A PENALTY SCHEME FOR THE TCHEBYCHEFF SCALARIZATION METHOD TO OPTIMIZE THE SINGLE SCREW EXTRUSION

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Abstract

The polymer single screw extruder optimal design has been involving the optimization of six objectives. Multi-objective optimization methods, in particular those based on the weighted Tchebycheff Scalarization (wTS) function, have provided reasonable solutions in a way that good trade-offs between conflicting objectives are identified. In this work, a new penalty term is added to the wTS function aiming to guide the solution toward the Pareto front. The corresponding formulation works similarly to the penalty-based boundary intersection function. The goal of the proposed penalty parameter scheme is to balance convergence and diversity. Since six objectives are simultaneously optimized, the penalty scheme provides large as well as small penalty parameter values to enlarge the improving region. The results show that the set of solutions obtained by the penalty-based wTS algorithm can reasonably well cover the Pareto front.

1. Introduction

The polymer Single Screw Extrusion (SSE) design is concerned with defining the optimal screw operating conditions and geometry in such a way that some relevant objectives achieved their best values. The most relevant objectives in the SSE design are: mass output (Q), length of the screw required for melting the polymer (Z_t), melt temperature at die entrance (T_{melt}), mechanical power consumption (*Power*), distributive mixing quantified by the Weighted Average Total Strain (*WATS*) and viscous dissipation (*Visco*). The objective values depend on two sets of parameters, geometrical and operating conditions. The geometrical parameters are the internal screw diameter of the feed zone (D_1) and metering zone (D_3), the axial lengths of the feed (L_1), compression (L_2) and metering (L_3) zones, the flight thickness (e) and the screw pitch (p). The operating parameters that correspond to the operating conditions of the extruder are the screw speed (N) and the temperature profile of the heater bands in the barrel (Tb_1, Tb_2, Tb_3).

The SSE optimal design can be efficiently obtained using an optimization procedure. However, the optimization of more than one conflicting objective simultaneously is not an easy task since improving one objective leads to another objective degradation [1]. A Multi-Objective Evolutionary Algorithm (MOEA) has been used [2] to simultaneously optimize some relevant objectives. More recently, a weighted Tchebycheff Scalarization (wTS) method [3] was applied to the six-objective simultaneous optimization and an approximate Pareto front was obtained [4]. The wTS method finds optimal values for the operating parameters, represented by the vector $x = (N, Tb_1, Tb_2, Tb_3)$, in such a way that the objectives Q and *WATS* are maximized and

Z_t, T_{melt}, *Power* and *Visco* are minimized. It is also assumed that the geometrical parameters are previously fixed. The range of variation of the screw speed depends on the characteristics of the extruder's motor and the reduction gear. The lower and upper bounds for the range of temperatures of the heater bands are the polymer melting temperature and the polymer onset of degradation, respectively. Thus, taking into consideration the extruder size range and layout, and assuming the processing of typical thermoplastic polyolefin (High Density Poyethylene - HDPE), the lower and upper bound vectors for the operating parameters are for N 10 and 60 rpm and, for Tb_1, Tb_2, and Tb_3 150 and 210 °C, respectively.

In the line of the work presented in [4], and to guide the solution towards the Pareto front, the present study incorporates a penalty parameter scheme into the wTS approach. The proposed formulation works similarly to the penalty-based boundary intersection function [5] by balancing the convergence and diversity of the obtained solutions.

2. SSE Design Optimization

When two or more conflicting objectives need to be optimized simultaneously, the problem is recognized as a multi-objective optimization (MOO) problem with the general form

$$\text{Find } x^* \in \Omega \subseteq \mathbb{R}^n \text{ that minimizes the functions vector } (f(x)_1, f_2(x), \ldots, f_m(x)), \quad (1)$$

where $x \in \mathbb{R}^n$ is the vector of the decision variables, n is the number of decision variables, Ω is the feasible search region, $\mathbb{R}^n$ is the decision space, the components of the vector $f = (f(x)_1, f_2(x), \ldots, f_m(x))$ are the $m > 1$ objective functions to be optimized and $\mathbb{R}^m$ is the objective space. When the objective functions are conflicting, does not exist one single optimal solution, but a set of alternatives - the nondominated solutions - called Pareto optimal set. The decision-maker then selects one (or more) compromise solution, among the alternatives, that better satisfies his/her preferences [6].

Using a scalarization approach to optimize the vector f, in particular the wTS method [3], a weighted aggregation of the objective functions f_i is minimized:

$$\begin{aligned} &\text{minimize } W_{\max}(x;\, w) \equiv \max\{w_1|f_1(x) - z_i^*|, \ldots, w_m|f_m(x) - z_m^*|\} \\ &\text{subject to } x \in \Omega \end{aligned} \quad (2)$$

where $z^* = (z_1^*, \ldots, z_m^*)$ is the ideal point in the objective space, i.e., $z_i^* = \min\{f_i(x) \text{ such that } x \in \Omega\}$ for $i = 1, \ldots, m$ and $w = (w_1, \ldots, w_m)$ is a vector of weights. By varying the weights, the solutions of problem (2) can approximate the complete Pareto optimal front. In order to improve the diversity of the obtained solutions and the convergence of the solutions towards the Pareto front, an equality constrained optimization problem can be defined as follows:

$$\text{minimize } D \quad \text{subject to} \quad f - z^* = D\, w \quad \text{and} \quad x \in \Omega \quad (3)$$

where D stands for the length of the projection of the vector f to the ideal point on the weight vector w and the constraint $f - z^* = D\, w$ ensures that the f value is always on the line with direction w passing through the ideal point. The goal is to push f as low as possible so that it reaches the boundary of the attainable objective set. To deal with the equality constraints, a penalty method may be used and a bound constrained optimization problem is solved for a user defined penalty parameter μ [5]. By using $D = W_{\max}(x; \widetilde{w})$, $\widetilde{w} = \frac{w}{\max w_i}$, problem (3) can be reformulated as follows:

$$\begin{aligned} &\text{minimize } \widetilde{W}(x;\, \widetilde{w}, \mu) = W_{\max}(x; \widetilde{w}) + \mu\, \widetilde{D}_{\max}(x; \widetilde{w}) \\ &\text{subject to } x \in \Omega \end{aligned} \quad (4)$$

and $\widetilde{D}_{\max}(x;\widetilde{w}) \equiv \max\{f_1(x) - (z_1^* + W_{max}(x;\widetilde{w})\widetilde{w}_1), \ldots, f_m(x) - (z_m^* + W_{\max}(x;\widetilde{w})\,\widetilde{w}_m)\}$ is the length of the perpendicular distance from f to w. Thus, solving problem (4) for a set of weight vectors, the solutions approximate the points of the intersection of each weight vector and the true Pareto front. The smaller the $W_{max}(x;\widetilde{w})$, the closer the solution is to the true Pareto front, determining convergence. On the other hand, $\widetilde{D}_{\max}(x;\widetilde{w})$ is penalized by the factor μ and determines diversity. A small value of μ emphasizes convergence and a large value encourages solution diversity. Setting the μ value for the best performance of the method is not an easy task. It depends on the problem and the number of objectives. In general, experiments are carried out with several values to select the best-performing μ value.

3. Results and Discussion

The weighted Tchebycheff algorithm was coded in MATLAB® (a registered trademark of MathWorks, Inc.) and the subproblems (4) are solved using the SA solver - *simulannealbnd* function - from the Global Optimization Toolbox of MATLAB. This solver uses the modelling software of the SSE process to provide the objective function values Q, Z_t, T_{melt}, *Power*, *WATS* and *Visco* (the output) given a set of values of the decision variables (the input).

To improve the diversity of solutions obtained by the method, problem (4) is solved for a large μ value (10^3), over 5 runs. Seventy-seven nondominated solutions were obtained, from a total of 105 solutions (5 runs, each one with 21 weight vectors). Table 1 shows the maximum and minimum values obtained for each objective (points A to F). Points C, G and J represent the three solutions that achieved the smallest $\widetilde{W}(x;\ \widetilde{w},\mu)$ values and point H is an intermediate solution. The more balanced solutions in terms of all objectives, in particular Q and *WATS*, are solutions C and J. It is possible to conclude that the penalty strategy provides the solutions uniformly distributed over the objective space.

Table 1. Optimized results when solving the problem (4) for $\mu = 10^3$

	operating conditions				objectives						
	N (rpm)	Tb_1 (°C)	Tb_2 (°C)	Tb_3 (°C)	Q (kg/hr)	Z_t (m)	T_{melt} (°C)	*Power* (W)	*WATS*	*Visco*	$\widetilde{W}$
A	41.4	209	210	195	9.72	0.793	207	794	51	1.06	670.6
B	11.5	210	210	188	2.81	0.249	202	295	231	1.07	554.9
C	23.1	208	151	159	4.83	0.629	162	868	145	1.06	368.5
D	10.7	152	210	164	2.98	0.540	193	200	160	1.17	458.2
E	15.0	210	159	163	2.98	0.259	169	721	262	1.11	383.7
F	11.8	167	209	210	3.23	0.459	209	258	178	1.00	615.5
G	27.4	207	151	196	6.10	0.720	176	891	92	1.06	387.2
H	31.0	157	209	182	7.69	0.627	200	846	138	1.10	594.0
J	25.1	206	158	152	5.31	0.657	163	863	129	1.07	375.6

To illustrate this optimization process Figure 1 shows, as an example, the two-dimensional projections of the Pareto fronts obtained considering the Q and T_{melt} (on the left) and Q and *WATS* (on the right) as objectives. In this figure, the red large circles refer to the non-dominated solutions obtained over five runs, i.e., the optimal solutions. Due to a lack of space, the remaining two-dimensional plots were not represented here.

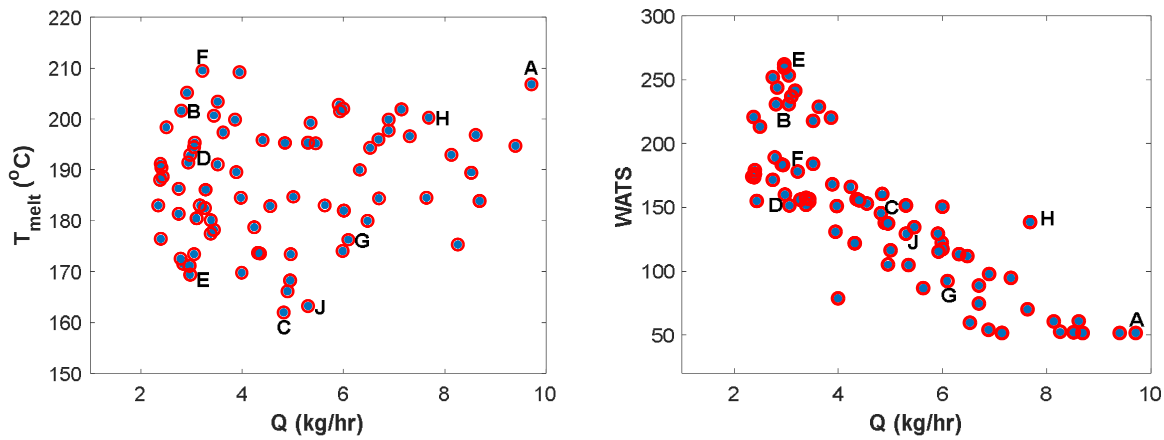

Fig.1. The two-dimensional projections of the Pareto front that are obtained when solving the problem (4) for $\mu = 10^3$

4. Conclusions

In this study, a penalty-based weighted Tchebycheff scalarization algorithm is applied to find a polymer SSE optimal design throughout the simultaneous optimization of six relevant objectives. Although the choice of the penalty parameter value remains an issue to address in future papers, the selection of a large value provided a good distribution of solutions. Also, it was demonstrated that the Pareto solutions obtained were a good starting point towards the selection of a more equilibrated solution considering the relative importance of the objectives.

REFERENCES

[1] Covas, J. A., Gaspar-Cunha, A., Polymer Extrusion - Setting the Operating Conditions and Defining the Screw Geometry, In: Gaspar-Cunha, A., Covas, J. A. (Eds.), Optimization in Polymer Processing, Nova Science Publishers, pp. 87–113, 2011.

[2] Gaspar-Cunha, A., Covas J. A., RPSGAe - A multiobjective genetic algorithm with elitism: application to polymer extrusion, In: Gandibleux, X., Sevaux, M., Sörensen, K., Tkindt, V. (Eds.), Metaheuristics for Multiobjective Optimisation, Lecture Notes in Economics and Mathematical Systems vol. 535, Springer-Verlag, Berlin, pp. 221–249, 2004.

[3] Steuer, R.E., & Choo, E.U. (1983). An interactive weighted Tchebycheff procedure for multiple objective programming. *Mathematical Programming*, 26, 326–344.

[4] Rocha A.M.A.C., Matos M.A., Costa M.F.P., Gaspar-Cunha A., & Fernandes E.M.G.P., Polymer single screw extruder optimization using Tchebycheff scalarization method and simulated annealing algorithm. In: Gaspar-Cunha, A., Sikora, J. (Eds.), *Technological and design aspects of the processing of composites and nanocomposites*: vol. III, pp. 118-136, 2020.

[5] Guo, J., Yang, S., & Jiang, S., An adaptive penalty-based boundary intersection approach for multiobjective evolutionary algorithm based on decomposition, 2016 IEEE Congress on Evolutionary Computation, pp. 2145–2152, 2016.

[6] Miettinen, K.M.: A posteriori methods. In: Nonlinear Multiobjective Optimization. International Series in Operations Research & Management Science, vol 12. Springer, Boston, MA, pp. 77–113, 1998.

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