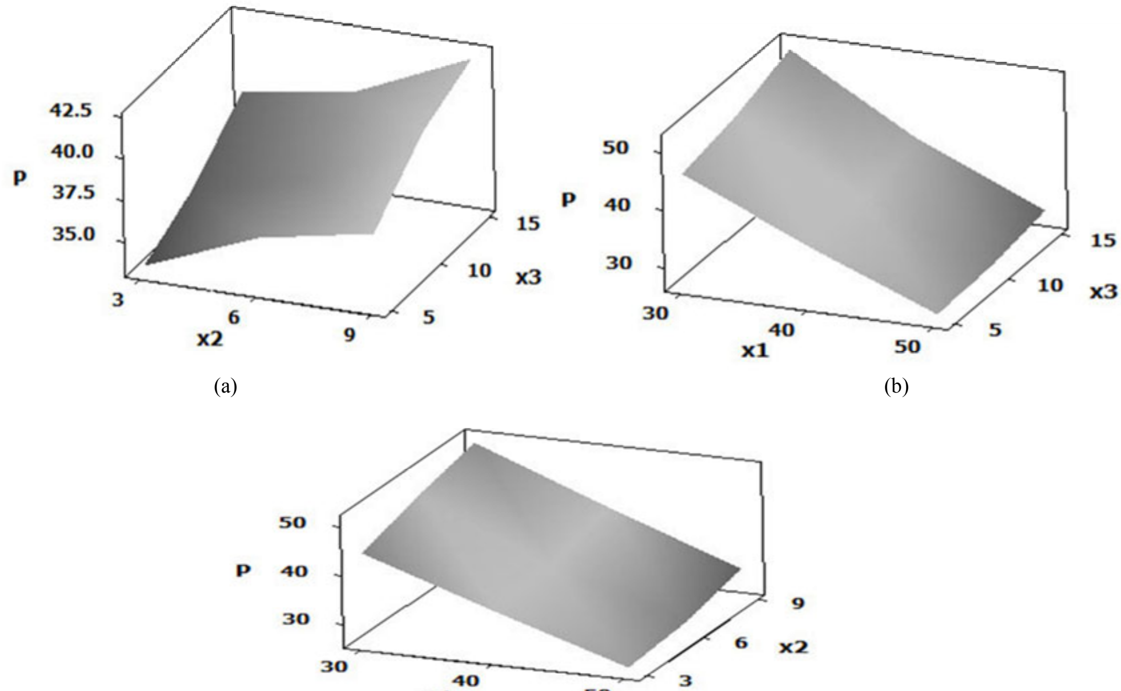
Fig 6 (a) shows the dependence of porosity on ratio of monomers (x_2) and monomer content (x_3) when the solid loading (x_1) is kept constant at 40 vol%. It can be seen that even though both factors have influence on the porosity ratio of monomers is a more dominant factor. The combination of low value of ratio of monomers and monomer content provide the lowest porosity. The influence of solid loading (x_1) and monomer content (x_3) for the constant ratio of monomers (x_2) of 6:1 is shown in Fig. 6 (b). Both the factors show similar intensity of influence on porosity. The Porosity decreases if solid loading increases. Monomer content has the opposite effect, that is, porosity decreases if monomer content decreases. Fig. 6 (c) shows how the porosity depends on the solid loading (x_1) and ratio of monomers (x_2) in the case when the monomer content (x_3) of10 wt% is kept constant.

4.5 Formulation of multi objective optimization

The two objective functions considered in this study are
1) Maximization of flexural strength, 2) Minimization of porosity, which are given in the equations (1) and (2) respectively.
Subject to

$$20 \leq x_1 \leq 60, 2 \leq x_2 \leq 20, 2 \leq x_3 \leq 20 \quad (3)$$

Tournament selection, binary crossover and polynomial mutation operators were selected as the genetic operators of the real-coded NSGA-II algorithm. The control parameters required for implementation of the algorithm are listed in table 5. The algorithm found the Pareto optimal front of conflicting objective functions with good diversity of solutions, as shown in Fig. 7. The optimal input variables and their corresponding objective function values are presented in table 6.



(c)

Fig. 6. Surface plots of effect of solid loading, ratio of monomers and monomer content on porosity

Table 5. NSGA-II control parameters

Population size	50
Number of generations	200
Crossover probability (%)	0.9
Mutation probability (%)	0.1
Selection method	Tournament

From the experimental results of Table 3, manufacturing parameters listed in the first experiment lead to the flexural strength of 116.93 MPa and porosity of 43.01%. After optimization, flexural strength is increased to 130.1447 MPa at the same value of porosity in Table 6, fifth experiment. Similarly, manufacturing parameters listed in the fifth experiment (Table 3) lead to the flexural strength of 98.69 MPa and porosity of 48.1%. After optimization, porosity decreased to 43.390% at the same value of flexural strength in Table 6, 40th experiment.

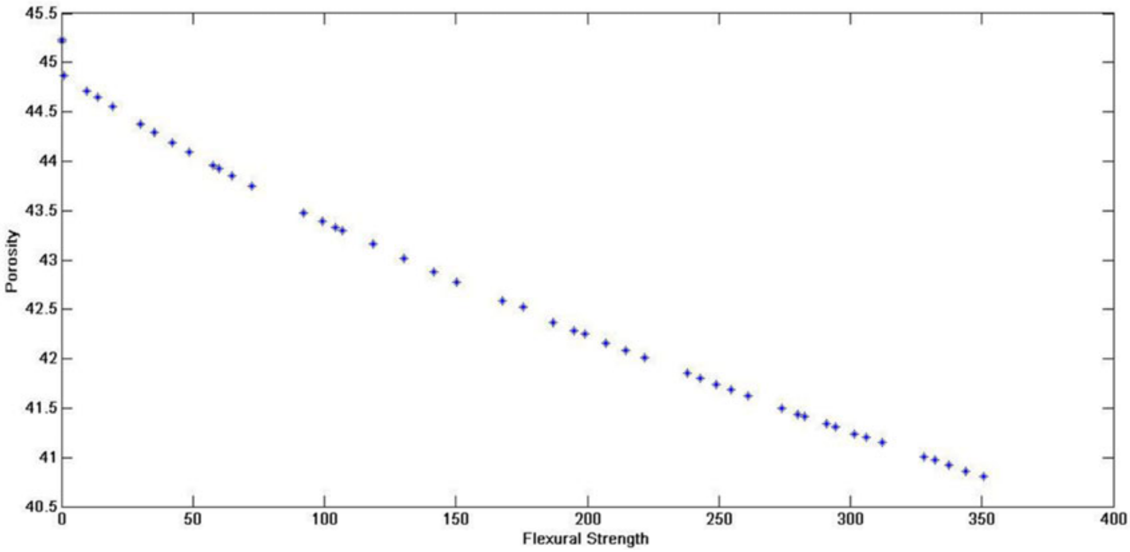


Fig. 7. Pareto optimal front

Table 6. Final optimal solutions

S. No	Solid loading (vol %)(x_1)	Ratio of monomers (x_2)	Monomer content (wt%)(x_3)	Flexural strength (MPa)	Porosity (%)
1	28.0000	2.0013	5.1152	0.0023	45.2326
2	60.0000	2.0000	2.0000	350.6114	40.8083
3	49.0000	2.0000	2.1702	199.2284	42.2517
4	28.0000	2.0000	2.0107	0.8020	44.8718
5	43.0000	2.0032	2.0113	130.1447	43.0117
6	47.0000	2.0100	2.1683	175.4547	42.5221
7	54.0000	2.0020	2.0738	261.0168	41.6270
8	58.0000	2.0021	2.0000	327.9407	41.0078
9	55.0000	2.0029	2.0000	274.0924	41.4967
10	51.0000	2.0022	2.0748	221.5842	42.0147
11	57.0000	2.0022	2.0000	312.0033	41.1489
12	52.0000	2.0020	2.0685	237.8938	41.8507
13	29.0000	2.0000	2.0050	9.8120	44.7112
14	48.0000	2.0000	2.0596	187.0310	42.3689
15	49.0000	2.0000	2.0631	206.8899	42.1602
16	28.0000	2.0012	4.9623	0.2792	45.2106
17	37.0000	2.0001	2.0223	72.4983	43.7476
18	40.0000	2.0013	2.0002	106.8646	43.2933
19	36.0000	2.0001	2.0000	64.9480	43.8507
20	46.0000	2.0000	2.1312	167.7087	42.5872

21	44.0000	2.0034	2.0005	141.5503	42.8760
22	39.0000	2.0001	2.0000	92.1967	43.4800
23	42.0000	2.0032	2.0606	118.5579	43.1575
24	42.0000	2.0032	2.0606	118.5579	43.1575
25	60.0000	2.0000	2.0000	344.0260	40.8647
26	60.0000	2.0000	2.0000	350.6114	40.8083
27	32.0000	2.0002	2.0043	35.4060	44.2902
28	56.0000	2.0028	2.0000	290.9973	41.3400
29	59.0000	2.0000	2.0191	337.4603	40.9235
30	57.0000	2.0020	2.0000	301.6934	41.2412
31	55.0000	2.0029	2.0000	282.4895	41.4185
32	34.0000	2.0000	2.0000	48.4847	44.0898
33	56.0000	2.0020	2.0000	294.4617	41.3069
34	32.0000	2.0002	2.0042	30.0628	44.3746
35	52.0000	2.0021	2.0667	242.9669	41.8008
36	44.0000	2.0033	2.0007	150.3087	42.7745
37	30.0000	2.0000	2.0060	19.3570	44.5489
38	53.0000	2.0021	2.0694	254.5149	41.6889
39	59.0000	2.0020	2.0003	332.1472	40.9708
40	40.0000	2.0013	2.0002	99.2608	43.3903
41	35.0000	2.0001	2.0000	59.8832	43.9229
42	33.0000	2.0010	2.0030	42.2167	44.1862
43	53.0000	2.0020	2.0693	248.8620	41.7436
44	35.0000	2.0001	2.0000	57.6175	43.9557
45	48.0000	2.0000	2.0642	194.9796	42.2849
46	55.0000	2.0028	2.0000	280.0529	41.4410
47	30.0000	2.0002	2.0146	13.6108	44.6471
48	50.0000	2.0023	2.0740	214.5512	42.0862
49	40.0000	2.0012	2.0010	104.2811	43.3261
50	57.0000	2.0022	2.0000	306.0409	41.2023

Conclusions

Si_3N_4 ceramic samples were prepared by gelcasting method with varying solid loading, ratio of monomers and monomer content at 3 levels using full factorial experimentation. Flexural strength and porosity of gelcast ceramic composite were measured. It results shows that flexural strength increases as solid loading increases and decreases as ratio of monomers and monomer content increases, porosity decreases as solid loading increases and increases as ratio of monomer to cross linking agent and monomer content increases. The process is modelled with genetic programming is a domain independent methodology which does not assume any prior functional form of the solution and hence it can accurately model the complex relationships of the process. The high R^2 (for flexural strength is 0.99453 and porosity is 0.98934) value of the models proves the effectiveness of the GP approach to establish substantially valid models. Non-dominated sorting genetic algorithms-II has been used to simultaneously optimize the conflicting objectives of flexural strength and porosity. The Pareto optimal front and solution set is generated and presented.

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