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Investigating Performance and Reliability of Stochastic Methods for Optimization of Low Temperature Gas Separation Processes

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The synthesis and optimization of low-temperature gas separation processes is complex owing to the large number of design options. In this paper, we have verified the performance of two popular stochastic methods, Genetic Algorithm and Simulated Annealing, in optimization of sub-ambient systems. GA has been applied to many problem areas, but evidently not previously to low-temperature problems. Despite the feasibility of GA optimizer in low-temperature processes, which has recently been addressed, here we have studied the quality of GA answers in this subject. We designed a very large experimental data set to systematically explore a range of parameter settings in genetic algorithm and simulated annealing and afterwards we have investigated the potential of achieving global optima. In other words, the optimization task is not only to converge in a feasible region, but also to give the best qualitative solution. Having identified the GA and SA parameters and also optimized the solutions in three different case studies, we observed that: (1) SA is more robust and reliable than GA when applying to low temperature gas separation processes. (2) By adjusting the key parameters in SA method, the optimization process will avoid pre-mature convergence and will be able to give the best near-global results.

1- Introduction

In the chemical process industry, there are many processes, such as natural gas liquefaction, gas separation and ethylene production that operate partially or totally below ambient temperature[1]. In these systems, it is desirable to develop a conceptual methodology for designing the refrigeration and separation systems simultaneously, including heat integration within and between the systems. Figure 1 shows a typical scheme showing existing interactions to design an efficient process that produces desired products from a given feed. Comprehensive exploration of various options within its separation and with utility system is required. The synthesis problem is complex and contains the following five issues: (1) Selection of the optimum sequence to separate a feed into desired products. (2) Selection of the separation device to carry out each task. (3) Determination of suitable operating conditions for each unit. (4) Design of associated refrigeration cycles and heat exchanger networks. (5) Effective using of different refrigeration configurations and refrigerant options or various pressure levels for satisfying the hot utility requirement. "Smith (2005), Wang et.al (2004, 2005)"

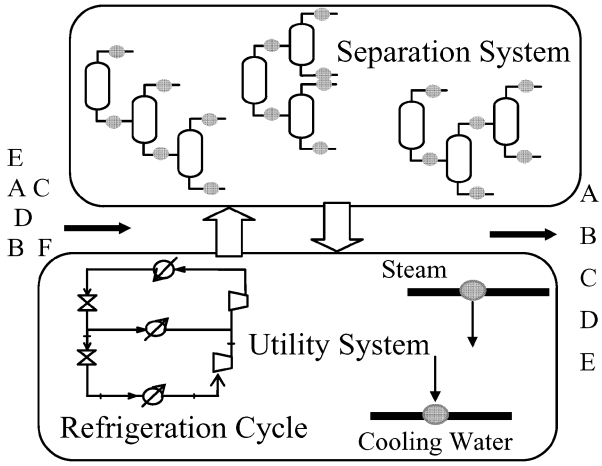


Figure 1. Heat integration within and between the separations systems should be explored in order to design an energy efficient system.

2- Stochastic Search Techniques – Genetic Algorithms, Simulated Annealing and Their Parameters

The stochastic methods rely on random decisions to explore the solution space. The most important feature of stochastic methods is that the optimization result given from the algorithm is not a single global optimum but a set of improved solutions towards the best one. For a complex system, providing a set of 'good' or 'satisfying' solutions is more important than attaining a single optimum point. "Golberg, (1989)."

Genetic algorithm is the famous stochastic search algorithm which begins with a random initialization of the population. The transition of one population to next (is called generation) takes place via the application of the genetic operators: selection, crossover, and mutation. The application of the genetic operators upon the individuals of the population continues until a sufficiently good solution of the optimization problem is found. Many efforts have been done on choosing values for GA parameters. Making a decision to set the values for different parameters is still adventurous. These parameters typically interact with each other non-linearly, so they cannot easily be optimized. "Jamshidi et.al.(2002), Lawrence (1991)"

Simulated Annealing is another important stochastic search algorithm. The algorithm uses a control parameter to guide the optimization, called annealing temperature. At the beginning, it is set to a high temperature. The trial solution is then generated by a random change in the current solution. The objective function of this new solution is calculated and compared with the objective function of the current trial solution. This may be accepted regarding of being the best solution or not. At each annealing temperature, this process is repeated a number of times, before the annealing temperature is reduced based on a pre-specified schedule, and then the whole cycle is repeated. The algorithm stops when a pre-established termination condition is met. An infinite Markov chain length will guarantee the convergence towards the global optimum. However, it is not practical to specify the Markov chain length to an infinite value. Instead, a sufficient long Markov chain length will be suitable. Long Markov chain length increases the computational time more quickly; however, short Markov reduces the probability of obtaining the optima. The trade off between the quality of solution and computational time should be exploited. "Lawrence (1987), Dolan et.al. (1989), Rodriguez (2005), Kah Loong Choong,2002"

3- Parameterization of GA and SA for Optimization of Separation Processes

We have a homogeneous multi-component fluid mixture that needs to be separated into some products. As explained previously, there are many choices for distillation arrangement and their associated heat exchanger networks and refrigeration systems. Thus, the best near optimum options should be found by a robust and reliable optimizer. Indeed, the idea of heat integration between separation and refrigeration systems in such industries is not too novel, but there is still a big question on which optimizer can explore the interactions properly. A random walk that searches and saves the best scheme through a space solution is a highly explorative search optimizer, which we use here. The goal of this research is verifying which of these two random optimizers, GA or SA, is more successful in gas separation and liquefaction processes to find the best solutions. Hence, we need to explore the appropriate parameters in GA and SA to avoid the premature convergence and improve the hill-climbing ability.

In this section, two sub-ambient industrial examples are presented to analyze the parameter values for GA and SA optimization. Case 1 is a LNG separation train. Typical specifications of the feed and product requirements are shown in Table 1.

Table 1. Problem data for LNG separation train

i	Component	Composition (mol %)	Product	Product Specification
1	Methane	0.3019	A	99% recovery of ethane
2	Ethane	0.2587		
3	Propane	0.2648	B	98% purity of propane
4	Butane	0.1198	C	98% purity of butane
5	Pentane	0.0358	D	97% purity of pentane
6	Hexane	0.0190	E	99% recovery of hexane
Flow rate		4313 kmol/hr, saturated liquid at 20 bar		

Also, case 2 is a live case study for Exxon Mobile Company. Table 2 shows the compositions of stream achieved from non-associated gas. "Farry (1998)"

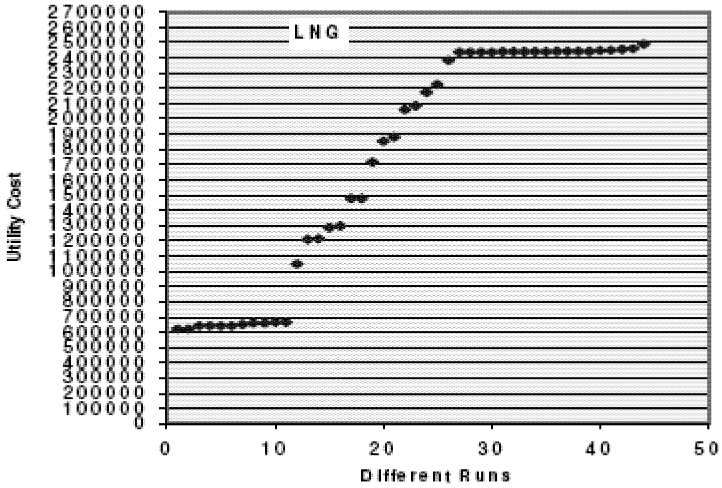
Table 2. Problem data for natural gas stream originated from non-associated gas

i	Component	Composition (mol %)	Product	Product Specification
1	Ethane	0.7750	A	98% recovery of ethane
2	Propane	0.1250	B	98% purity of propane
3	iso-Butane	0.0250	C	98% purity of iso-Butane
4	n-Butane	0.0250	D	98% purity of n-Butane
5	iso-Pentane	0.0150	E	99% purity of pentane
6	n-Pentane	0.0200		
7	Hexane	0.0150		
Flow rate		3600 kmol/hr, saturated liquid at 8 bar		

Now, two stochastic models, GA and SA, are implemented to design an optimum sequence that recovers desired products from a given feed, optimizing all synthesis issues simultaneously. Note that the objective function is utility cost. Both techniques should be parameterized to avoid converging prematurely before the best solution has been found. We have applied colom software, a program for analyzing a variety of separation problems. “Centre for Process Integration, 2006)

a) Parameter Sensitivity Analysis in GA and SA Optimization

The value of generation, population, mutation and crossover play a very important role in quality of result and speed of convergence in GA. Effective values of the parameters used in the running of genetic algorithms in separation systems have been explored in this work.



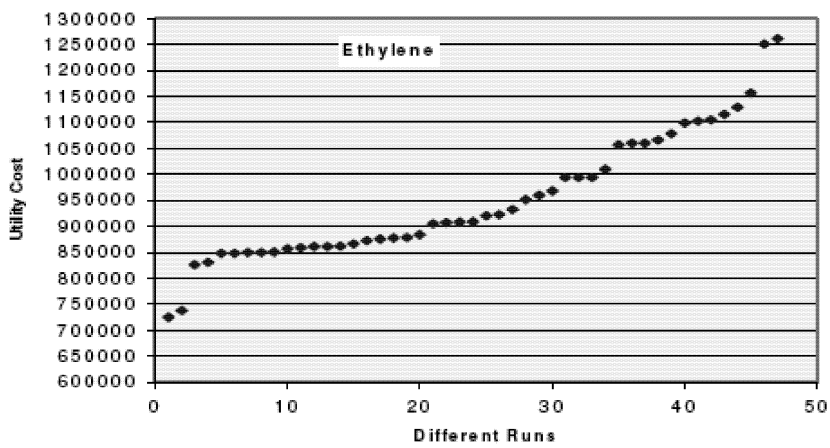


Figure 3. The utility cost achieved with different blending of parameters

It has been found that the larger population size, the better the optimization performance, however, it requires more generation and more computation efforts to yield a near-optimum solution. According to a big set of data, we have recommended a moderate population size (say 250) and a big generation (at least 2000) for robust optimization of such systems. Also, we have used a well-known recommendation in our work given by Grefenstette, which is 0.75-0.95 for crossover and 0.005-0.01 for mutation rate. “Mitchell (1998)”

Moreover, cooling parameter; Markov Chain Length and maximum iteration are key issues in SA. It would be interesting to explore the relationship between parameters, which bias the results. It has realized that there is a negative power relationship between cooling parameter and iteration and a linear relationship between iterations and Markov Chain Length. After several runs, we have suggested Markov 150 and cooling parameter 0.005 in such systems.

Figure 3 depicts the utility cost for two case studies in different runs done with different blending of parameters. As illustrated, needless to say that different set of parameters in SA may lead to different result cluster of an objective function. The following section provides a set of quantitative results for comparison between the two optimizers, GA and SA, in a low temperature gas separation system.

b) Comparison of GA and SA for Design and Optimization of Low-temperature Separation Processes

Table 3. The results of synthesis and optimization of Exxon mobile case study for different available set of refrigerants using GA, with population 250 ,generation 3000, mutation 0.005 and crossover 0.9.

Different Refrigerants	Utility cost	Time	Sequence	Pressure
0-Methane+Ethylene+Propylene	1,230,987	20:55:12	Sstrip PreFrTC	4.00 9.2
1-Methane+Ethylene+Propane	1,195,777	25:16:30	Simple Sstrip Simple	4.00 5.73 17.87
2-Methane+Ethane+Propylene	1,166,139	16:23:51	Simple DivWall Dephleg	4.00 7.47 10.93
3-Methane+Ethane+Propane	1,199,227	17:52:45	Sstrip DivWall	4.00 9.2

Table 4. The results of synthesis and optimization of Exxon mobile case study for different available set of refrigerants using SA, with Markov 150 and cooling parameter 0.005

Different Refrigerants	Utility cost	Time	Sequence	Pressure	Iteration
0-Methane+Ethylene +Propylene	863,111	8:54:10	Simple PreFrTC Dephg	4.47 8.77 6.37	1933
1-Methane+Ethylene +Propane	856,161	9:30:30	Simple PreFrTC Dephg	4.59 9.01 7.12	1985
2-Methane+Ethane +Propylene	858,124	7:25:38	Simple DivWall Dephg	4.30 8.48 5.82	2053
3-Methane+Ethane +Propane	784,851	9:12:49	Simple Simple Simple Simple	6.13 9.23 11.84 4.00	2159

As we explained before, the optimal synthesis of low temperature separation sequences, associated heat recovery network and refrigeration cycles should be considered simultaneously. One of the important factors in cost reduction is selection of the best refrigerants that satisfy a set of process cooling duties at different temperatures. Consequently, the configuration design for the refrigeration cycle, the best selection of refrigerants, and the opportunities of integration with the process streams are explored simultaneously.

Here, in order to verify the quality of Genetic Algorithm and Simulated Annealing optimization, we have investigated the effect of applying different refrigerants to get minimum utility cost. The results shown in Tables 3 and 4 are related to synthesis and optimization of Exxon Mobile case study using GA and SA

4- Discussion and Conclusion

In this study, we designed a very large experimental data set to systematically explore a range of parameter settings in Genetic Algorithms and Simulated Annealing. The resulting data will be useful not only in better perception of fundamental nature of GA and SA, but also in right decision for seeking the best solutions in gas separation and liquefaction processes.

Although GA has long been applied in many problem areas successfully, but we have presented a systematic series of runs showing the poor performance of GA in low-temperature gas separation. Despite the feasibility of GA optimizer in low-temperature processes, which has recently been addressed by others, here we have studied the quality of GA answers in this subject. Our study has shown that GA is not robust in finding a comprehensive search space compared to SA. Moreover, GA is a more time-intensive method and the convergence speed of genetic algorithm is far slower than Simulated Annealing.

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