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A REVIEW OF GENETIC ALGORITHMS AND ITS APPLICATIONS IN CHEMICAL ENGINEERING RESEARCH

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ABSTRACT
This paper presents a review of Genetic Algorithms (GAs) and its applications within the field of Chemical Engineering. The primary applications of GAs in Chemical Engineering date back to the 1970s, and within the last decades, they have been more and more often used to solve various complex problems, even when the objective functions don't possess properties like continuity, differentiability and so on. These algorithms manipulate and maintain a set or population of solutions and implement a “survival of the fittest” strategy in their search for better solutions. GAs are very helpful for the optimization and variable selection in modeling and calibration due to the strong effect of the relationship between presence/absence of variables in a calibration model and the prediction ability of the model itself. This review is an outline of the concept of GA and in fact, it does not present all applications of Genetic Algorithms to Chemical Engineering problems; its goal is to rather point out to the researchers, the important fields of application of GAs along with providing a list of references on the topic.

KEYWORDS: Genetic Algorithm, Chemical Engineering, Evolutionary Algorithm, Optimization.

INTRODUCTION
Genetic algorithms are classed as global search heuristics and represent one branch of the field of study called Evolutionary Computation or Evolutionary Algorithms. These algorithms make use of the principle of evolution that was originally propounded by Charles Darwin. They emulate the biological processes of natural selection and reproduction to get the fittest solutions. A genetic algorithm is a search technique employed in computing to obtain precise or approximate solutions to optimization and search problems. They employ the use of techniques inspired by evolutionary biology like selection, crossover, mutation and inheritance. Like in evolution, a lot of processes in genetic algorithms are random; however this technique permits one to set the level of randomization and also the level of control. These algorithms are much more powerful and economical than random search and exhaustive search algorithms, yet require no additional data concerning the given problem. This feature permits them to find solutions to problems that other optimization methods cannot handle because of a lack of continuity, derivatives, linearity, or other features

Evolutionary algorithms are used in solving such problems which don't have a well outlined economical solution. They are used to solve optimization problems such as scheduling, shortest path, etc and in modeling of systems wherever randomness is involved (e.g. the stock market). It is an adaptive heuristic search methodology based on population genetics.

Genetic algorithm is started with a collection of solutions referred to as population. a solution is represented by a chromosome. The population size is maintained throughout each generation. At every generation fitness of every chromosome is evaluated and then chromosomes for consecutive generation are probabilistically chosen according to their fitness values.

Nowadays, the utilization of Multi-Objective evolutionary Algorithms in all disciplines has become widespread and chemical engineering is, by no means, an exception.

HISTORY OF GA

The idea of evolution-inspired algorithms to optimize functions was put forth by G.E.P. Box, G.J. Friedman, W.W. Bledsoe and H.J. Bremermann independently but their work was not much impressive and had little follow-up. The first possible mention of evolutionary algorithm is present in the PhD thesis of Rosenberg of Technical University of Berlin, who introduced a technique and named it evolution strategy but this technique was more similar to hill climbers than to genetic algorithms. The technique performed mutation of a parent and produced two offspring of which the better was kept and it became the parent for the next round of mutation. Also it had no population or crossover. The idea of crossover and other recombination operators was first put forth by John Holland. He produced the most important work in the field of genetic algorithms in the year 1975 in the form of a landmark book titled Adaptation in Natural and Artificial Systems. This book was the first to present rigorously and systematically, the concept of adaptive digital systems by the use of mutation, selection and crossover, imitating the processes of biological evolution, as a problem-solving strategy. The book introduced the notion of Schemata and thus provided a firm theoretical support to Genetic Algorithms. In that same year, the potential of GAs was established by Kenneth De Jong in his important dissertation by showing that GAs could perform well on a wide variety of test functions that included discontinuous, noisy and multimodal search landscapes. Goldberg provided the first advancement on the Schema theory in the form of a crucial and popular proposition which was known as Building Block Hypothesis. It stated that the major source of Genetic Algorithm performance is the crossover. The first international conference of genetic algorithm was held in USA in the year 1985.

The early use of genetic algorithm in the field of chemical engineering was done to solve reaction kinetics and estimation of kinetic parameters. The availability of powerful optimization techniques based on GA has provided a strong boost to studies on optimization involving multiple objectives, of several key Chemical Engineering processes in the last decade.

The success of GAs as search procedures is attributed to some of its unique characteristics. They manipulate a population (set) of solutions simultaneously and thus reduce the probability of getting confined in local optima by a greater extent, when compared with other methods that move linearly from one point to other in the solution region. Parallelization can also be suitably done because of this feature. Second, the operators used by GAs act on parameter space coding rather than the parameters themselves, which enables their simplified implementation. Third, they can handle almost any kind of objective function because the continuity or differentiability of the function to be optimized is not required. This is suitable for problems which are evaluated by simulation and also those with complex objectives. However, GAs are not without limitations in that they can suffer from premature convergence and make fine tuning of search less effective. Thus, solutions could get worse or stagnate if not handled properly. A successful implementation of GA should aim to reduce these difficulties.

In the language of genetic algorithms, the function variables are called genes. These can be real or binary values. If they are binary, they have certain encoding functions which convert the value of gene to real value in output. This is also named genotype-phenotype mapping. Different values of a gene are called alleles. A Chromosome or Individual is a set of genes or set of variables of the model. A set of individuals is called population. Many different populations may co-exist, as in real evolution. These population groups are isolated and they are called subpopulations. The isolation helps to maintain the variety in the whole population. The subpopulations move between other subpopulations every now and then to get new genes. The GA derives most of its terminology from evolution biology which are listed here:

Initial population: A matrix of population size (number of individuals x number of genes) created by generating random numbers of selected range. To some variables with large range of possible values, logarithmic scale can be used.

Fitness value: The goodness of an individual, how well the candidate model matches the experimental data is calculated using fitness function.

Stopping condition: It is the condition of stopping the algorithm. It can be a maximum number of generations or achieving certain fitness.

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Ranking: To give values to individuals according their fitness values. The better the individual, the better is value in ranking. The ranking value can be understood as a probability to survive to the next generation.

Selection: To choose the parents for the next generation. The individuals with high ranking value can be parents for many offspring while the individuals with worst ranking values should not be able to survive. The selection is based on stochastic methods.

Crossover: The production of offspring. The chosen parents are set to pairs and each pair are changing alleles according the conditions of crossover.

Mutation: A gene in a chromosome is replaced by new random number from the defined area. The mutation occurs relatively seldom but is really important to maintain the variety in population. By mutation the algorithm can find new and better alleles that lead to global minimum.

Migration: Individuals or genes of different subpopulations are changing place bringing new alleles to subpopulations.

Next generation: The next generation consists of the best offspring and best parents so that the number of individuals in population stays constant.

The steps involved in developing genetic algorithm are as follows:

Initialization
It is the first step in which a population of suitable pop size of binary strings of suitable chromosome length is created. All the strings are evaluated for their fitness values using specified fitness function. The objective function is interpreted in the light minimization and maximization & becomes the fitness function.

Reproduction
It involves selection of the chromosomes from the current population to form a mating pool for the next generation production. The selection procedure is stochastic wherein fitter chromosomes have a better chance of getting selected.

Crossover
This step results in creating two offspring chromosomes from each parent pair selected randomly. The two parent chromosomes selected are cut at same randomly selected crossover points to obtain two sub-strings per parent string. The second sub-string is then mutually exchanged and combined with the respective first sub-string to form two offspring chromosomes.

Mutation
Among the members of the population generated, randomly as many elements of the offspring are mutated with probability equal to Pmut. This is usually very small & avoids creation of entirely different search sub-spaces. This prevents the GA search from becoming absolutely random.

The new population undergoes the fitness test. The steps are repeated & finally, the values of the variables obtained hereby represent the optimized solution.

In one generation crossover and mutation operators are applied only once. Thus generation means the number of times the crossover and mutation must operate on the population. Generation is synonymous to iteration. The flow diagram of a genetic algorithm is given below.

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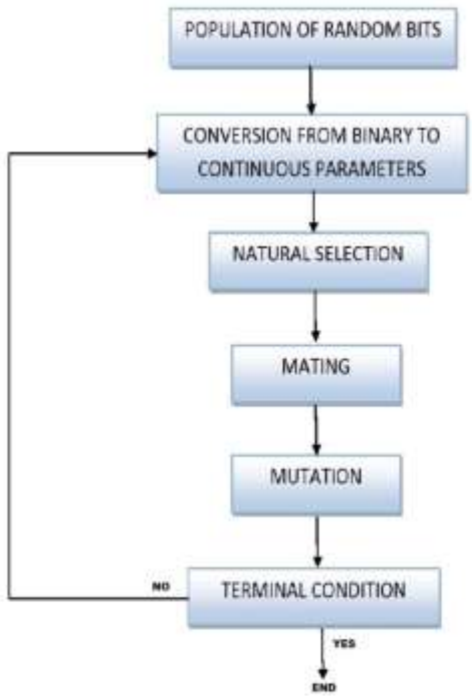

Fig 1: Flowchart Of Genetic Algorithm

APPLICATIONS OF GAs IN CHEMICAL ENGINEERING

Chemical Engineering in the present day is linked to core competencies in the area of reaction engineering, transport phenomena, separations science, and process and systems science. This discipline has developed a lot over the years with technological advancements and paradigm shifts. These embody the introduction of mathematical modeling in its varied forms such as process control, systems approach, etc., the shift to transport phenomena from unit operations, the recent gradation towards bio-systems, etc. However, one aspect of chemical engineers that still remains unchanged is that they have a duty of integrating the core chemical engineering constituencies with economic parameters in order to attain commercial success. in this context, optimization of processes play a major role in chemical engineering.

The main focus and practical application of improvement of chemical processes involve many objectives to be considered at the same time. These objectives can include profit, payback period, operating cost, capital cost/investment, quality, selectivity, and/or recovery of the product, energy required, process safety and/or quality, conversion, efficiency, robustness, operation time, etc. Recent publications cover differing types of optimization problems in a variety of disciplines of chemical engineering: they vary from single objective optimization to multiple-objective optimization, from parameter estimation to plant design,, from pure integer programming to mixed integer-nonlinear-programming (MINLP), from problems with specific objective functions to problems with simulation-determined objective functions, from optimization under well-defined conditions to optimization under uncertainty.

With the application of GA, multi objective functions of chemical engineering processes have been easily tackled and optimized. most areas of Chemical Engineering have used GA optimization technique be it maximization or minimization however the foremost use of GA has been in estimation of kinetic parameters of chemical reactions.

A few examples of use of GA in various chemical engineering applications are summarized in table 1. The list doesn't represent essentially all the research done with GA in chemical engineering. However, it is aimed toward giving an outline of the broad reach and flexibility of the technique.

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Table 1: Examples of applications of Genetic Algorithms in Chemical Engineering

S.NO	Author	YEAR	Details
1	Mitra et al.	1998	Minimization of the reaction time and the cyclic dimer concentration in an industrial semibatch nylon 6 reactor.
2	Garg and Gupta,	1999	Minimization of total reaction time and the polydispersity of the PMMA product
3	Gupta and Gupta,	1999	Minimization of the reaction time and the cyclic dimer concentration in an industrial semibatch nylon 6 reactor system.
4	Rajesh et al.	2000	Minimization of the methane feed rate and maximization of the flowrate of CO in the syngas for a fixed production rate of hydrogen in an existing side-fired steam
5	Bhaskar et al.	2000	Minimization of the residence time of the polymer melt and the concentrations of the undesirable side products formed in the industrial continuous wiped film PET reactor. Equality constraint on the desired degree of polymerization imposed.
6	Ravi et al.	2000	Maximization of the overall collection efficiency and minimization of the pressure drop / overall cost of the cyclone separators
7	Chan et al.	2000	Maximization of the percentage removal of the alcohol from beer and minimization of the removal of the 'extract' (taste chemicals)
8	Zhou et al.	2000	Maximization of the monomer conversion (cross-section average value) and minimization of the length of the film reactor in the continuous casting process for PMMA
9	Chan et al.	2000	Two cases: maximization of alcohol removal from beer while minimizing (a) Removal of 'taste chemicals or extract' and (b) Removal of 'taste chemicals or extract' as well as cost.
10	Zhou et al.	2000	Maximization of average monomer conversion in the product while minimizing length of the film reactor.
11	Chen and Ramaswamy	2002	Simultaneous minimization of surface cook values (i.e. Maximization of final product quality) and minimization of processing time.

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12	Li et al. Yee et al.	2003	Five cases using two or three objectives from (1) maximization of styrene produced, (2) maximization of styrene selectivity, (3) maximization of styrene yield, and (4) minimization of amount of steam used.
13	Subramani et al. (2003a) Yu et al. (2004)	2004	Two cases: (a) maximization of both purity and productivity of fructose, and (b) maximization of productivity of both glucose and fructose.
14	Inamdar et al.	2004	Three cases: (a) maximization of profit while minimizing energy cost, (b) maximization of total distillates produced while minimizing energy cost, and (c) maximization of profit while minimizing cumulative deviation of all the properties from the plant/desired values.
15	Silva and Biscaia	2003 and 2004	Minimization of the initiator concentration in the product and the deviation from the desired conversion in a batch free radical polymerization of Styrene
16	Anderson et al.	2005	Maximization of waste feed rate and minimization of carbon content in ash.
17	Guria et al.	2005	Maximization of both the recovery of the concentrated ore and valuable mineral content in the concentrated ore.
18	Kurup et al.	2006	Maximization of sum of purity A and purity C, and maximization of purity B in a reaction multi-component reaction involving three products A, B and C.
19	Sarkar et al.	2006	Three problems with two or three objectives from (1) maximization of the weight mean size of the crystal size distribution, (2) minimization of the nucleated product, (3) minimization of total time of operation, and (4) minimization of coefficient of variation.
20	Dietz et al.	2006	Four cases of 2 or 3 objectives from minimization of investment and environmental impact (EI) due to biomass and EI due to solvent.

21	Bhutani et al.	2006	Three cases: (a) maximization of kerosene produced while minimizing hydrogen makeup, (b) maximization of diesel produced while minimizing hydrogen makeup, and (c) maximization of more valuable, heavy end products while minimizing light end products.
22	Sarkar et al.	2007	Maximization of weight mean size while minimizing coefficient of variation.
23	Dietz et al.	2007	Three cases with one or more objectives from maximization of net present value (NPV) and optimizing two other criteria: (1) production delay/advance and (2) flexibility criteria.
24	Hou et al.	2007	Maximization of the aromatic yield and minimization of the yield of heavy aromatics.
25	Wu et al	2007	Molecular design of extractive distillation
26	Yang et al	2007	Optimization of fuzzy neural network in FCC of gasoline
27	Masoori et al	2007	Rates of reaction in chemical reacting systems
28	Tao and Wang	2007	Parameter estimation
29	Cao et al	2007	Minimum freshwater consumption
30	Jezowski et al	2007	Superstructure optimization of retrofit problem in heat exchanger network
31	Young et al	2007	MINLP in the design of chemical systems
32	Elliott et al	2007	A reduced mechanism to simulate fuel combustion
33	Agrawal et al	2007	Two-objective low-density polyethylene reactor
34	Istadi and Amin	2007	ANN-based model for plasma reactor
35	He and Hui	2007	Large multi-stage multi-product scheduling
36	Jung et al	2007	Search for blue phosphors in seven cation systems
37	Till et al	2007	Two-stage stochastic integer programs
38	Cubillos et al	2007	Process optimization of grey-box neural models
39	G. N. Xie	2008	Optimization of compact heat exchangers by a genetic algorithm
40	S. K. Lahiri and K. C. Ghanta	2008	Prediction of Pressure Drop of Slurry Flow in Pipeline by Hybrid Support Vector Regression and Genetic Algorithm Model
41	Ayla Altinten et al	2008	Self-tuning PID control of jacketed batch polystyrene reactor using genetic algorithm
42	B. Saha et al	2008	Hybrid genetic algorithm to find the best model and the globally optimized overall kinetics parameters for thermal decomposition of plastics

43	Javier Causa et al	2008	Hybrid fuzzy predictive control based on genetic algorithms for the temperature control of a batch reactor
44	G. Milani and F. Milani	2008	Genetic algorithm for the optimization of rubber insulated high voltage power cables production lines
45	Jose M. Ponce-Ortega et al	2009	Use of genetic algorithms for the optimal design of shell-and-tube heat exchangers
46	Xiao Chen and Ning Wang	2009	A DNA based genetic algorithm for parameter estimation in the hydrogenation reaction
47	Jose Antonio Vazquez-Castillo et al	2009	Design and optimization, using genetic algorithms, of intensified distillation systems for a class of quaternary mixtures
48	Giovanna Fiandaca et al	2009	A multi-objective genetic algorithm for the design of pressure swing adsorption
49	Benoit Allen et al	2009	Optimizing heat exchanger networks with genetic algorithms for designing each heat exchanger including condensers
50	Jawed Iqbal and Chandan Guria	2009	Optimization of an operating domestic wastewater treatment plant using elitist non-dominated sorting genetic algorithm
51	T. Hatami et al	2010	Mathematical modeling and genetic algorithm optimization of clove oil extraction with supercritical carbon dioxide
52	Kangtai Wang and Ning Wang	2010	A novel RNA genetic algorithm for parameter estimation of dynamic systems
53	J. C. Curvelo Santana et al	2010	Optimization of Corn Malt Drying by Use of a Genetic Algorithm
54	A. Rahimi et al	2010	Development of an optimized chemical kinetic mechanism for homogeneous charge compression ignition combustion of a fuel blend of n-Heptane and natural gas using a genetic algorithm
55	Thadikamala Sathish Andreddy Shetty Prakasham	2010	Enrichment of Glutaminase production by Bacillus Subtilis RSP-GLU in submerged cultivation based on neural network—genetic algorithm approach
56	Hamidreza Najafi et al	2011	Energy and cost optimization of a plate and fin heat exchanger using genetic algorithm
57	Debanga Nandan Mondal et al	2011	Cu—Zn separation by supported liquid membrane analyzed through Multi-objective Genetic Algorithms

58	H. Safikhani et al	2011	Modeling and multi-objective optimization of cyclone separators using CFD and genetic algorithms
59	Masamoto Arakawa, Yosuke Yamashita and Kimito Funatsu	2011	Genetic algorithm-based wavelength selection method for spectral calibration
60	Miha kovacic and Bozidar Sarler	2011	Genetic Algorithm-Based Batch Filling Scheduling in the Steel Industry
61	R. Abbasi et al	2012	Kinetics of methane combustion over Pt and Pt–Pd catalysts
62	Feng Qian et al	2012	Development of a Free Radical Kinetic Model for Industrial Oxidation of p-Xylene Based on Artificial Neural Network and Adaptive Immune Genetic Algorithm
63	A. Ghaee et al	2012	Adsorption of copper and nickel ions on macroporous chitosan membrane: Equilibrium study
64	E. B. Gueguim Kana	2012	Modeling and optimization of biogas production on saw dust and other co-substrates using Artificial Neural network and Genetic Algorithm
65	Ali Taheri Najafabadi et al	2012	Kinetic modeling and optimization of the operating condition of MTO process on SAPO-34 catalyst
66	Fatemeh Bashipour and Seyyed M. Ghoreishi	2012	Experimental optimization of supercritical extraction of β-carotene from Aloe Barbadensis Miller via genetic algorithm
67	Lim Kai Tun and Hideyuki Matsumoto	2013	Application Methods for Genetic Algorithms for the Search of Feed Positions in the Design of a Reactive Distillation Process
68	Li Zhang and Ning Wang	2013	A modified DNA genetic algorithm for parameter estimation of the 2-Chlorophenol oxidation in supercritical water
69	Ali Nejad Ebrahimi et al	2013	Genetic algorithm-based pore network extraction from micro-computed tomography images
70	Maria Vazquez Ojeda et al	2013	Design and optimization of an ethanol dehydration process using stochastic methods
71	Amin Shokrallahi et al	2013	Intelligent model for prediction of CO_2 – Reservoir oil minimum miscibility pressure
72	Dorianna M. D'Addona and Roberto Teti	2013	Genetic Algorithm-based Optimization of Cutting Parameters in Turning Processes

73	Seyyed Mohammad Ghoreishi , Ehsan Bataghva	2014	Supercritical extraction of essential oil from Echium Amoenum seed : Experimental, modeling and genetic algorithm parameter estimation
74	M. Susana Moreno et al	2014	Parameter Estimation of an Empirical Kinetic Model for CO Preferential Oxidation
75	Matheus P. Porto et al	2014	Genetic optimization of heat transfer correlations for evaporator tube flows
76	H. Safari and M. Jamialahmadi	2014	Estimating the kinetic parameters regarding barium sulfate deposition in porous media: a genetic algorithm approach
77	Ramin Badmezhad and Behrooz Mirza	2014	Modeling and optimization of cross-flow ultrafiltration using hybrid neural network-genetic algorithm approach
78	M. Ghaedi et al	2014	Principal component analysis-artificial neural network and genetic algorithm optimization for removal of reactive orange 12 by copper sulfide nanoparticles-activated carbon
79	Ridong Zhang et al	2014	Temperature Modeling in a Coke Furnace with an Improved RNA-GA Based RBF Network
80	Mohammad-Ali Ahmadi et al	2014	Gas Analysis by In Situ Combustion in heavy oil Recovery Process: Experimental and Modeling Studies
81	Arash Kamari et al	2015	Compositional Model for Estimating Asphaltene Precipitation Conditions in Live Reservoir Oil Systems
82	Donatas Levišauskas et al	2015	Optimization of biomass production in fed-batch culture by feed and dilution control actions
83	Elaheh Neshat and Rahim Khoshbakhti Saray	2015	An optimized chemical kinetic mechanism for HCCI combustion of prfs using multi-zone model and genetic algorithm
84	Pedro J. Casanova Pelaez et al	2015	Olive Cake Improvement for Bioenergy: the Drying Kinetics
85	Job S. Kasule et al	2015	Very Large Scale Droplet Microfluidic Integration (VLDMI) using Genetic Algorithm
86	Naser Hadi et al	2015	An intelligent approach to design and optimization of M-Mn/H-ZSM-5 (M: Ce, Cr, Fe, Ni) catalysts in conversion of methanol to propylene

87	Xinqiang You et al	2015	Investigation of Separation Efficiency Indicator for the Optimization of the Acetone–Methanol Extractive Distillation with Water
88	Mohammad-Ali Ahmadi et al	2015	Estimation of the silica solubility in the superheated steam using LSSVM modeling approach
89	Kasat et al. (2002) Sankararao and Gupta (2007a)	2002, 2007	Four problems with two or three objectives from (1) maximization of gasoline yield, (2) minimization of air flow rate, and (3) minimization of percent carbon monoxide in the flue gas.

CONCLUSION

A brief introduction of Genetic Algorithms has been presented in this review. The method of working of GA is explained together with its application in the field of Chemical Engineering. Several improvements can be made to increase the applicability of GA in chemical engineering and other engineering disciplines as well. It is concluded that GA is a very promising optimization technique which can be and has been applied successfully in problems involving multi-variable systems and complex engineering systems commonly encountered in chemical engineering processes. With the increase in the awareness about GA, we hope to see wider applicability and more research using this technique.

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