GENETIC ALGORITHMS APPLIED TO THE OPTIMIZATION OF GASIFICATION FOR A GIVEN FUEL

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Keywords: Gasification, Genetic Algorithms, Optimisation

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 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 may vary in composition from shipment to shipment, and from lot to lot. If operating conditions are kept constant, this could result in lost of efficiency. This paper presents an application of Genetic Algorithms to optimise the operating parameters of a gasifier processing a given fuel. Two different objective functions are used: one to be used if hydrogen production is the main goal of gasification; other to be used when power/heat production is the aim of the process. Results show that the optimisation method developed is fast and simple enough to be used for on-line adjustment of the gasification operating parameters, for each fuel composition and gasification aim, thus improving the overall performance of the industrial process.

1 INTRODUCTION

This paper presents an application of 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 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 become an agent of gasification for the remaining fuel. There will exist 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 pneumatic transportation of the fuel. Some heat can be recovered from the gasification chamber (gasification is an overall

Caldas M., Caldas L. and Semião V. (2004).
GENETIC ALGORITHMS APPLIED TO THE OPTIMIZATION OF GASIFICATION FOR A GIVEN FUEL.
In *Proceedings of the First International Conference on Informatics in Control, Automation and Robotics*, pages 58-63
DOI: 10.5220/0001140400580063

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 (Haupt *et al.*, 2000). It also permits 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 Operating Pressure, Oxygen to Fuel ratio, Steam to Fuel ratio, and Heat Recovered.

Two different objective functions are used, since the goals to be reached are different if the gasification process is intended to produce an 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). Thermal efficiency (defined as the quotient between: 1) the sum of the heat recovered in the process and the heating capacity of the syngas; and 2) the fuel heating capacity), which is a parameter closely related to Cold Gas Efficiency, is also analyzed.

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 overall performance of the industrial process.

Genetic Algorithms (GAs) have been used to determine optimal operational parameters for several industrial processes and other practical applications (for example, Dickinson and Bradshaw, 1995; Wright, 1996; Huang and Lam, 1997). They are particularly suitable for problems that are either multimodal (*i.e.*, present several local extremes), or discontinuous, since in these cases conventional optimization methods based on calculus, like gradient methods, tend to fail. GAs are also effective in smother problems that could be solved using more traditional methods, what makes them very flexible and adaptable to a variety of solution spaces. In the present work, it is suspected that the objective functions are in fact multimodal, what lead to the choice of GAs as the search procedure.

The structure of the paper is the following: in section 2 the gasification modeling is briefly described, section 3 verses on the search and optimization process using GAs, section 4 presents the main results of this work, and section 5 draws conclusions.

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 (Govind and Shah, 1984; Liu *et al.*, 2000; Benyon, 2002). Each phenomenon has its one rate of reaction and a full CFD, heat transfer and chemical kinetic simulation is required to perform a detailed simulation of the process. See Benyon (2002) 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 Benyon (2002) for details.

In the gaseous phase there will be combustion reactions that will tend to convert all of the hydrocarbons into CO_2 and H_2O 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 and detailed heat transfer modeling. Therefore, all the reactions are assumed to attain their equilibrium concentrations at the reaction temperature. This assumption is very justifiable, since industrial gasifiers are designed in such a way that irreversible gasification reactions proceed to their completion and reversible ones attain equilibrium within the reaction chamber and within the reactants residence time. Therefore, in industrial gasifiers that are commercially available, we can expect to have a homogeneous temperature and equilibrium conditions at the gasifier's exit. Of course, this model will not allow for an in depth analysis of the intermediate stages of the gasification complex phenomena, but that is not the purpose of the present research, which focus on the overall exit conditions only.

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).

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

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

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

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

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

Each element mass balance provides one equation. The enthalpy equation offers another one. Each of the equilibrium reactions (1) to (5) provides an equation for the species concentration. See any standard text book, *e.g.*, Levine (1988), for details on chemical equilibrium.

Therefore, we have eleven equations (five for elements mass balance, one for enthalpy and five for equilibrium reactions) and eleven unknowns: the temperature, *T*, and the mass flow of the syngas constituents (H_2, CO, H_2O, CO_2, N_2, H_2S, COS, CH_4, HCN and NH_3). The result is a determined system of non-linear equations that can be solved through any of the standard numerical techniques available in the literature.

Having the mass flow of all the elements in the resulting syngas, it is straight forward to compute their respective percentage in the syngas composition, both in terms of mass and in terms of volume.

The Cold Gas Efficiency is defined, as said before, as the quotient between the heating capacity of the syngas and the original fuel heating capacity. This quotient is expressed in Eq.(6) where the index *i* ranges over all syngas constituents, LHV means Lower Heating Value, and *m* with an over dot means mass flow.

$$CGE = \frac{\sum_i \dot{m}_i \; LHV_i}{\dot{m}_{Fuel} \; LHV_{Fuel}} \tag{6}$$

Of course that, besides the parameters that will be manipulated (oxygen to fuel ratio, steam to fuel ratio, etc…), the fuel elementary composition, fuel mass flow and fuel LHV must be supplied as inputs to the model.

Again, notice that, although this model is much simpler than the full numerical approach presented in, *e.g.*, Govind and Shah (1984), Liu *et al.* (2000) or Benyon (2002), it retains the major effects of the influence of the parameters that are being manipulated in the objective functions under analysis, being therefore well suited for the purpose at hand. Also, being much simpler, this model is more manageable, has reduced computational times, and is thus better suited for linking with Genetic Algorithms.

3 SEARCH AND OPTIMISATION PROCESS

The search and optimization method used is a Genetic Algorithm. 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. Since a GA searches from a population of points, not a single point, the probability of the search getting trapped in a local extreme is limited. GAs start searching by randomly sampling within the solution space, and then use stochastic operators to direct a hill-climbing process based on objective function values. Genetic Algorithms were first presented by Holland (1975), and made familiar to a broader audience by Goldberg (1989).

A standard Genetic Algorithm was used, with a total population of 30 individuals per generation, evolution being carried out through 100 generations. This means that for each run, 3000 possible solutions are evaluated, even though there will be some degree of repetition among them. One of the sources of solution overlapping among generations is elitism, a strategy used in this study, in which the best individual of a generation is always copied to the following population. A simple kind of memory can thus be implemented to reduce computational time, so that when the GA is confronted with a previously evaluated solution, it automatically retrieves its objective function values. Uniform crossover, which works allele by allele, was used throughout the experiments. The probability of crossover was 0.5, and the probability of mutation was kept as 0.04.

The study also compares results using a micro-GA and the conventional GA. The main difference between the two methods relies on the population size used. Typical population sizes for GAs range from 30 to 200, based on earlier studies such as those of Grefenstette (1986), where suggestions for optimal population choices based on parametric studies are presented. In this study we use a strategy named micro-GA (Krishnakumar 1989), which starts with a small population (in this case, of only 5 individuals) and quickly makes it converge to a solution. Convergence is measured by comparing the chromosomes of the individual solutions. If they differ by less that 5%, it is considered the population has converged. When that happens, the micro-GA restarts a new random population while carrying over the individual with the best fitness in the previous generation (elitism). This way, new individuals are often brought into the search, without loosing track of the ones that did better until that point. An advantage of using the micro-GA procedure is that the algorithm tends to perform a local search around the best solutions during the generations prior to convergence, since at that stage solutions only differ by a few alleles. This local search is important in finding local minima around good solutions, and is usually hard to implement in conventional GAs. Another advantage is that the search procedure is faster, since the micro-GA does not have the inertia of the large populations associated with conventional GAs.

4 RESULTS AND DISCUSSION

Two different fuels for gasification were studied: Visbreaker Tar and Petcoke. These are refinery residues and a common fuel for gasification. Their elementary analysis and Lower Heating Value can be seen in Table 1.

Table 1: Properties of the fuels under study.

	Visbreaker Tar	Petcoke
C (% wt)	86.1	88.6
H (% wt)	10.4	2.8
O (% wt)	0.5	0
N (% wt)	0.6	1.3
S (% wt)	2.4	7.3
LHV (kJ/kg)	40,938	33,680

Lower and upper bounds for each variable used in this study are shown in table 2. Please note that the fuel load considered was 3.6 ton/h, or 1 kg/s, which mean that the total fuel heat capacity is about 40,000 kW for Visbreaker Tar and around 33,500 kW for Petcoke. Therefore, the upper bound of the heat recovered is around 25% of the total fuel heat capacity.

Table 2: Lower and upper bounds for each variable.

	Press. (bar)	Oxigen/ Fuel	Steam / Fuel	Heat Recov. (kW)
Lower bound	20	0	0	0
Upper bound	57.5	2	2	9000

Results converge independently of the starting population, which is random. This can be seen in Fig.1, which depicts the Cold Gas Efficiency (CGE) of the population's best individual solution plotted against the number of elapsed generations for 3 different initial populations. Fig.2 shows the search evolution for the best individual Cold Gas Efficiency, for 500 generations. It can be seen that the quality of the solutions improved sharply during the first generations, a tendency which continued steadily, though in a less prominent fashion, until approximately generation 100, after which improvements were only marginal.

As can be seen from Table 1, the best Cold Gas Efficiency the 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 (22.5 bar, 0.89, 0.41, 0 kW). For this solution the Dry Hydrogen Percentage (DHP) in the gas is 44%.

If, conversely, we maximize the DHP, a value of 52% is reached for this parameter. The operating conditions are (20 bar, 1.02, 1.94, 0 kW) and the

CGE is 83%. As can be seen, the largest change in the operating parameters between these two cases occurs in the Steam/Fuel ratio.

It was interesting to find out that thermal efficiency, although being a relevant parameter to measure the overall efficiency of the process, should not be used as an objective function. The reason for this is that an excessive weight will be placed in the heat recovered, hurting both the CGE and the DHP in the syngas. The gasification process would then be shaped almost as a heat generating process, and this is not the intention. As an example, if thermal efficiency was to be maximized in the above case, the operating parameters would be (20 bar, 1.43, 0, 9575 kW), resulting in a thermal efficiency of 92%. However, the CGE would only be 68% and the DHP would equal 29%. As it can be seen, these parameters are worse than either of the previous cases, thus confirming that this solution should be avoided.

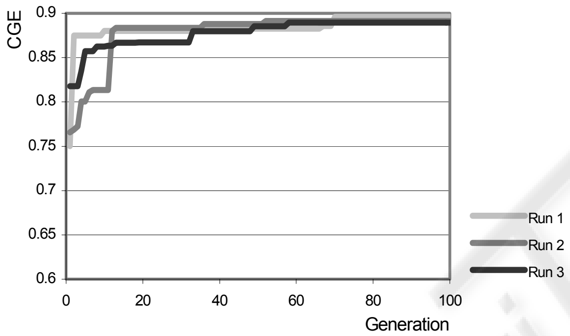

Figure 1: Evolution of the best individual Cold Gas Efficiency for three random initial populations.

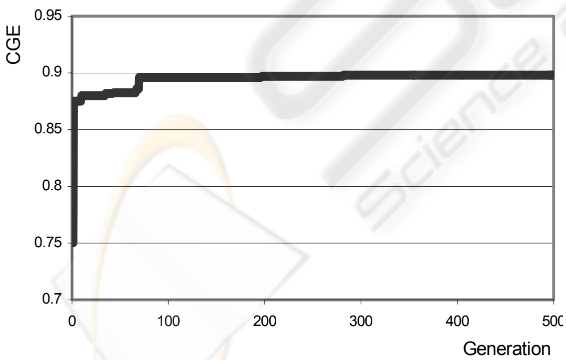

Figure 2: Evolution of the best individual Cold Gas Efficiency (CGE) throughout 500 generations.

If the two previous operating conditions - (22.5 bar, 0.89, 0.41, 0 kW) and (20 bar, 1.02, 1.94, 0 kW) - were to be used for a different fuel (in the present case Petcoke), the resulting CGE and DHP would be 88%, 29% for the first case and 79%, 41% for the second. In case the operating conditions were maximized for Petcoke, the solutions obtained would be (20 bar, 0.83, 0.51, 0 kW), CGE=89%, DHP=30% if CGE is maximized and (20 bar, 1.02, 2.0, 540 kW), CGE=79%, DHP=42% if DHP is maximized. These operating condition do not differ significantly from those obtained when Visbreaker Tar was being considered, so, at least for these two petrochemical products, optimum operating conditions are rather independent of fuel composition. Table 3 summarizes the results obtained using a standard GA. Note that the 540 kW present in the last line of Table 3 are under 1.5% of the total fuel heat capacity of this case, being therefore almost negligible.

Table 3: Results obtained using a standard GA. Values in bold indicate the objective function being maximized.

	Variables				**Objective Functions**	
Fuel	**Press. (bar)**	**Oxigen / Fuel**	**Steam / Fuel**	**Heat Recov. (kW)**	**CGE**	**DHP**
Visbreaker Tar	22.5	0.89	0.41	0	**89%**	44%
Visbreaker Tar	20	1.02	1.94	0	83%	**52%**
Petcoke	20	0.83	0.51	0	**89%**	30%
Petcoke	20	1.02	2	540	79%	**42%**

Finally, the Micro-GA technique was tested in the same cases. Results were equivalent to those obtained using a conventional GA. Therefore, no apparent advantage resulted from the local search features introduced by the Micro GA. In fact, slightly inferior results were observed when using the Micro GA. The evolution of the cold gas efficiency of the population's best individual solution for Visbreaker Tar is presented in Fig.3 as an example, which compares almost exactly with Fig.1. Again, three random and independent initial population solutions are presented.

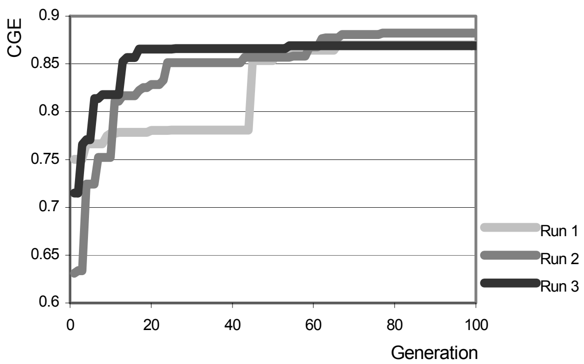

Figure 3: Evolution of the best individual Cold Gas Efficiency (CGE) for three random initial populations, using a Micro GA.

5 CONCLUSIONS

The optimisation 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 overall performance of the industrial process.

Thermal efficiency should not be chosen as an objective function to be maximized under the penalty of placing too much emphasis on the heat recovered, thus compromising both the CGE and DHP of the syngas.

The fundamental parameter that will influence the best operating conditions for heat/power production or hydrogen production is the Steam/Fuel ratio, the Oxygen/Fuel ration being correspondently adjusted.

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

Results seem to be rather insensitive of pressure. However, even if pressure is a less important parameter for CGE and DHP, it is fundamental in the operational aspects of the gasification. Furthermore, and most importantly for industrial applications, pressure is determinant for determining the gas production capacity of the gasifier. Therefore, operating pressure is a parameter that should not be overlooked.

For the two studied fuels, the best operating conditions to maximize CGE or DHP seem to be independent of the fuel. Further work is required to evaluate if this feature remains in a broader range of fuels, including biomass and other non-petrochemical fuels.

The Micro-GA technique was also used with identical results than those obtained through regular GA, no benefits resulting from the local search features of the Micro-GA.

Future work will include the expansion of these methods to multicriteria optimization, using Pareto-based techniques.

ACKNOWLEDGEMENTS

This work has been partially performed with the financial support of: 1) Fundação para a Ciência e a Tecnologia, Programa PRAXIS XXI, under the PhD scholarship SFRH/BD/4833/2001; 2) the European Commission's 5th Framework Programme for RTD, under the contract NNE5-2001-00670 (Migreyd project). 3) Fundação para a Ciência e a Tecnologia, project POCTI/AUR/42147/2001, and the European Union, FSE/ FEDER.

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