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A K A P I T

COMPUTER METHODS IN MATERIALS SCIENCE
Informatyka w Technologii Materiałów

Vol. 11, 2011, No. 3

HYBRID MULTI-OBJECTIVE DIFFERENTIAL EVOLUTION FOR MULTI-OBJECTIVE OPTIMIZATION OF INDUSTRIAL POLYMERIC MATERIALS

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Abstract

MOO of industrial case studies involving process design decisions [namely, styrene reactor, polyethylene terephthalate (PET) reactor, and low density polyethylene (LDPE) tubular reactor] is carried out using the newly developed algorithms. The performance of newly developed algorithms is checked with respect to the effects of dominant decision variables on the Pareto front. The Pareto fronts obtained using the algorithms developed in this study are compared among themselves, with the industrial data, and the data reported in the literature. The newly developed strategies of MODE algorithm are able to converge to a better Pareto front as compared to the Pareto fronts obtained using MODE and NSGA for styrene reactor. For PET reactor, where NSGA algorithm gave a single point solution, the strategies of MODE algorithm resulted in a Pareto front (consisting of setoff solutions). For LDPE tubular reactor, the results obtained in this study show that MODE III algorithm is able to give a wide range of solutions on the Pareto front as compared to those obtained using other strategies of MODE. The points on the Pareto front are of interest to the decision makers (plant engineers) involved in process design decisions.

Key words: multi-objective optimization; evolutionary algorithms; multi-objective differential evolution; hybrid algorithms; pareto front; industrial problems

1. INTRODUCTION

An optimization problem involving more than one objective to be optimized simultaneously is referred as multi-objective optimization (MOO) problem (Deb, 2001). The expected outcome of MOO algorithm is a set of solutions which are non-dominated with respect to each other. Such a set of solutions is called the Pareto optimal front. Unlike single objective optimization problems, MOO problems involve two search spaces, namely the decision variable space and the objective space. Two major goals that need to be achieved in any MOO algorithm are, (1) to converge to the true Pareto front, and, (2) to have a diverse set of solutions on the Pareto front. Due to these multiple goals and multiple search spaces, the MOO problems are considered to be more difficult to solve, as compared to the single objective optimization problems. Both traditional and population based MOO search algorithms have been used to obtain solutions for MOO problems. However, each category of algorithms has its own limitations in obtaining a well diverse and converged Pareto front. Multi-objective differential evolution (MODE) algorithm is used successfully for obtaining the Pareto front for the industrial- and test- problems. In this study, successful application of hybrid MODE algorithm is made on industrial

 ISSN 1641-8581

real world problems [namely, styrene reactor, polyethylene terephthalate (PET) reactor, and low density polyethylene (LDPE) tubular reactor]. The outcome of hybrid MODE algorithms is compared with the results obtained using other popular strategies of MODE algorithm.

2. STRATEGIES OF MULTI-OBJECTIVE DIFFERENTIAL EVOLUTION (MODE)

MODE is an extension of Differential Evolution (DE). DE (Price & Storn, 1997) is found to give better results than Genetic Algorithm (GA) (Goldberg, 1989) for many optimization problems. Multi-objective optimization of industrial styrene reactor, PET reactor and LDPE tubular reactor is carried out using several newly developed strategies of MODE (namely, MODE III, elitist-MODE, and hybrid MODE). Detailed working principles of newly developed strategies of MODE are available in the literature (Gujarathi et al., 2009; Gujarathi, 2010, Gujarathi & Babu, 2009a, 2009b, 2010).

Hybrid MODE algorithm consists of hybridization of evolutionary and deterministic methods. Both the evolutionary and deterministic methods of optimization in isolation have their own limitations and advantages over the other. For example, the evolutionary optimization algorithms start with multiple population points. All the population points usually converge to a single point in case of single objective optimization. In case of MOO problems non-dominated optimal set of solutions is obtained after the specified number of generations are met. However, the deterministic methods often start with a single initial guess. The new point is created either by the method of gradient or by certain perturbation law (in case of direct search methods) and the new point is compared with the existing point. If the new point is found to be better than the current point, then it replaces the current point. The outcome of these methods is often dependent on initial guess and the method of perturbation or the step size of the gradient. It may be possible in the deterministic methods that it may get converged to local minima, if the initial guess is selected wrongly. But at the same time it has the advantage of faster convergence. The evolutionary based optimization methods, due to multiple function evaluations in a single run, are more accurate at the cost of slower convergence. In case of hybrid multi-objective differential evolution algorithm advantage of both the deterministic local search method and the evolutionary approach based optimization method is obtained. The deterministic sequential simplex method is used for local search, whereas one of the evolutionary multi-objective differential evolution strategies (MODE-III algorithm) is used for global search. Detailed working principle of hybrid multi-objective differential evolution can be found in the literature (Gujarathi, 2010; Gujarathi & Babu, 2009b).

3. RESULTS AND DISCUSSION

3.1. Multi-objective optimization of industrial styrene reactor using strategies of MODE algorithm

Pareto fronts (a set of equally good solutions) obtained using various strategies of MODE algorithms is shown in figure 1. Simultaneous maximization of selectivity and yield is considered. The decision variables (i.e., T_{EB}, P, SOR, and F^0_{EB}) corresponding to the Pareto solutions in figure 1 are shown against one of the objective functions in figures 2a - 2h. Figures 2a - 2b show the effect of the temperature of ethyl benzene on the objective functions (namely, selectivity and yield, respectively). Because the main reaction is reversible and endothermic in nature, a high temperature favours the rate of the forward reaction. This is apparent from the plot of yield versus temperature (figure 2b). However, at higher temperature, side products such as toluene and benzene are also formed, thus reducing the selectivity value (figure 2a).

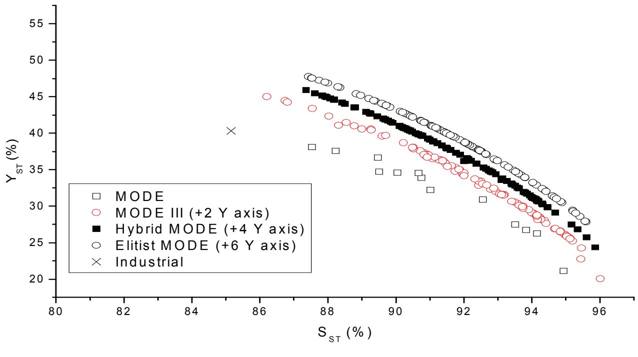

Fig. 1. The results are plotted with vertical shift in value of ordinate by +2 in MODE III, +4 in Hybrid MODE, and +6 in Elitist MODE data points.

Thus a clear conflicting behaviour is observed in both the objectives, which is attributed to the dominance of temperature on the objectives and hence it is termed as a dominant variable. To select a particular value of yield, the user has to sacrifice for the selectivity, and vice versa. If a too high value of yield is selected, then the corresponding value of

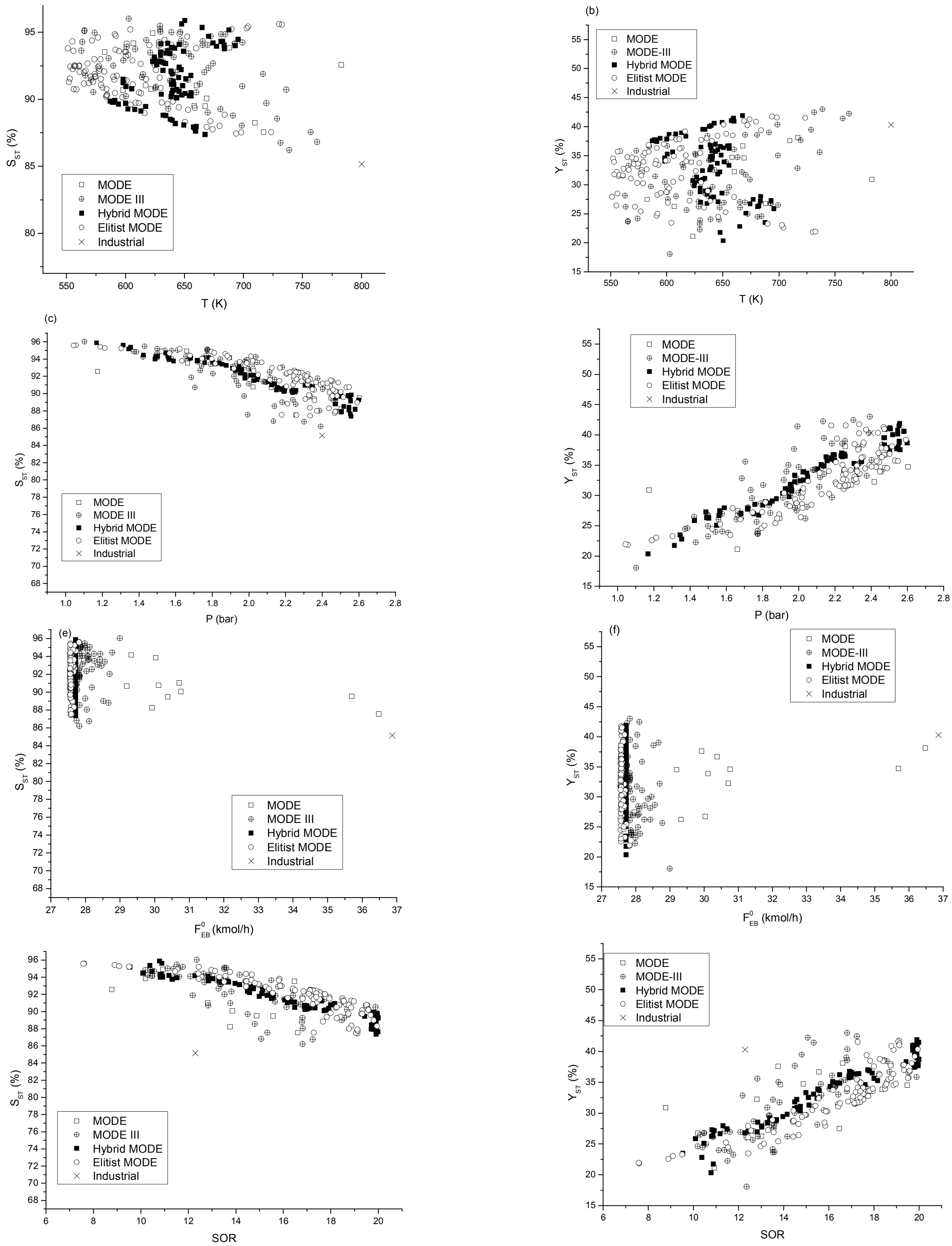

Fig. 2. *(a-h) Decision variables (T, P, F^0_{EB}, and SOR) plotted against one of the objective functions.*

selectivity would be on lower side, thus increasing the cost of separation incurred on the separation of side products from the main product, i.e., styrene. Operating pressure also affects desired values of objective functions. According to the Li-Chatelier's principle, the low pressure favours the formation of main product. By lowering the value of the operating pressure, the selectivity is increased while the yield is decreased (figures 2c - 2d). The feed flow rate of ethyl benzene has approached a lower bound because the lower flow rate is also responsible for generating relatively low pressure. If an initial ethyl benzene flow rate is maintained at a lower value, the mixture of ethyl benzene and the steam would produce a relatively higher temperature (as per energy balance of mixing streams). High temperature and low pressure are favored at lower initial flow rate of ethyl benzene and therefore all the points corresponding to the Pareto optimal solutions belong to the lower initial ethyl benzene flow rate (figures 2e - 2f). The steam over reactant ratio (*SOR*) also controls the desired objectives. Higher *SOR* value is favored for high value of yield and vice versa for the selectivity.

Figures 2a–2h also show the comparison of decision variables corresponding to the Pareto optimal solutions obtained using MODE III, hybrid MODE, and elitist MODE algorithms and industrial operating point (Sheel & Crowe, 1969; Elnashaie & Elshishini, 1994; Yee et al., 2003). A comparatively better trend of decision variables is observed in case of hybrid MODE, and elitist MODE algorithms whereas the decision variables are slightly scattered in case of MODE and MODE III algorithms. Figures 2b and 2f show that for few of the points, MODE algorithm approached lower bound of temperature and upper bound of initial flow rate of ethyl benzene. This resulted in a lower combined inlet temperature of the steam and the ethyl benzene mixture. MODE algorithm resulted in local Pareto solutions due to high value of initial ethyl benzene flow & lower steam temperature. Thus, in order to reach towards the global Pareto solutions, it is necessary to attain a relatively high temperature of the combined stream of mixture of steam and ethyl benzene to the inlet of reactor.

3.2. Multi-objective optimization of PET reactor using strategies of MODE algorithm

In this case, the optimization problem of simultaneous minimization of acid and vinyl end groups is solved using four decision variables namely, temperature, pressure, dimensionless time and the dimensionless agitator speed. Figure 3 shows the Pareto optimal fronts obtained using the strategies of MODE algorithm for MOO of PET reactor.

In the earlier studies, Bhaskar et al. (2001) and Babu et al. (2007), it was observed that the NSGA algorithm converged to a single optimal point. But MODE algorithm was able to give sufficient number of Pareto optimal points (9 points in this case) against the single point obtained using NSGA code. In this study, newly developed strategies are used to obtain the set of non-dominated solutions for PET reactor. MODE algorithm resulted in local Pareto fronts as compared to the Pareto fronts obtained using MODE II, hybrid MODE, and elitist MODE algorithms. The solutions obtained using MODE III, hybrid MODE, and elitist MODE algorithms lie on the same front. However the diversity and range of solutions vary. The Pareto fronts obtained using MODE III, hybrid MODE and elitist MODE algorithms are well spread with uniform diversity which covers a wide range of objective function values against that obtained using simple MODE algorithm. NSGA study resulted in a single optimum point for the same problem, when same set of decision variables and constraints were used. It is more important in any MOO study to generate large number of wide spread points, which can serve the purpose of decision making. NSGA algorithm resulted in the lowest value in terms of vinyl end group objective function as compared to the solutions obtained using strategies of MODE. However, NSGA algorithm could not capture the range of solutions in terms of another objective, i.e., the minimization of acid end group. Further description of obtained results with respect to the set of decision variables can be found in the literature (Gujarathi, 2010).

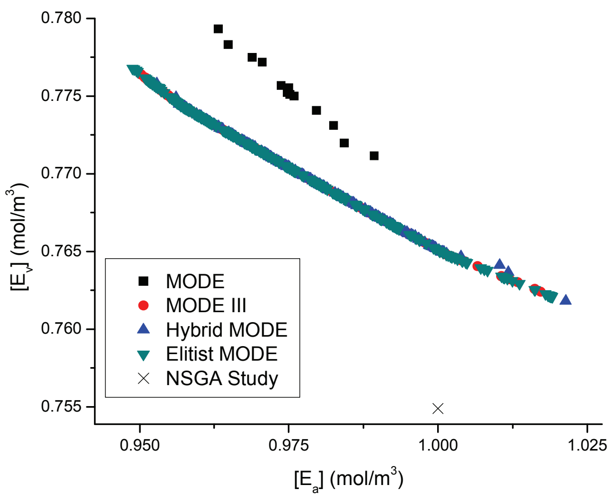

Fig. 3. *Pareto optimal solutions obtained using strategies of MODE algorithms.*

3.3. Multi-objective optimization of LDPE tubular reactor using strategies of MODE algorithm

Multi-objective optimization of two objectives, namely maximization of conversion and minimization of sum of normalized side products is carried out using the algorithms developed in this study.

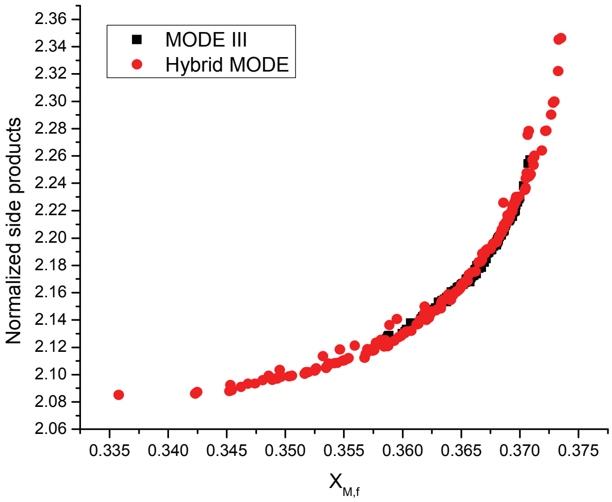

Fig. 4. *Pareto optimal solutions for case 1 using MODE III and hybrid MODE algorithms for a reference case ($M_{N,f}$ = 21,900 ± 200 kg/kmol).*

A set of eleven decision variables, which consists of operating variables, namely, inlet temperature (T_{in}), inlet pressure (P_{in}), the feed flow rates of -oxygen (F_o), -solvent (F_S), -initiators ($F_{I,1}$, $F_{I,2}$), and the five average jacket temperatures ($T_{J,1}$ - $T_{J,5}$), is considered. The Pareto fronts obtained using MODE III, and hybrid MODE algorithms are shown in figure 4. The equality constraint on number-average molecular weight is relaxed by ± 2, ± 20, ± 200, and ± 1100 kg/kmol from its original value of 21, 900 kg/kmol. However, the constraint with $M_{N,f}$ = 21,900 ± 200 kg/kmol, is considered as a reference case and the results are discussed with respect to the reference case. Both hybrid MODE and MODE III algorithms converged to the same front. However, the diversity of solutions obtained using both the algorithms is different. MODE III algorithm covered a range of conversion of 0.335-0.375 on the abscissa (figure 4). If the constraints on number average molecular weight is relaxed to a higher value (e.g. >200) the better distribution of solutions is obtained (Gujarathi, 2010). With a strict constraint, i.e., $M_{N,f}$ = 21, 900 ± 2, it is difficult to obtain a smooth Pareto front and the solutions obtained have a typical nature of high value of side chain products and a low conversion (Gujarathi, 2010).

3. CONCLUSIONS

In this study successful application of improved strategies of MODE algorithm is carried out on problems related to real world industrial polymeric materials.

1. For case-1 (Maximization of Y_{ST} and S_{ST}) of styrene reactor, all the strategies of MODE algorithm (except MODE) converged to the same front. However the diversity of solutions on the Pareto front varies.
2. In case of styrene reactor, a comparatively better trend of decision variables is observed in case of hybrid MODE, and elitist MODE algorithms whereas the decision variables are slightly scattered in case of MODE and MODE III algorithms.
3. In case of styrene reactor, the global Pareto front solutions can be obtained only when a relatively high temperature of the combined stream of mixture of steam and ethyl benzene to the inlet of the reactor is attained.
4. For case of PET reactor, the Pareto fronts obtained using MODE III, hybrid MODE and elitist MODE algorithms are well spread with uniform diversity which covers a wide range of objective function values against that obtained using trigonometric MODE algorithm. NSGA study resulted in a single optimum point for the same problem, when same set of decision variables and constraints were used.
5. For LDPE reactor MOO study, both hybrid MODE and MODE III algorithms converged to the same front. However, the diversity of solutions obtained using both the algorithms is different.
6. In general it is observed that hybrid strategy of MODE algorithm is able to give a well spread and converged Pareto front for the industrial problems as compared to the stand alone evolutionary MOO method.

REFERENCES

Babu, B.V., Mubeen, J.H.S., Chakole, P.G., 2007, Modeling, simulation, and optimization of wiped film poly ethylene terephthalate (PET) reactor using multi-objective differential evolution (MODE), *Mater. Manuf. Processes*, 22, 541-552.

Bhaskar, V., Gupta, S.K., Ray, A.K., 2001, Multi-objective optimization of an industrial wiped film poly(ethylene terephthalate) reactor: some further insights, *Compu. Chem. Engng.*, 25, 391–407.

Deb, K., 2001, *Multi-objective optimization using evolutionary algorithms,* John Wiley and Sons Limited, New York.

Elnashaie, S.S.E.H., Elshishini, S.S., 1994, *Modeling, simulation and optimization of industrial fixed bed catalytic reactors*, Gordon and Breach Science Publisher, London.

Goldberg, D.E., 1989, *Genetic algorithms in search, optimization, and machine learning*, Reading, MA: Addison-Wesley.

Gujarathi, A.M., 2010, *Pareto Optimal Solutions in process design decisions using evolutionary multi-objective op-*

timization, Ph.D. Thesis, Birla Institute of Technology and Science (BITS), Pilani, India.

Gujarathi, A.M., Babu B.V., 2009a, Improved Multi-Objective Differential Evolution (MODE) Approach for Purified Terephthalic Acid (PTA) Oxidation Process, *Mater. Manuf. Processes*, 24, 303-319.

Gujarathi, A.M., Babu, B.V., 2009b, Optimization of adiabatic styrene reactor: A hybrid multi-objective differential evolution (H–MODE) approach, *Ind. Engng. Chem. Res.*, 48, 11115-11132.

Gujarathi, A.M., Babu, B.V., 2010, Multi-objective Optimization of Industrial Styrene Reactor: Adiabatic and Pseudo-isothermal Operation, *Chemi. Engng. Sci.*, 65, 2009-2026.

Gujarathi, A. M., Lohumi, A., Mishra, M., Sharma, D., Babu, B.V., 2009, Multi-objective optimization using Trigonometric mutation multi-objective differential evolution algorithm, *Proc. Int. Symp. & 62nd Ann. Sess. IIChE in asso. with Inter. Part.(CHEMCON-2009)*, Andhra University, Visakhapatnam.

Price, K.V., Storn, R., 1997, Differential evolution - a simple evolution strategy for fast optimization, *Dr. Dobb's J.*, 22, 18-22.

Sheel, J.G.P., Crowe, C.M., 1969, Simulation and optimization of an existing ethyl benzene dehydrogenation reactor, *Can. J. Chem. Engng*, 47, 183-187.

Yee, A.K.Y., Ray, A.K., Rangiah, G.P., 2003, Multi-objective optimization of industrial styrene reactor, *Compu. Chem. Engng.*, 27, 111-130.

WIELOKRYTERIALNY RÓŻNICOWY ALGORYTM EWOLUCYJNY DLA WIELOKRYTERIALNEJ OPTYMALIZACJI PRZEMYSŁOWYCH PROCESÓW DLA MATERIAŁÓW POLIMEROWYCH

Streszczenie

W pracy przeprowadzono wielokryterialna optymalizację (ang. Multi-objective Optimization – MOO) procesów przemysłowych obejmującą decyzje związane z projektowaniem tych procesów [przykładowo, reaktor styrenu (winylobenzenu), reaktor termoplastycznej żywicy polimerowej (ang. polyethylene terephthalate - PET), i rurowy reaktor polietylenu o niskiej gęstości (ang. low density polyethylene - LDPE)]. W tym celu wykorzystano opracowane, nowe algorytmy. Efektywność tych algorytmów została sprawdzona przez ocenę wpływu głównych zmiennych decyzyjnych na front Pareto. Front Pareto otrzymywany stosując różne opracowane w niniejszej pracy algorytmy porównywano między sobą oraz z danymi przemysłowymi i danymi wziętymi z literatury. Opracowane nowe strategie wielokryterialnego algorytmu ewolucyjnego (MODE) zbiegają się do lepszego frontu Pareto niż uzyskiwany klasycznymi algorytmami MODE i NSGA dla reaktora styrenu. W przypadku reaktora PET, dla którego algorytm genetyczny NSGA dawał pojedyncze rozwiązanie, strategia oparta o algorytm MODE daje front Pareto składający się ze zbioru rozwiązań. Wyniki uzyskane w niniejszej pracy dla reaktora rurowego LDPE wykazują, że algorytm MODE III może dać szerszy obszar rozwiązań we froncie Pareto w porównaniu do uzyskanego innymi strategiami MODE. Punkty na froncie Pareto są interesujące dla inżynierów podejmujących decyzje produkcyjne.

Submitted: May 16, 2011
Submitted in a revised form: May 17, 2011
Accepted: May 17, 2011