CHEMICAL ENGINEERING TRANSACTIONS
VOL. 71, 2018

A publication of AIDIC
The Italian Association of Chemical Engineering
Online at www.aidic.it/cet

Guest Editors: Xiantang Zhang, Songrong Qian, Jianmin Xu

ISBN 978-88-95608-68-6; **ISSN** 2283-9216
DOI: 10.3303/CET1871209

Safety Production Management of Hazardous Chemical Products Based on Optimized Genetic Algorithm

Meiyan Du

Department of General Education,Shandong University of Arts, Shandong 250014, China
meiyandu7712@163.com

The improvement of genetic algorithm and its application in Hazardous chemical production are discussed in order to improve the production efficiency of Hazardous chemical industry. The genetic algorithm is improved by using ASPEN method. An improved genetic algorithm is proposed to optimize the Hazardous chemical production process and reduce the generation complexity. The improved genetic algorithm is simulated and analysed by MATLAB. The results show that compared with the traditional genetic algorithm, the improved genetic algorithm can simplify the production process, which improve the production efficiency by 20%, and save production costs. Therefore, the improved genetic algorithm is of great significance to improve the production efficiency of chemical industry and promote the development of Hazardous chemical industry.

1. Introduction

In the face of increasingly severe issues about ecological environment, the Chinese government has successively proposed the "energy conservation and emission reduction" policy and the concept of ecological civilization construction, which aim to further control the emission of pollutants and reduce energy consumption. As everyone knows, chemical industry is characterized by high energy consumption, heavy pollution and high emission, while chemical distillation consumes most in the Hazardous Chemical Products process. It is therefore absolutely essential to investigate the optimization measures against emissions and increasing costs in the distillation process of Hazardous Chemical Products. Genetic algorithms have been widely used in the chemical industry thanks to its unique advantages. However, traditional genetic algorithm requires optimizing since it is prone to local optimum solutions. This paper describes the basic principle of genetic algorithm, followed by it, the optimization algorithm based on the process simulator and genetic algorithm is proposed. Here also involves how to simulate the application of the improved genetic algorithm in the separation process of divided wall distillation column.

2. Literature review

Modern industrial enterprise production is a typical manufacturing industry. It is faced with the problems of how to use information technology to improve the adaptability, real-time and flexibility of workshop production planning, enhance the effectiveness of production organization and management, improve production efficiency, shorten contract delivery time and improve product quality. The design and implementation of manufacturing execution system is the only way for enterprises to develop and improve their core competitiveness. Production planning and production scheduling optimization is the core issue of manufacturing execution system in chemical industry, which plays a key role in improving the efficiency and economic benefits of enterprises. In order to explore the genetic algorithm and its application in Hazardous Chemical Products, Liu and Huang studied two multi-objective scheduling problems involving economic- and environmental-related criteria. The first one is a batch-processing machine scheduling problem to minimise the total weighted tardiness and carbon footprint simultaneously. The other is a triple-criteria scheduling problem involving of a hybrid flow shop consisting of a batch-processing machine followed by two parallel-processing machines, in which the shop attempts to minimise the total weighted tardiness, carbon footprint and peak power. Then, they implemented the non-dominated sorting-based genetic algorithm II (NSGA-II), which

Please cite this article as: Du M., 2018, Safety production management of hazardous chemical products based on optimized genetic algorithm, Chemical Engineering Transactions, 71, 1249-1254 DOI:10.3303/CET1871209

identifies the set of approximate efficient schedules to both multi-objective scheduling problems. The research results prove that the adaptive multi-objective genetic algorithm is effective in converging to the true Pareto-optimal set (Liu and Huang, 2014). Bio-based production of chemical building blocks from renewable resources is an attractive alternative to petroleum-based platform chemicals. Metabolic pathway and strain engineering is the key element in constructing robust microbial chemical factories within the constraints of cost effective production. Therefore, Chen and Nielsen discussed how the development of computational algorithms, novel modules and methods, omics-based techniques combined with modeling refinement are enabling reduction in development time and thus advance the field of industrial biotechnology. They further explored how recent technological developments contribute to the development of novel cell factories for the production of the building block chemicals. The results show that the computational algorithms have great impact on the Hazardous Chemical Products (Chen and Nielsen, 2013). At present, the production-distribution planning problems are usually modeled as single-objective bilevel programming problems. In order to solve this problem, Jia et al. constructed a multi-objective bilevel production-distribution planning model with equilibrium between supply and demand, in which the distribution company is the leader who controls the distributing process with the aims to minimize its overall cost, and the manufacturer is the follower who controls the production process with the aims to minimize its overall cost and storage cost. Then, the lower level problem (follower's problem) is transformed into an equivalent single-objective programming problem by a weighted aggregation method. As a result, the multi-objective bilevel optimization problem is transformed into a single-objective bilevel optimization problem. The research results suggest that the proposed algorithm is efficient and feasible in solving the production-distribution planning problems (Jia et al., 2014). Huang et al. put forward an iteration optimization approach integrating back propagation neural network with genetic algorithm. The main idea of the approach is that a back propagation neural network model is first developed and trained using fewer learning samples, then the trained back propagation neural network model is solved using genetic algorithm in the feasible region to search the model optimum. The result of verification conducted based on this optimum is added as a new sample into the training pattern set to retrain the back propagation neural network model. They also proposed four strategies in the approach to deal with the possible deficiency of prediction accuracy due to fewer training patterns used. The proposed approach is then applied to optimize the thickness of blow molded polypropylene bellows used in cars. The results show that the optimal die gap profile can be obtained after three iterations (Huang et al., 2015). In order to estimate the proton exchange membrane fuel cell (PEMFC) model parameters, Zhang and Wang put forward an adaptive RNA genetic algorithm (ARNA-GA) which is inspired by the mechanism of biological RNA. To maintain the population diversity and avoid premature convergence, on the basis of the dissimilarity coefficient, they also proposed the adaptive genetic strategy that allows the algorithm dynamically select crossover operation or mutation operation to execute. They also conducted numerical experiments, and the results indicated that ARNA-GA had better search capability and a higher quality of solutions (Zhang and Wang, 2013).

To verify whether the prediction ability of classification models can be improved by using pre-processing in order to remove unwanted variance in the spectra, Devos et al. put forward a new methodology based on genetic algorithm for the simultaneous optimization of support vector machine parameters and pre-processing. Then, they tested the method for the discrimination of the geographical origin of Italian olive oil (Ligurian and non-Ligurian) on the basis of near infrared or mid infrared spectra. The research results verify that even support vector machine models have to be developed on the basis of well-corrected spectral data in order to obtain higher classification rates (Devos et al., 2014). In order to find the location and the dimensions of the facilities such that the sum of the weighted distances between the centroids of the facilities is minimized, Gonçalves and Resende presented a biased random-key genetic algorithm for the unequal area facility layout problem where a set of rectangular facilities with given area requirements has to be placed, without overlapping, on a rectangular floor space. Then, they developed a hybrid approach combining a biased random-key genetic algorithm, to determine the order of placement and the dimensions of each facility, a novel placement strategy to position each facility, and a linear programming model to fine-tune the solutions. The results show that the quality of the approach can be validated by the improvement of the best known solutions of the extensively studied benchmark datasets (Gonçalves and Resende, 2015). Vu et al. presented a computational assessment of bioHazardous Chemical Products in Synechococcus sp. PCC 7002 (Synechococcus 7002), a fast growing cyanobacterium whose genome has been sequenced, and for which genetic modification methods have been developed. Subsequently, they evaluated the maximum theoretical yields of producing various chemicals under photoautotrophic and dark conditions using a genome‐scale metabolic model of Synechococcus 7002. They also examined the effects of photon and CO_2 limitations on Hazardous Chemical Products under photoautotrophic conditions and identified gene‐knockout mutants that are predicted to improve Hazardous Chemical Products under photoautotrophic and/or dark anoxic conditions. The results show that the computational results are useful for metabolic engineering of cyanobacteria to synthesize value - added products (Vu et al., 2013). As the implementation of life cycle assessment with other management tools can help life cycle assessment practitioners to evaluate agri-food systems from different viewpoints, Khoshnevisan et al. combined life cycle assessment, multi-objective genetic algorithm, and data envelopment analysis and investigated and the advantages and disadvantages of their application. The results show that life cycle assessment and data envelopment analysis can be used to reveal that if all farmers operate on the efficient frontier (suggested values) impacts in all three categories can be reduced by 8% (Khoshnevisan et al., 2015).

To sum up, genetic algorithm plays an essential role in Hazardous Chemical Products. MATLAB is combined with ASPEN to improve the genetic algorithm. First of all, the principles and methods of genetic algorithm are introduced. The definition of multi-objective optimization is given and the multi-objective decision-making problem is compared with other schemes. Then, an integrated platform of Matlab and Aspen FPlus is established and the results of using the optimization method of NSGA-II combined with Aspen FPlus for the optimization solution are analyzed.

3. Principle and method

Genetic algorithm is a computation model for biological evolution process. It attempts to simulate how the Darwinian genetics and biological evolution complete the natural selection, referring to a way to find the optimal solution mainly by simulating the natural evolution process. There are two main types of chromosome coding modes, i.e. direct and indirect coding.

The goal optimization refers to the problem that multiple objectives in one system are simultaneously made optimal under certain constraints. In such problems, there are always more complex relationships between objectives and constraints, so that it is often more cumbersome to solve them than the common single-objective optimization problem. When compared with other solutions, there are three possibilities of feasible solution to multi-objective decision problem: 1) all objectives are optimal, called the overall optimum solution, which rarely appears. 2) all objectives are the worst solution, called inferior solution, which can be eliminated immediately. 3) all objectives have superior and inferior solutions. It is neither sure that the program is optimal nor can be eliminated immediately, called non-inferior solution, or effective solution or Pareto optimal solution.

Multi-objective optimization is calculated based on the NSGA-II algorithm. The following describes the implementation of the NSGA-II algorithm. The main process of NSGA-II is as follows: 1) Set the population size and genetic generations. First, we need to determine the population size pop and the genetic generations gen in the genetic algorithm; the population size represents the number of individuals included in the population, that is, the number of chromosomes. 2) Initialize the parent population. The value is assigned randomly; the number of objective functions is Multi-objective (M), and the number of decision variables is Variable (V); in the process of how to randomly select chromosomes to evolve into the population, there will be individuals who do not satisfy the constraints. In this case, the individuals should be weeded out tore-select others, and determine whether the constraints are met. 3) fast non-dominated sorting, it is the essence of the algorithm. Individuals are sorted by comparing the objective functions of individuals in the parent population. 4) Calculate the crowded distance. After grading the individuals, the crowded distance are calculated for those individuals at one level. 5) Select the operator. The operator will select a certain number of parents from the population and include them into the breeding pool for sexual reproduction. The operator’s choice occurs in the form of a tournament. 6) genetics and mutation. In this algorithm, commonly used SBX and multiple mutation methods are employed. 7) restructure options.

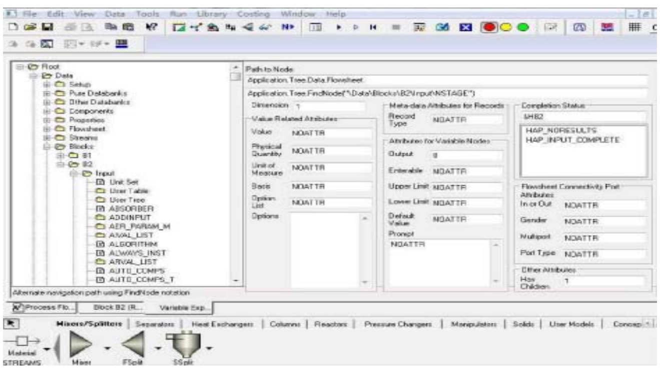

Figure 1: Aspen Plus Variable Browser

This paper intends to build a platform integrated with Matlab and Aspen FPlus, where, the multi-objective genetic algorithm is used to optimize the Aspen FPlus simulation process of the Hazardous Chemical Products in order to achieve the overall program. The data transmission between Matla b and Aspen FPlus is implemented by COM technology. ActiveX is a component integration protocol based on Microsoft FWindows OS. With ActvieX, senders and end users can select the application-oriented Actvie X components released by different developers and integrate them seamlessly into their own applications. The path code can be available from the Variable Fexplorer under the variable manager Tools provided by Aspen Plus, as shown in Figure 1.

The FCOMF objects of Aspen FPlus F mainly include IHapp, IH Node, IHNodeCol, and IHAP Enging. The roles of each are shown in Table 1.

Table1: Main objects of Aspen Plus

Object	Description
Happ IP	Aspen F Plus customer object
IH Node	Input and output data on the Aspen Plus tree structure diagram
IH Node Col	Each IH Node object can have its own other nodes, which are organized in an M Node Col collection object
IHAP Engine	Provide an interface to Aspen Plus's simulation engine

The basic process of integrated NSGA-FII and Aspen is shown in Figure 2.

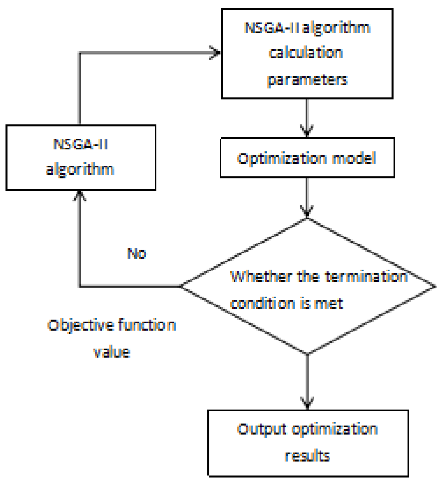

Figure 2: Calculation flow chart of the combination of Aspen and NSGA-II

Unlike many gradient-based algorithms, genetic algorithm does not depend on objective function and constraints, and can converge to the global optimal solution. Therefore, it has become a powerful tool for solving constrained optimization problems. For now, the penalty function method is the most commonly used to treat with the constraints, but the optimized search efficiency has a clear dependence on the choice of penalty factors. There is also no general criterion for selecting the penalty factor, making it more difficult to select the penalty factors.

Min F(x)=(fl(x), f2(x),...,fn(x))

X=(xl, Fx2, xm)

S.t.g(x)<0, i=1, 2,…,q

hj(x)=0, j=1, 2,…,p

x∈X modifies the objective function:

:miny=F (x) +J1*MAX1+J2*MAX1

The F(x) function is usually regarded as an objective function; set X is usually the area defined by the upper and lower bounds for the variable; vector x∈X also satisfies all constraints, called a feasible solution to the problem. Otherwise, it is the infeasible solution. All infeasible solutions make up an infeasible domain.

Although the penalty function method seems more convenient, there is nogeneral selection criterion for penalty factors, making the selection of the penalty factor very difficult. Therefore, we can use AspenPlus functions, such as design rule, to limit the range of independent variables, quickly find the feasible domain, and effectively improve the performance to solve problems. The design rule is shown in Figure 3.

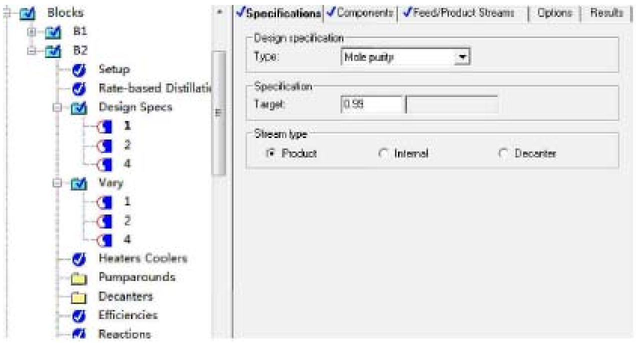

Figure 3: Design Specs

4. Results and analysis

The optimization model that integrates NSGA-II and Aspen FPlus is used to find the optimal solution from the above model. The number of populations is set to 100 and evolutionary generations to 30 in the NSGA-II algorithm to solve the three-objective optimization model with five optimization variables and one constraint. The calculated Pareto frontier curve is shown in Figure 4.

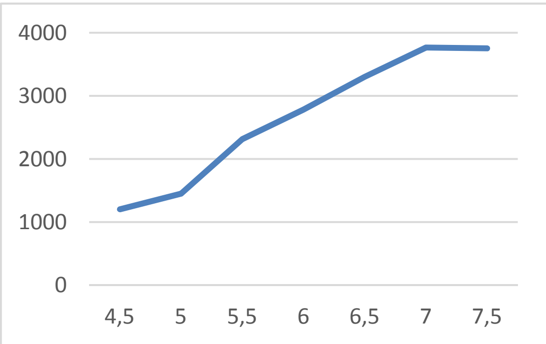

Figure 4: Tert-butanolre coverya mount Pareto front curve

As shown in Figure 4, as the energy consumption increases, the product yield t-butanol at the bottom continues to grow up; when the energy consumption increases to 6.9 MW, the yield of t-butanol does not increase.

Table 2: Multi-objective optimization of the smallest TAC and simulated process comparison

Optimization target value	Original process value	Optimization value	Reduce the proportion
C2 tower reboil ratio	5.53614	7.35056	
Tower Cost Shell	3.8746E+05	2.1026E+05	
Total heat transfer investment cost hx	3.3019E+05	2.8685E+05	13.13%
Operating energy costs Energy	5.1285E+05	4.1302E+05	19.47%
Capital expenditure Capita	8.0197E+05	5.5210E+05	31.16%
Total energy consumption	4.7438	4.54723	4.14%
TAC	7.8017E+05	5.9667E+05	23.52%

As shown in Table 2, there are results from comparison between the optimized and original processes of the genetic algorithm. In the table, we can see that, after the multi-objective optimization calculation by genetic algorithm, provided that the separation requirements are met, when the minimum TAC is taken, the energy consumption of the equipment is 4.54723MW, whereas, in the divided wall distillation column, energy consumption of the simulation process is 4.7438 MW, reduced by 4.14%of the total energy consumption. Similarly, after multi-objective optimization calculation, the total TAC of the equipment is 5.9667e+005, while the simulation process in divided-wall distillation column is 7.807e+005, reduced by 23.52% of the total TAC.

The mathematics software Matlab integrates the process simulation software Aspen FPlur to build a multi-objective optimization platform. To maximize the total yield of tert-butanol, minimize the energy consumption of the separation tower and the TAC, a mathematical model should be built to separate tert-butanol and water. The multi-objective optimization is performed on this model by the NSGA-II, so that the multi-objective Pareto optimal frontier is available. It is revealed by analyzing the frontier curve that there is a law on how the energy consumption of the distillation column affects the yield of tert-butyl alcohol, providing the clue for the design and operation optimization of the tert-butanol separation process.

5. Conclusion

Taking the recovery rate, TAC, etc., as optimization targets, this paper makes a comparison between the calculated values from the multi-objective optimization of genetic algorithm and the simulation value from traditional algorithm. It is obvious that the multi-objective optimization presents an outstanding performance in energy conservation. Adequate programs will be available for the designer, in conjunction with the basis for comparing the investment cost and design parameters to facilitate the designer to select; the relationship between the decision variable and the objective function, providing the clues for the designer to select the design value.

Due to limited knowledge and time, there are still gaps to be filled in the future work, including the following aspects: 1) The non-dominated genetic algorithm (NSGA-II) takes relatively much time and can further optimize the genetic algorithm, or attempt to apply a variety of optimization algorithms for calculations. 2) detailed production data and operation parameters should be incorporated for simulation to test it in practice, so that the results seem more accurate and reliable.

Reference

Chen Y., Nielsen J., 2013, Advances in metabolic pathway and strain engineering paving the way for sustainable production of chemical building blocks, Current opinion in biotechnology, 24(6), 965-972, DOI: 10.1016/j.copbio.2013.03.008

Devos O., Downey G., Duponchel L., 2014, Simultaneous data pre-processing and SVM classification model selection based on a parallel genetic algorithm applied to spectroscopic data of olive oils, Food chemistry, 148, 124-130, DOI: 10.1016/j.foodchem.2013.10.020

Gonçalves J.F., Resende M.G., 2015, A biased random-key genetic algorithm for the unequal area facility layout problem, European Journal of Operational Research, 246(1), 86-107, DOI: 10.1016/j.ejor.2015.04.029

Huang H.X., Li J.C., Xiao C.L., 2015, A proposed iteration optimization approach integrating backpropagation neural network with genetic algorithm, Expert Systems with Applications, 42(1), 146-155, DOI: 10.1016/j.eswa.2014.07.039

Jia L., Wang Y., Fan L., 2014, Multiobjective bilevel optimization for production-distribution planning problems using hybrid genetic algorithm, Integrated Computer-Aided Engineering, 21(1), 77-90, DOI: 10.3233/ica-130452

Khoshnevisan B., Bolandnazar E., Shamshirband S., Shariati H.M., Anuar N.B., Kiah M.L.M., 2015, Decreasing environmental impacts of cropping systems using life cycle assessment (LCA) and multi-objective genetic algorithm, Journal of Cleaner Production, 86, 67-77, DOI: 10.1016/j.jclepro.2014.08.062

Liu C.H., Huang D.H., 2014, Reduction of power consumption and carbon footprints by applying multi-objective optimisation via genetic algorithms, International Journal of Production Research, 52(2), 337-352, DOI: 10.1080/00207543.2013.825740

Vu T.T., Hill E.A., Kucek L.A., Konopka A.E., Beliaev A.S., Reed J.L., 2013, Computational evaluation of Synechococcus sp. PCC 7002 metabolism for Hazardous Chemical Products, Biotechnology journal, 8(5), 619-630, DOI: 10.1002/biot.201200315

Zhang L., Wang N., 2013, An adaptive RNA genetic algorithm for modeling of proton exchange membrane fuel cells, International Journal of Hydrogen Energy, 38(1), 219-228, DOI: 10.1016/j.ijhydene.2012.10.026