Multicriteria Optimization of Gasification Operational Parameters Using a Pareto Genetic Algorithm

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ABSTRACT

Gasification is a well-known technology that allows for a combustible gas to be obtained from a carbonaceous fuel by a partial oxidation process (POX). The resulting gas (synthesis gas or syngas) can be used either as a fuel or as a feedstock for chemical production. Recently, gasification has also received a great deal of attention concerning power production possibilities through IGCC process (Integrated Gasification Combined Cycle), which is currently the most environmentally friendly and efficient method for the production of electricity. Gasification allows for low grade fuels, or dirty fuels, to be used in an environmental acceptable way. Amongst these fuels are wastes from the petrochemical and other industries, which vary in composition from shipment to shipment, and from lot to lot. If operating conditions are kept constant this could result in lose of efficiency. This paper presents an application of Genetic Algorithms to optimize the operating parameters of a gasifier processing a given fuel, so that the system achieves maximum efficiency for each particular fuel composition. A Pareto multiobjective optimization method, combined with a Genetic Algorithm, is applied to the simultaneous maximization of two different objective functions: Cold Gas Efficiency and Hydrogen Contents of the syngas. Results show that the optimization method developed is fast and simple enough to be used for on-line adjustment of the gasification operating parameters for each fuel composition and aim of gasification, thus improving overall performance of the industrial process.

Keywords: Gasification, Pareto Genetic Algorithms, Multicriteria Optimization

1. INTRODUCTION

This paper presents an application of Pareto Genetic Algorithms to optimize the operating parameters of a gasifier processing a given fuel.

Gasification is a well-known technology that allows for a combustible gas to be obtained from a carbonaceous fuel by a partial oxidation process (POX). The resulting gas (synthesis gas or syngas) can be used either as a fuel or as a feedstock for chemical production. The major constituents of syngas are CO, H_2, CO_2 and H_2O. From these, only H_2 and CO are combustible and only H_2 is interesting as chemical feedstock.

Formally defined, gasification is the conversion of solid and liquid materials into a gas through reaction with oxygen, steam and carbon dioxide, or a mixture of these gases at a temperature exceeding 700 ºC. In industrial applications, a solid or liquid fuel is conveyed to a vessel (the gasifier) and mixed with oxygen and steam. The CO_2 and H_2O resulting from the combustion of a fraction of the fuel will also be an agent of gasification of the remaining fuel. There will also be some N_2 present in the gasifier because the oxygen stream is not 100% pure and also, possibly, because N_2 can be used as a conveying gas for the transportation of the fuel. Some heat can be recovered from the gasification chamber (gasification is an overall exothermic reaction, which will generate heat) to produce steam.

Traditionally, gasification has been used as a means of producing heating gas for domestic and industrial needs (town gas) and as a source of hydrogen for the heavy chemical industry. Recently, gasification has received a great deal of attention concerning power production possibilities, since it is the core of the IGCC process (Integrated Gasification Combined Cycle). IGCC is the most environmentally friendly method for the production of electricity since it allows for all the pollutants to be removed in a pre-combustion stage, at the gas cleanup [1].

It also allows for any fuel to be used in a combined cycle, thus greatly increasing electricity production efficiency.

One of the major advantages of gasification is that it allows for less noble fuels, or dirty fuels, to be used for the above mentioned purposes. Amongst these are wastes from the petrochemical and other industries. In the latter case, each shipment of wastes supplied to be gasified usually presents a different composition. This is quite understandable since the waste supplier industry will deal with different feedstocks of prime matter or will produce different products in a given time span. So, naturally, the waste produced will present a different composition from case to case.

In the present work we determine the optimum operational parameters for the gasification of a given fuel, as characterized by its elementary composition and Lower Heating Value (LHV). The parameters to be optimized are the oxygen to fuel ratio, steam to fuel ratio, operating pressure and heat recovered.

Different goals are to be reached if the gasification process is intended to produce a hydrogen rich gas for chemical feedstock or a combustible gas for power/heat production. In the former case, the syngas Hydrogen Percentage will be maximized, while in the latter the gasification Cold Gas Efficiency is the parameter to be maximized (cold gas efficiency is the quotient between the heating capacity of the syngas and the original fuel heating capacity; the heating capacity is the product of the lower heating value and the mass flow). In order to investigate the interrelation between these two goals, maximization procedures were carried out for these two different objective functions and a Pareto optimization scheme was set up to investigate the existence of eventual trade offs between them.

The optimization method developed could be used for on-line adjustment of the gasification operating parameters for different fuel compositions and gas final purpose, thus improving the overall performance of the industrial process.

2. GASIFICATION MODELLING

Gasification is a complex chemical process that involves a multitude of phenomena, like devolatization, pyrolysis, heterogeneous gas-solid reactions and homogeneous gas-gas reactions – see [2], [3] or [4]. Each phenomenon has its own rate and a full CFD, heat transfer and chemical kinetic simulation is required to perform a detailed simulation of the process. See Benyon's work [4] for an excellent dissertation on the subject. A brief description of the process follows.

The first part of the gasification process is the pyrolysis of the fuel. When solid fuels are concerned, the term devolatilization is usually utilized. During pyrolysis, some gaseous constituents are released from the fuel. These include CO, CO_2, H_2, H_2O, H_2S, COS, HCN, NH_3, CH_4, C_2H_2 and some other heavier hydrocarbons in lesser quantities.

After pyrolysis a char residue containing fixed carbon and ash will remain and will undergo further oxidation. The volatiles released will react in the gaseous phase.

The main char heterogeneous reactions are reactions between the char's fixed carbon and O_2, H_2, H_2O and CO_2 producing CO, H_2, CO_2 and CH_4. Reactions with O_2 and H_2 are exothermic and those with H_2O and CO_2 are endothermic. See [4] for details.

In the gaseous phase there will be combustion reactions that will tend to convert all of the hydrocarbons into CO2 and H2O, and some equilibrium reactions, noticeably the water-gas shift and the methanation reactions, to be described below – Eqs. (1) and (3).

In the present paper, a simplified gasification model was used. It is an equilibrium model that assumes a homogenous temperature throughout the reaction zone and neglects chemical kinetics effects. Therefore, all the reactions are assumed to attain their equilibrium concentrations at the reaction temperature. This model is based on mass balances for each atomic species (C, H, O, N and S), an energy balance in order to compute the gasification's final temperature, and on the equilibrium between the species using reactions (1) to (5).

$$CO + H_2O \longrightarrow CO_2 + H_2 \tag{1}$$

$$H_2S + CO_2 \longrightarrow COS + H_2O \tag{2}$$

$$CO + 3H_2 \longrightarrow CH_4 + H_2O \tag{3}$$

$$3H_2 + N_2 \longrightarrow 2\ NH_3 \tag{4}$$

$$HCN + 3H_2 \longrightarrow NH_3 + CH_4 \tag{5}$$

Notice that in the present model no chemical kinetic effect is considered and no heat transfer is modeled. But, although this model is much simpler than the full numerical approach presented, *e.g.*, in [2], [3] or [4], it retains the major effects of the influence of the parameters that are being manipulated in the objective functions under analysis, being therefore perfectly suited for the purpose at hand. Also, being much simpler, this model is much more manageable and better suited for linking with Genetic Algorithms.

3. SEARCH AND OPTIMIZATION PROCESS

The search and optimization method used is a Genetic Algorithm [5,6]. The use of a GA was suitable for the problem under study due to its non-linearity, and to the possible existence of local minima, where a conventional optimization procedure might become trapped. Genetic Algorithms have been used to determine optimal operational parameters for several industrial processes and other practical applications, such as building operation parameters [7,8,9]. As mentioned above, the problem under study can be optimized according to two objective functions: hydrogen percentage, and cold gas efficiency. The method used was to first optimize individually for each of the objective functions, using a standard GA, and then use a multicriteria Pareto GA to perform the optimization for the two objectives simultaneously, and look for the trade-offs among them.

The most common multicriteria optimization methods are plain aggregating approaches, which provide a single figure of merit that aims at characterizing the quality of a solution, by combining the several criteria using weighting factors. The problem with this approach is twofold: the final result is heavily dependent on the weights attributed to each factor, and it provides little insight into performance according to each criteria.

Pareto optimization is based on the work of Italian economist Vilfredo Pareto (1848-1923). It moves away from the search for single, optimal solutions, and avoids artificial aggregations using weighting factors. Instead, it supplies decision-makers with information on the best trade-offs achievable within a specific problem formulation and constraints. This information is provided under the form of Pareto fronts. The decision maker will then chose where in the front will the final solution be located, that is, what compromises will be made in the final choice. This seems a particularly suitable approach to handle multicriteria problems since there is usually no single solution that performs best in terms of all the criteria, meaning there is no 'best' or 'optimal' solution. Optimal performance according to one objective often implies a lower performance in one or more of the other objective dimensions, creating the need for a compromise to be reached. Nevertheless, there are solutions that represent better trade-offs than others, and it is this valuable information that Pareto fronts can provide.

Pareto optimality makes use of the concept of dominated and non-dominated solutions: x dominates y if x is better than y for at least one objective function, and is at least as good on all the others [10]. A solution is Pareto optimal if it is not dominated by any other solution. A Pareto front is formed only by Pareto solutions. Another way of understanding Pareto optimality is that it describes a solution for multiple objectives where no part of the solution can be improved without making some other part worse. Hence the Pareto-optimal set is a family of points that is optimal in the sense that no improvement can be achieved in any objective without degradation in others.

4. PARETO GENETIC ALGORITHMS

Genetic Algorithms are methods for approximate optimization which have been successfully applied to several problems difficult to solve exactly by conventional optimization methods. Although GAs are most commonly used in single-criterion problems, their implicit parallelism makes them particularly suitable for multicriteria problems, since a GA searches a population of solutions in parallel instead of departing from a single point, as most optimization procedures do. As Pareto fronts are populations of optimal solutions, GAs prove to be very adequate procedures to locate them.

The Pareto algorithm used in this study uses a ranking method that assigns to each individual a 'dummy fitness' based on his Pareto optimality in the overall population [11, 12]. A rank (or dummy fitness) of 1 is assigned to non-dominated individuals in the population and these individuals are subsequently removed from the current population. A new set of non-dominated individuals is identified in the modified population (i.e. the original population without the rank 1 individuals), assigned a rank of 2, and then removed from the population. This process continues until all individuals in the population have been ranked. The usual genetic operators of reproduction and crossover are then applied using this 'dummy fitness' ranking, instead of the usual fitness values used in standard GAs.

Pareto-based ranking only does not guarantee that the Pareto set will be uniformly sampled. Finite populations tend to converge to only some of these solutions, due to stochastic errors in the selection process. Additionally, recombination and mutation may be less likely to produce individuals in certain regions of the trade-off surface (for example, the extremes) than in others, causing the population to cover only a small part of the surface. Using niching induction techniques to solve multiobjective GA improves over the previous method by promoting the sampling of the entire Pareto set. The maintenance of diversity is important since diversity along the non-dominated frontier helps in the search for new and improved trade-offs, thus extending the frontier. The clustering of solutions around small areas of the Pareto front, leaving much of the remaining front unexplored, is a phenomenon known as *genetic drift*, which has been observed in natural as well as in artificial evolution. Niching techniques avoid it by degrading the fitness of a given individual if many other similar individuals share the same niche. This exerts a spreading pressure over the population, making the final population become more diverse, composed of individuals that have different characteristics and thus exploiting different niches, which spread along the entire Pareto front. This final method incorporating the niche induction technique is known as a Nondominated Sorting Genetic Algorithm (NSGA) [13]. There are different possible implementations of niching described in the literature. The one used in this study is known as sharing, and works in the following way: solutions ranked 1 are given an initial fitness value F_1, and then their niche counts n are calculated, that is, the number of individuals that are within a predetermined distance of that solution (meaning they are similar individuals to the one being evaluated). The shared fitness of each individual is then calculated using the expression $F_{shared,}= F_1/n$. Solutions ranked 2 are then assigned an initial fitness value F_2, less than the lowest shared objective function value of those ranked 1, and then undergo sharing themselves. This process is repeated until all members of the population are assigned a fitness value, and then the usual genetic operators are used to create the next population. This niche induction technique is more complex to implement computationally, but it effectively finds optimal solutions along all the Pareto front, maintaining high diversity in the population and providing the most options to the decision-maker.

5. RESULTS AND DISCUSSION

Four different fuels for gasification were studied: Vacuum Residue, Visbreaker Tar, Asphalt and Petcoke. All of these are refinery residues and a common fuel for gasification. Their typical elementary analysis and Lower Heating Value can be seen in Table 1.

	Vac. Res.	Vis. Tar	Asph.	Pet coke
C (% wt, dry)	84.9	86.1	85.0	88.6
H (% wt, dry)	10.4	10.4	9.1	2.8
N (% wt, dry)	0.5	0.6	0.7	1.1
S (% wt, dry)	4.2	2.4	5.1	7.3
O (% wt, dry)	0.0	0.5	0.0	0.0
Ash (% wt, dry)	0.0	0.0	0.1	0.2
LHV (kJ/kg, dry)	39,007	40,938	38,263	33,680

Table 1 – Properties of the fuels under study.

For both the standard Genetic Algorithm and the Pareto GA, a total population of 30 individuals per generation was used, evolution being carried out through 100 generations in the standard GA and through 200 generations for the Pareto case. This means that for each standard GA run, 3000 possible solutions are evaluated, while 6000 solutions are evaluated for each Pareto GA run. The probability of crossover used through all the experiments was 0.5, and the probability of mutation was 0.04.

Lower and upper bounds are shown in table 2. In this table TFHC means Total Fuel Heat Capacity and is equal to the product of the fuel load and the fuel LHV. In every case considered, the fuel load was equal to 1 kg/s, which means that the upper bound of the heat recovered changed from case to case, according to the fuel's LHV.

	Press. (bar)	Oxigen / Fuel	Steam/ Fuel	Heat Recov. (kW)
Lower bound	20	0	0	0
Upper bound	57.5	2	2	20% TFHC

Table 2 – Lower and upper bounds for each variable.

Results converge independently of the starting population, which is random. This as can be seen in Fig.1, which depicts the Cold Gas Efficiency (CGE) – for Visbreaker Tar - of the population's best individual solution plotted against the number of elapsed generations, for three different initial populations.

As can be seen from Fig.1, the best cold gas efficiency the standard GA was able to attain when gasifying Visbraker Tar was 89%. This value of CGE is reached when the pressure, Oxygen/Fuel ratio, Steam/Fuel ratio and Heat Recovered have the following values (37.5 bar, 0.86, 0.44, 0 kW). For this solution, the gas hydrogen percentage (% vol, wet) in the gas is 40%.

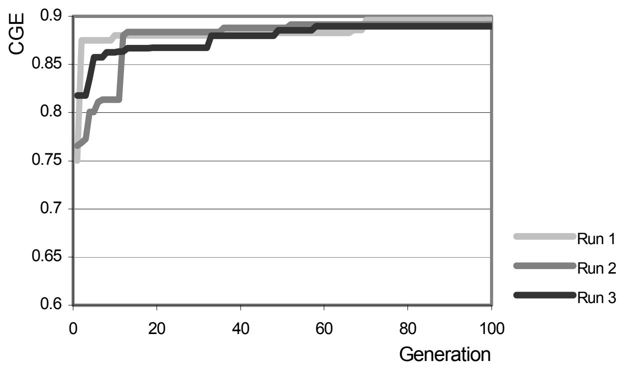

Fig.1 – Evolution of the best individual Cold Gas Efficiency for three random initial populations – Standard GA, Visbreaker Tar.

In order to test whether 100 generations are sufficient to attain accurate results, a run of 500 generations was performed. Results can be seen in Fig.2 and confirm that after 100 generations improvements in the solution are marginal.

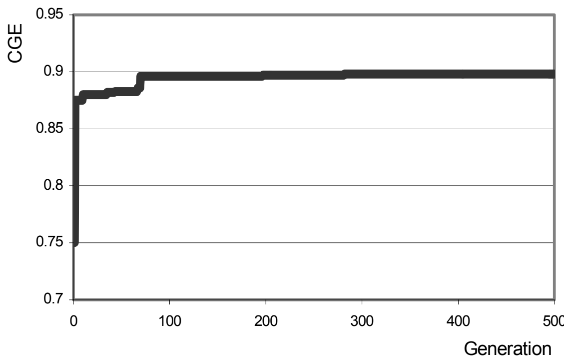

Fig.2 – Evolution of the best individual Cold Gas Efficiency throughout 500 generations – Standard GA, Visbreaker Tar.

If, conversely, we maximize the Hydrogen Percentage of the gas, a value of 44% is reached for this parameter. The operating conditions are (20 bar, 1.02, 0.29, 0 kW) and the CGE is 87%.

Finally, a multi-objective Pareto analysis was performed. It was curious to find out that the Pareto optimization scheme managed to locate better solutions, even if only marginally, than the standard GA did. A plot of the syngas' Hydrogen wet percentage against the CGE (for Visbreaker Tar) is presented in Fig.3. It can be seen clearly that three Pareto solutions were found (highlighted in Fig.3), even though presenting very similar fitness values.

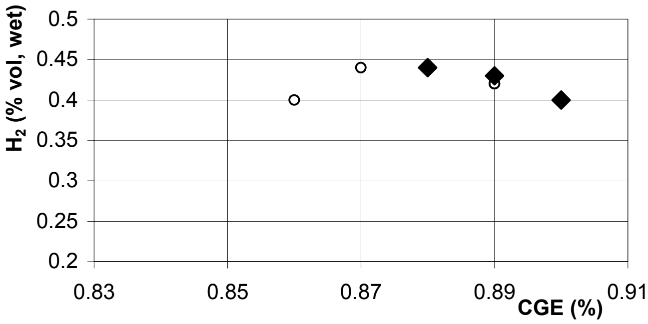

Fig.3 – Pareto plot for Visbreaker Tar. Pareto solutions depicted in Table 3.

A Pareto plot for Petcoke is shown in Fig.4. Notice that in spite of the differences in fuel composition (see Table1), the CGE is quite similar to the one concerning Visbreaker Tar – Fig.3, changing only the level of syngas' Hydrogen contents, which is considerably lower in the case of Petcoke.

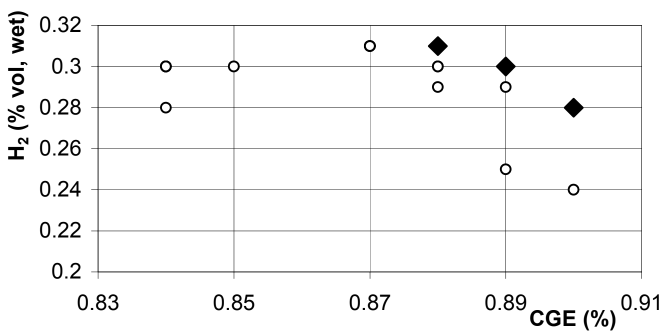

Fig.4 – Pareto plot for Petcoke. Pareto solutions depicted in Table 3.

Table 3 summarizes the Pareto solutions obtained for all fuels under consideration. The first four columns depict the solution's operating conditions, the next two columns present the values of the objective functions to be maximized, i.e., the Cold Gas Efficiency and the syngas' Hydrogen volume percentage (wet). The last column present the final gasification temperature attained when gasifying the considered fuel under those operating conditions.

Observing Table 3, some features become evident and allow for some generalization. The first feature that calls the attention is that all Pareto solutions are attained at zero heat recovery. This clearly indicates that heat removal from the gasifier does not contribute for the increase of either parameter. This is not a surprise, since the recovered heat is not accounted for in neither of the considered objective functions. However, an objective function that accounts for this recovered heat, like thermal efficiency, should be avoided since, if it was used, an excessive weight would be placed in the heat recovered, shaping the gasification process as a heat generating process, which is not the intention.

	Pr. (bar)	Ox./ Fuel	Stm/ Fuel	Heat Rec. (kW)	CGE	H_2 (wet)	T (ºC)
Vac.	20	1.08	0.25	0	**88%**	**42%**	1132
	20	1.02	0.25	0	**89%**	**41%**	1047
Vis.	20	0.98	0.32	0	**88%**	**44%**	1147
	20	0.92	0.32	0	**89%**	**43%**	1072
	20	0.83	0.48	0	**90%**	**40%**	1186
Asph	20	0.98	0.25	0	**89%**	**40%**	1087
	20	0.89	0.44	0	**90%**	**37%**	946
Pet	20	0.86	0.7	0	**88%**	**31%**	987
	20	0.86	0.51	0	**89%**	**30%**	1038
	20	0.79	0.6	0	**90%**	**28%**	936

Table 3 – Pareto solutions found for the different fuels.

Another very clear feature of all the Pareto solutions is that the operating pressure always presents its minimum allowable value. The reason for this can be understand by inspection of equilibrium equations (3) to (5). These equations present 4 moles in the left hand side (where H_2 is present) and 2 moles in the right hand side. Therefore an increase in pressure would shift the equilibrium composition towards the right hand side, thus decreasing the hydrogen contents of the syngas.

One other feature worth noticing is that the two objective functions (CGE and H_2) are closely correlated and allow little room for trade offs at the Pareto border. Therefore all the Pareto solutions are very close to each other and a global optimum zone seams to be possible to define. However, a more significant variation occurs in what concerns the operating parameters that generate these optimum solutions.

Lastly, all the optimum solutions appear to happen at moderate temperatures.

6. CONCLUSIONS

The optimization method developed is fast, simple and robust enough to be used for on-line adjustment of the gasification operating parameters for each fuel composition and aim of gasification, thus improving the overall performance of the industrial process.

Genetic Algorithms proved to be a useful, efficient and appropriate toll for the purpose at hand, being able to locate high quality solutions in very little time. The Pareto GA showed slightly better results than the standard GA. Pareto solutions did not differ significantly among them, despite the niching strategies used, suggesting that an optimal area is clearly definable for this problem.

Heat recovered should be marginal in order to attain optimal conditions.

Results show that the two objective functions under study, *i.e.*, Cold Gas efficiency and Hydrogen Contents, are closely correlated and allow little room for trade offs at the Pareto border.

A high Cold Gas Efficiency (88%-90%) seems to be always attainable no matter what the fuel is, provided the operating parameters are the right ones. Conversely, the maximum Hydrogen content of the syngas is much more dependent on the fuel composition.

Results show that optimum solutions (particularly in what concerns hydrogen contents) appear at the minimum allowable operating pressure. However, pressure is a fundamental parameter in the operational aspects of the gasification. Namely, in industrial applications, pressure is determinant for gas production capacity of the gasifier, *i.e.*, by increasing operating pressure it is possible to produce more syngas in an equal volume gasifying vessel. Therefore, a trade off will exist between increased hydrogen contents of the syngas and increased syngas production. The existence of a point of maximum efficiency should be investigated in future work.

Besides this last point, future work would ideally include the derivation of explicit formulae, *i.e.*, correlations, to determine the optimum Oxygen to Fuel and Steam to Fuel ratios given the fuel's composition and LHV.

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REFERENCES

[1] Haupt, G., Zimmermann, G., Hourfar, D., Hirschfelder, A., Romey, I., Oeljeklaus, G., Folke C., and Semiao, V., IGCC - The best choice for producing clean power, **Proceedings of POWER-GEN Europe 2000**, Helsinki, Finland, 2000.

[2] Govind, R. and Shah, J., Modeling and Simulation of an Entrained Flow Coal Gasifier, **AIChE Journal**, 30 (1), 1984, pp. 79-92.

[3] Liu, G., Rezaei, H., Lucas, J., Harris, D. and Wall, T., Modelling of a Pressurised Entrained Flow Gasifier: the Effect of Reaction Kinetics and Char Structure, **Fuel**, 79, 2000, pp.1767-1779.

[4] Benyon, P.J., **Computational modelling of entrained flow slagging gasifiers**, PhD thesis, University of Sydney, Australia, 2002.

[5] Holland, J., **Adaptation in Natural and Artificial Systems**, The University of Michigan, 1975.

[6] Goldberg, D., **Genetic Algorithms in Search, Optimization and Machine Learning**, Addison-Wesley Publishing Company, 1989.

[7] Huang, W., Lam, H., Using genetic algorithms to optimize controller parameters for HVAC systems, **Energy and Buildings**, 26, 1997, pp. 277-282.

[8] Dickinson, S., Bradshaw, A., Genetic Algorithm Optimization and Scheduling for Building Heating Systems, **Genetic Algorithms in Engineering Systems: Innovations and Applications**, 12-14 September 1995,

(pp. 106-111), University of Sheffield: Conference Publication No. 414, Institution of Electrical Engineers.

[9] Wright, J., HVAC optimization studies: Sizing by genetic algorithm, **Building Services Engineering Research and Technology**, 17 (1), 1996, pp. 1-14.

[10] Tamaki, H., Kita, Hajime, Kobayashi, S., Multi-Objective Optimization by Genetic Algorithms: A Review, in **Proc. 1996 IEEE Int. Conf. on Evolutionary Computation**, pp.517-522

[11] Goldberg, D., Richardson, J., Genetic Algorithms with Sharing for Multimodal Function Optimization, in Grefenstette (ed.), **Genetic Algorithms and their Applications**, ICGA, 1987, pp. 41--49

[12] Deb, K., Goldberg D., An Investigation of Niche and Species Formation in Genetic Function Optimization. In Proceedings of the 3rd **ICGA**, 1989, pp. 42-50

[13] Srinivas, N., Kalyanmoy D., Multiobjective Optimization Using Nondominated Sorting in Genetic Algorithms, **Evolutionary Computation**, 2(3), 1995, pp. 221-248