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POLYMER SINGLE SCREW EXTRUDER OPTIMIZATION USING TCHEBYCHEFF SCALARIZATION METHOD AND SIMULATED ANNEALING ALGORITHM

Abstract. *The single screw extrusion optimal design involves the optimization of six criteria that can be efficiently handled by a weighted Tchebycheff scalarization method. The performance of the method has been analyzed for three different methods to generate weight vectors.*

The experimental results show that the tested strategies provide similar and reasonable solutions and supply a valuable procedure to identify good trade-offs between conflicting objectives.

Keywords: *Single screw extrusion, Multi-objective optimization, Tchebycheff scalarization, Simulated annealing method*

1. Introduction

The single screw extrusion (SSE) design is concerned with the definition of the optimal screw operating conditions and geometry in such a way that some selected criteria achieve their best values. The screw operating conditions and geometry can be established using empirical knowledge, combined with a trial-and-error approach until the desirable criteria values are attained. However, a more efficient approach is to handle the SSE design as an optimization problem. The optimization of the SSE design is a very difficult task since it deals with the optimization of several criteria that are conflicting [1,2,3,4], which means that the improvement of one criterion leads to another criterion degradation.

The SSE design has been addressed in the past and the resulting multi-objective optimization problem has been solved by a multi-objective evolutionary algorithm (MOEA) named reduced Pareto set genetic algorithm (RPSGA) [2,3,5]. Most MOEA treat the multi-objective optimization problem as a whole and find the entire set of promising and desirable solutions in a single run of the algorithm. They are, in general, stochastic methods that generate, handle and mutate a population of solutions at each

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iteration, like for example, the genetic algorithm, particle swarm optimization, differential evolution, ant colony optimization [6,7,8,9,10,11,12].

This paper aims to contribute to the research area of the SSE optimal design throughout a weighted Tchebycheff scalarization approach. The selected criteria of the SSE design problem are optimized using a scalarization function. A vector of weights has to be provided to construct the weighted Tchebycheff scalarization function and converge to a single solution. It is expected that with different weight vectors, the weighted Tchebycheff approach will converge to the trade-off solutions of the multi-objective optimization problem. Therefore, the success of the weighted Tchebycheff approach depends on an even distribution of the weight vectors. To analyze the performance and the effectiveness of the Tchebycheff approach, this paper tests three different methods to generate weight vectors. Although the differences are not significant, it is possible to identify the goodness of one relative to the others.

This paper is organized as follows. Section 2 describes the SSE problem exhibiting the six criteria to be optimized and the decision variables of the problem. Section 3 presents the basic concepts and a summary of some approaches to multi-objective optimization, Section 4 describes the proposed methodology to solve the SSE optimization problem and Section 5 contains a discussion of the obtained numerical results. Finally, Section 6 contains the conclusions of this study.

2. Single Screw Extrusion Problem

The most relevant criteria in the SSE design are the mass output (Q), the length of the screw required for melting the polymer (Z_t), the melt temperature at die entrance (T_{melt}), the mechanical power consumption (*Power*), the weighted average total strain (*WATS*) and the viscosity (*Visco*). These criteria, also called objective functions, depend on the values of two sets of parameters: the geometrical and the operating parameters. Given a set of parameter values, the corresponding objective function values are obtained using numerical modelling routines that describe the plasticizing SSE process [1]. Usually, the best design is attained by maximizing the objectives Q and *WATS*, and minimizing Z_t, T_{melt}, *Power* and *Visco*.

The geometrical parameters are related with 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 parameter L_3 can be obtained from the equation $L_3 = L - L_1 - L_2$, since L is the total length of the screw (corresponding to the Z_t objective function, which is to be minimized).

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 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 a typical thermoplastic polyolefin (High Density Poyethylene-HDPE), the lower and upper bound vectors for these operating parameters are (10,150,150,150) and (60,210,210,210), respectively.

The study in this paper assumes that the geometrical parameters are previously fixed. The aim is to find the optimal values for the operating parameters - herein also denoted as decision variables of the problem - represented generically 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. The multi-objective optimization formulation of the SSE problem is:

$$\begin{aligned}&\text{Find a set of values for the vector } (N, Tb_1, Tb_2, Tb_3) \in \Omega \subset \mathrm{R}^4 \\ &\text{such that the vector } (Q, Z_t, T_{melt}, Power, WATS, Visco) \text{ is optimized,}\end{aligned} \tag{1}$$

where the set Ω of feasible solutions is defined as $\Omega = \{(N, Tb_1, Tb_2, Tb_3) : 10 \le N \le 60, 150 \le Tb_i \le 210, i = 1,2,3\}$.

3. Multi-objective Optimization

Many problems emanating from industrial applications require the optimization of two or more objectives that are frequently conflicting. They are recognized as multi-objective optimization (MOO) problems and their solutions have been tackled by many researchers using a variety of methods. Assuming the minimization, the MOO problem can be formally defined as:

$$\text{Find } x^* \in \Omega \subseteq \mathrm{R}^n \text{ that minimizes the functions vector } (f_1(x),...,f_m(x)), \tag{2}$$

where $x \in \mathrm{R}^n$ is the vector of the decision variables, n is the number of decision variables, Ω is the feasible search region and the components of the vector $f : \mathrm{R}^n \rightarrow \mathrm{R}^m$ are the m objective functions to be optimized. The space R^n is called the decision space and R^m is called the objective space. When the objective functions are not conflicting, it is possible to find a solution where every objective function attains its minimum [12]. However, if the objectives are conflicting, i.e, the improvement of one objective leads to another objective deterioration, it does not exist one single optimal solution, but a set of alternatives - the non-dominated solutions - further ahead called Pareto optimal set. The decision-maker then selects one (or more than one) compromise solution, among the alternatives, that better satisfies his/her preferences.

3.1. Basic Concepts in MOO

The basic concepts in MOO are the following.

Definition 1. *A vector* $f = (f_1,...,f_m)$ *is said to dominate* $\bar{f} = (\bar{f}_1,...,\bar{f}_m)$ *if and only if*

$$\forall i \in \{1,...,m\}\ f_i \leq \bar{f}_i \ and\ \exists i \in \{1,...,m\}\ such\ that\ f_i < \bar{f}_i. \quad (3)$$

Thus, when two solutions $f^1 = f(x^1)$ and $f^2 = f(x^2)$, $x^1, x^2 \in \Omega \subseteq R^n$ are compared, one of these three cases holds: i) f^1 dominates f^2, ii) f^1 is dominated by f^2, iii) f^1 and f^2 are non-dominated.

Definition 2. *Let $f \in R^m$ be the objective functions vector. A solution $x^1 \in \Omega$ is said to be Pareto optimal if and only if there is no other solution $x^2 \in \Omega$ for which $f(x^2)$ dominates $f(x^1)$.*

Definition 2 says that x^1 is Pareto optimal if there is no other feasible solution x^2 which would decrease some objective f_i without causing a simultaneous increase in at least one other objective. Thus, it does not exist a single solution, but a set of solutions called Pareto optimal set (in the space of the decision variables) and the corresponding function vectors are said to be non-dominated.

Definition 3. *Given a MOO problem with objective function vector $f \in R^m$ and the Pareto optimal set X^*, the Pareto optimal front (PF^*) is defined as:*

$$PF^* = \{f = (f_1(x),...,f_m(x))\ such\ that\ x \in X^*\}.$$

The algorithms for MOO aim to find a good and balanced approximation to the Pareto optimal set (and Pareto optimal front PF^*). The goals are:

i) to find a manageable number of Pareto function vectors;
ii) to find Pareto function vectors that are evenly distributed along PF^*;
iii) to support the decision-maker to formulate his/her preferences and identify the compromise solutions.

3.2. General Approaches to MOO

Taking into consideration the point in time when the preferences of the decision-maker participate in the optimization process, methods for MOO can be classified as [6,7,12]:

- No preference participation: the preferences of the decision-maker are not taken into consideration. The solution obtained by a simple method will be accepted or rejected by the decision-maker.
- *A priori* participation: the preferences of the decision-maker are taken into consideration before the optimization process. These methods require that the decision-maker knows beforehand the priority of each objective.

- *A posteriori* participation: no preferences of the decision-maker are considered before the process. However, the decision-maker chooses a solution from the set of alternatives provided by the Pareto optimal front.
- Interactive participation: the decision-maker preferences are continuously used and adjusted during the optimization process.

MOO methods with *a priori* and *a posteriori* decision-maker participation are the most known and popular. The easiest ones are *a priori* methods that combine the multi-objective functions into a weighted scalar aggregation function, converting the MOO problem into a single objective optimization (SOO) problem. Simple and well-known SOO algorithms can then be used to find one optimal solution [6,7]. To obtain an approximation to the PF^*, the SOO method must be run as many times as the desired number of points using different weight vectors [13]. The most popular scalar aggregation function is the weighted sum. To solve problem (2) by the weighted sum method involves selecting a weight vector $w = (w_1, w_2, ..., w_m)$ and minimizing the aggregation function

$$W_{sum}(x; w) = \sum_{i=1}^{m} w_i f_i(x).$$

If all weights are positive, minimizing W_{sum} provides a sufficient condition for Pareto optimality that is the minimum of W_{sum} is Pareto optimal. However, if $w_i \geq 0$ and $w_1 + \cdots + w_m = 1$ are the assumed conditions, and any of the w_i is zero, the solution may be only weakly Pareto optimal [14,15]. It has been reported the inability of the weighted sum method to capture Pareto optimal points that lie on non-convex portions of the Pareto optimal front. This weighted sum method has been extensively used not only to compute a single solution that may reflect the decision-maker preference, but also multiple solutions that provide approximations to the Pareto optimal front, using different sets of weights.

It is expected that different weight vectors will produce different trade-off points on the Pareto front. However, different sets of weights can lead to the same point or points very close to each other. Thus, choosing the sets of weights is an important issue since the solutions depend on the weights. Ideally, they must be an evenly distributed set of weights in a simplex. Nevertheless, it has been observed that the weighted sum method may fail to produce solutions evenly distributed on the Pareto front.

It can also be the case that the relative value of the weights reflects the relative importance of the objectives representing the decision-maker preferences. Frequently, judgments of the decision-makers are vague and their preferences cannot be translated to numerical values. While setting exact weights to objectives may be difficult, it is expectable that rank ordering the importance of objectives be easier. Thus, rank order weight methods aim to convert the list of ranks into numerical weights. Each rank, r_i, is inversely related to the weight, e.g., $r_i = 1$ denotes the highest weight, $r_i = m$ means the lowest weight [16]. The rank exponent weight method produces the weights

$$w_i = \frac{(m - r_i + 1)^t}{\sum_{j=1}^{m}(m - r_j + 1)^t} \tag{4}$$

where r_i denotes the rank of the ith objective $i = 1,...,m$ and t is a parameter that can be estimated by the decision-maker. The value $t = 0$ assigns equal weights to the objectives, and as t increases, the weights distribution becomes steeper [16].

Classical uniform design methods for generating evenly distributed set of weights in a simplex include the popular simplex-lattice design and simplex centroid design [17]. In [18], a constructive method for the creation of a $\{m,q\}$-simplex lattice is presented and used to obtain the uniformly distributed weight vectors, in a MOEA context. For a weights vector of m components and assuming that q is a positive constant, representing the number of points equally distributed on each axis, the simplex consists of all valid mixture combinations - i.e., sum 1 - that can be created for the m components from the $q + 1$ levels $0, 1/q, 2/q, ..., (q - 1)/q, 1$. In general, it consists of $\binom{m+q-1}{q}$ design points [19].

Another scalarization method based on weights to model preferences is the weighted Tchebycheff method [20]. As opposed to the linear aggregation of the weighted sum method, the weighted Tchebycheff method relies on a nonlinear weighted aggregation of the functions f_i, as follows:

$$\begin{aligned}&\text{Minimize } W_{\max}(x;w) \equiv \max\ \{w_1\,|\,f_1(x) - z_1^*\,|, ..., w_m\,|\,f_m(x) - z_m^*\,|\}\\ &\text{subject to } x \in \Omega\end{aligned} \tag{5}$$

where $z^* = (z_1^*, ..., z_m^*)$ is the ideal point in the objective space, i.e., $z_i^* = \min\{f_i(x)$ such that $x \in \Omega\}$ for $i = 1,...,m$. Each term can be view as a distance function that minimizes the distance between the solution point and the ideal point in the objective space.

Minimizing $W_{\max}(x;w)$ can provide approximations to the complete Pareto optimal front by varying the set of weights [6,13]. Under some mild conditions, for each Pareto optimal $x^* \in X^*$ there exists a weight vector w such that x^* is the optimal solution of problem (5), and each optimal solution of problem (5) (associated with a weights vector w) is a Pareto optimal solution to problem (2) [6]. The weighted Tchebycheff method guarantees finding all Pareto optimal solutions with ideal solution z^*. One disadvantage of solving problem (5) is that $W_{\max}(x;w)$ is not smooth at some points, although this is easily overcame by implementing a derivative-free optimization method.

Methods from the class of *a posteriori* decision-maker participation compute a set of solutions to approximate the PF^* in a single run. They are, in general, stochastic population-based search techniques and are denoted by MOEA. These population-based meta-heuristics work reasonably well on difficult problems and are naturally prepared to produce many solutions from which the set of Pareto optimal solutions can be emanated. Known examples with industry applications are NSGA-II [8], SPEA-2 [21] and RPSGA [3]. The reader is referred to [6,7,22,23,24] for more details.

4. Weighted Tchebycheff Scalarization Algorithm

This section aims to present the herein implemented weighted Tchebycheff scalarization algorithm that is used to solve the MOO problem (2) throughout the minimization of the Tchebycheff function $W_{\max}(x;w)$, as shown in (5). To scale the objective values so that they are approximately of the same magnitude, the objectives must be normalized. Thus, each f_i is replaced by:

$$F_i(x) = \frac{f_i(x) - z_i^*}{z_i^{nad} - z_i^*}, \tag{6}$$

where z^* is the ideal objective vector and z^{nad} is the nadir objective vector. This way, the range of the normalized function is [0,1]. The vector z^{nad} is constructed with the worst objective function values in the complete Pareto optimal set X^*, i.e., $z_i^{nad} = \max\{f_i(x) \text{ such that } x \in X^*\}$ for $i = 1,\ldots,m$, which is a difficult task [25]. For normalized objectives, the maximization of $F_i(x)$ can be reformulated as a minimization objective as follows:

$$\max F_i(x) = \min\left(1 - \frac{f_i(x) - z_i^*}{z_i^{nad} - z_i^*}\right).$$

To solve the MOO problem in (1), the approximations to z_i^*, $i = 1,\ldots,m$ (see (6)) are found from empirical knowledge of the SSE equipment and the polymer material, which lead to the $f_i^{\min}$ values presented in Table 1. The table also displays the specific objectives of the function vector f and the estimator for the vector z^{nad}, the vector $f^{\max}$, obtained by empirical knowledge of the equipment and the polymer material.

Table 1. Objectives of the function vector f, $f^{\min}$ and $f^{\max}$

	Q	Z_t	T_{melt}	$Power$	$WATS$	$Visc$
$f^{\min}$	1.0	0.2	150.0	0.0	0.0	0.9
$f^{\max}$	20.0	0.9	220.0	9200.0	1300.0	1.2

Let $\{w^1, \ldots, w^{N_{weight}}\}$ be a set of N_{weight} weight vectors. According to the above stated, for each weights vector w^i, the minimizer of $W_{\max}(x;w^i)$ is an approximation to a Pareto optimal solution of the problem (2). Thus, our methodology to obtain an approximation to the PF^* is as follows. For each weights vector w^i, an approximation to $x^*(w^i)$ and the corresponding functions vector (approximation to $f(x^*(w^i))$) are computed by a SOO solver. The solution $x(w^i)$ obtained for the weights vector w^i is used as the initial approximation to the SOO solver for the next problem constructed with the next vector w^{i+1}. This process is repeated N_{runs} independent times. From the N_{runs} sets of function vectors (approximations to the Pareto optimal front), the non-dominated function vectors are selected to better represent the trade-off between the objectives. From there on the decision-maker may identify a set of compromise solutions. Algorithm 1 describes the main steps of the methodology.

Algorithm 1 Weighted Tchebycheff algorithm

Require: m (number of objectives), $N_{weights}$ (number of weight vectors), N_{runs} (number of runs)
1: Generate a set of N_{weight} weight vectors, w^i_j, $i = 1, \ldots, N_{weights}$, $j = 1, \ldots, m$
2: **for** $N = 1$ to N_{runs} **do**
3: Randomly generate $y \in \Omega$
4: **for** $i = 1$ to $N_{weights}$ **do**
5: Given y as initial approximation, compute $x(w^i)$ (approximation to $x^*(w^i)$)
6: Set $PF^{N,i} = f(x(w^i))$
7: Set $y = x(w^i)$
8: **end for**
9: **end for**
10: Select the non-dominated function vectors among the vectors $PF^{N,i}$, $i = 1, \ldots, N_{weights}$, $N = 1, \ldots, N_{runs}$.

In this study, the simulated annealing (SA) method is used to compute $x(w^i)$, in line 5 of the Algorithm 1. SA is a single solution-based meta-heuristic with origins in statistical mechanics. Meta-heuristics are approximate methods that can solve any complex optimization problem. As opposed to the exact methods, meta-heuristics do not require information about the properties of the mathematical functions involved in the problem formulation. They are not problem-dependent methods. They search the feasible region for a reasonable good solution to the problem although they do not guarantee to find an optimal solution [26].

The SA method models the physical process of heating a material and controls the reduction of the temperature - the cooling process - in order to minimize the system energy and reduce defects [27]. This process is known as annealing. At each iteration of the SA algorithm, a new point is randomly generated using a generating probability function that depends on the temperature. The algorithm accepts a new point if it improves the objective function, but also accepts, with a certain probability, a new point that deteriorates the objective. See [26,27,28] for details. The temperature is used to control the search for the global solution, e.g., a higher temperature allows more new points to be accepted which lead to the exploration of different regions of the search space. On the other hand, a lower temperature favors the acceptance of improving new points which result in the local exploitation of a promising region. Along the iterative process, the temperature is systematically decreased through a cooling schedule. Algorithm 2 presents the main steps of the SA algorithm.

Algorithm 2 SA algorithm

Require: T_0 (initial temperature), $It_{\max} = 50$ (maximum number of iterations), w (the weights vector), x (initial approximation), $0 < \kappa < 1$ (cooling rate), N_t (number of trials per temperature)

Evaluate $W_{\max}(x; w)$
Set $T = T_0$, $It = 0$
repeat
  for $j = 1$ to N_t **do**
    Generate a new point $\bar{x}$ in the neighborhood of x using a generating probability, and evaluate $W_{\max}(\bar{x}; w)$
    if $\bar{x}$ is accepted according to the probability $P(x, \bar{x}; T)$ **then**
      Set $x = \bar{x}$
    end if
  end for
  Set $T = \kappa T$, $It = It + 1$
until $It \geq It_{\max}$

5. Experimental Results

The weighted Tchebycheff algorithm was coded in MATLAB® (MATLAB is a registered trademark of the MathWorks, Inc.). For each weights vector, the function $W_{\max}(x;w)$ is minimized using the SA solver from the Global Optimization Toolbox of MATLAB - the *simulannealbnd* function. On the other hand, the solver *simulannealbnd* invokes the *computerized simulator of the SSE process* that provides the objective function values *Q*, Z_t, T_{melt}, *Power*, *WATS* and *Visco* (output) given a set of values of the decision variables (input) [1].

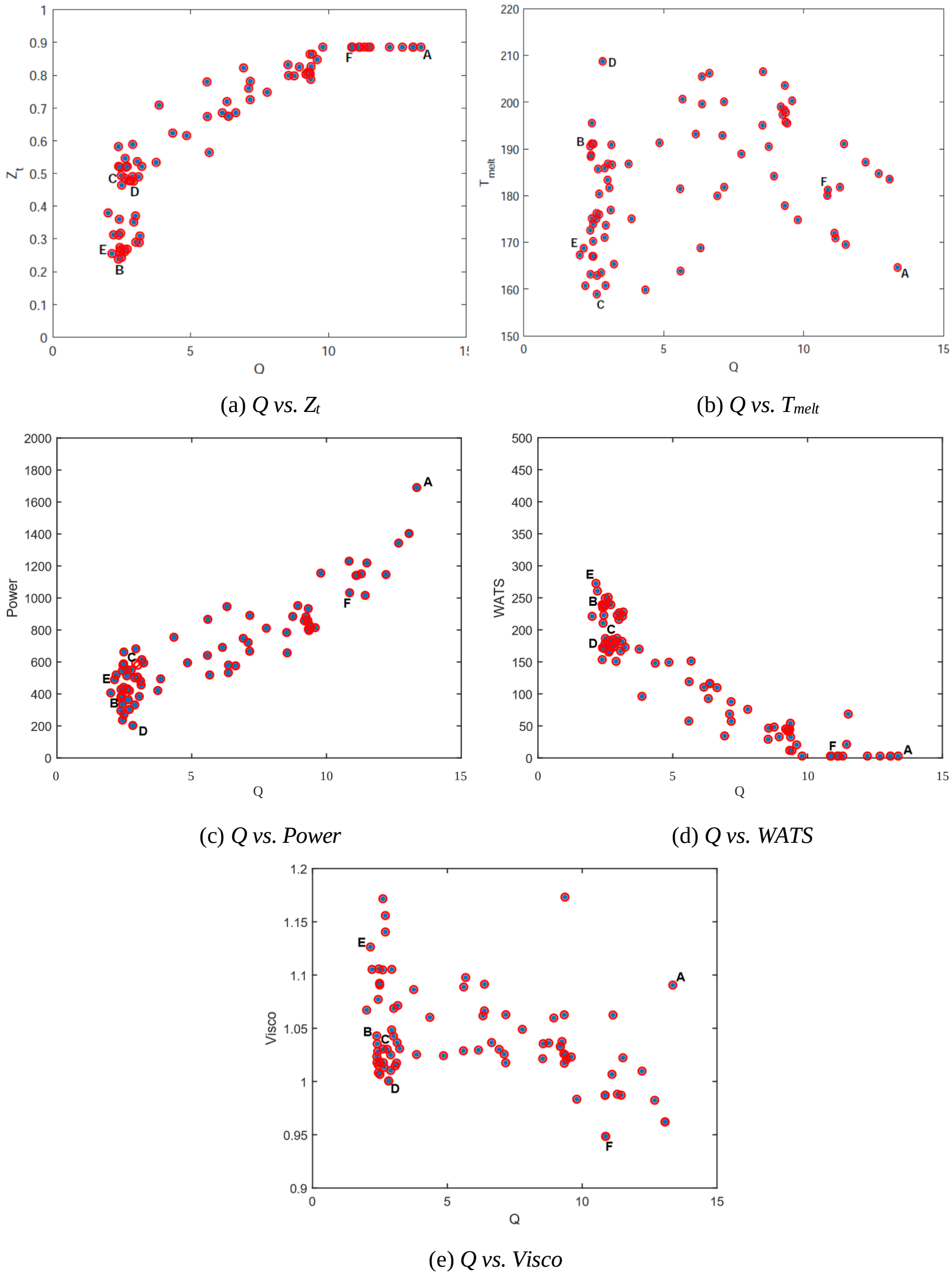
For the experimental results the parameter values are set as follows: $It_{\max} = 50$ (adopted stopping criterion for *simulannealbnd*), $T_0 = 100$ (default value), $\kappa = 0.95$ (default value) and $N_{runs} = 5$ with $N_{weights} = 21$. We note that the use of a high number of weight vectors increases the computational complexity of MOO methods and, in some applications, they become impractical. The fixed values assigned to the geometrical parameters are: $L_1 = 300$, $L_2 = 300$, $D_1 = 20.0$, $D_3 = 26.0$, $p = 30.0$ and $e = 3.60$.

This study aims to analyze the performance of the Algorithm 1 when three different methods are used to generate the set of $N_{weights}$ weight vectors, to solve the MOO problem throughout the minimization of $W_{\max}(x;w)$. Setting weights is an approach to articulate preferences and may be applied to different methods [14].

The first implemented technique applies the rank exponent weight method, see (4), with $t = 1$ and the sequence of ranks $r = (1,2,3,4,5,6)$. When $t = 1$ is set the method reduces to the *rank sum weight method*. With the generated weights vector, the technique constructs all permutations (without replacement), a total of 6! vectors, and randomly selects 21 vectors. With the six objectives optimized simultaneously, the weighted Tchebycheff algorithm produces a set of six-dimensional non-dominated solutions, the Pareto front.

Since the most relevant objective is the mass output Q, to visualize the trade-offs between Q and the others, five two-dimensional projections of the Pareto front are drawn and shown in Figure 1. The (blue) small full circles represent the solutions obtained for all the sets of weight vectors, over 5 runs, and the (red) large circles are the non-dominated solutions among the whole set. Figures 1(a) and 1(c) show that as Q decreases, the lower are Z_t and *Power* respectively. It is observed from Figure 1(d) that as Q decreases, the greater is *WATS*. The tendency shown by the cloud of non-dominated solutions in Figure 1(b) indicates that for lower Q values there are several solutions with lower T_{melt} values but there are also solutions with larger T_{melt} values. From Figure 1(e) we can also see a considerable number of solutions with lower Q values but with moderate *Visco* values. The solution with the lowest value of *Visco* has a reasonable large value of Q.

Table 2 shows the values of the decision variables and the corresponding objective values for the six identified and selected solutions from the Pareto front. They are the extremes of the Pareto front. Point A corresponds to the solution with the highest Q value, B, C, D and F are the Pareto solutions where Z_t, T_{melt}, *Power* and *Visco* attain their lowest values respectively, and point E corresponds to the Pareto solution with the highest value of *WATS*.



(a) Q *vs.* Z_t

(b) Q *vs.* T_{melt}

(c) Q *vs. Power*

(d) Q *vs. WATS*

(e) Q *vs. Visco*

Fig.1. Two-dimensional projections of the Pareto front, when *rank sum weight method* and random selection are used

Table 2. Solutions with the best values of the objectives, when *rank sum weight method* and random selection are used

	operating parameters				optimized objectives					
	N	Tb_1	Tb_2	Tb_3	Q	Z_t	T_{melt}	$Power$	$WATS$	$Visco$
A	59.9	179	150	151	**13.36**	0.886	165	1689	3	1.09
B	10.1	205	176	202	2.38	**0.238**	191	377	239	1.04
C	12.9	187	153	159	2.62	0.486	**159**	550	183	1.03
D	10.0	157	208	210	2.82	0.478	209	**201**	174	1.00
E	10.3	208	151	174	2.15	0.255	169	488	**273**	1.13
F	46.5	187	168	191	10.87	0.886	181	1031	3	**0.95**

Another technique to generate the weight vectors is based on the *rank exponential weight method*, and uses the formula in (4) with the sequence of ranks r = (1,2,3,3,2,3) and the 21 values of t starting at 0, ending at 10, with a step of 0.5. The five two-dimensional projections of the Pareto front are shown in Figure 2.

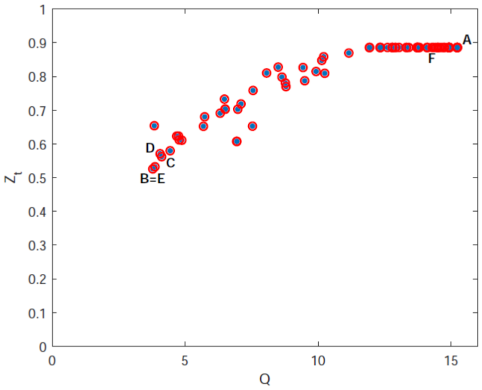
Similar conclusions can be withdrawn relative to the behavior of the solutions, although with this weight generating method, the concentration of solutions is more expressive for large values of Q. Table 3 shows the values of the decision variables and the corresponding objective function values from the six extreme points of the Pareto front.

Table 3. Solutions with the best values of the objectives for the *rank exponential weight method*

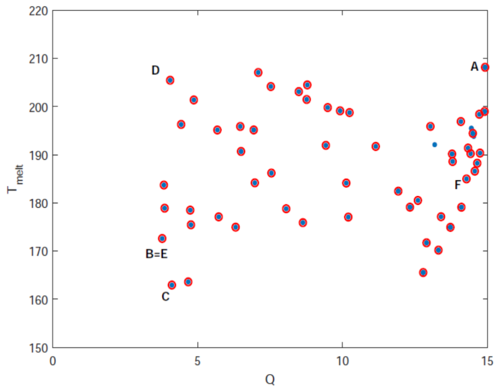
	operating parameters				optimized objectives					
	N	Tb_1	Tb_2	Tb_3	Q	Z_t	T_{melt}	$Power$	$WATS$	$Visco$
A	59.9	177	210	210	**15.23**	0.886	209	1274	3	1.00
B	17.9	210	172	162	3.78	**0.526**	173	594	173	1.06
C	20.0	210	158	156	4.12	0.562	**163**	761	164	1.05
D	15.3	165	207	201	4.06	0.571	205	**334**	151	1.02
E	17.9	210	172	162	3.78	0.526	173	594	**173**	1.06
F	59.7	165	168	199	14.29	0.886	185	1580	3	**0.95**

The third technique, to generate the weight vectors, is based on the *simplex lattice design*. It starts by creating a $\{m,q\}$-simplex lattice, as presented in [18], where m = 6 and q = 8. Since the great majority of the created design points contain null components, we only select the design points that have all components positive to compose a set of 21 weight vectors.

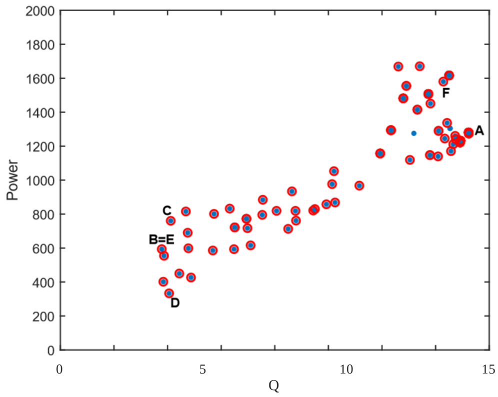
The five two-dimensional projections of the Pareto front are shown in Figure 3. We note that the concentration of solutions is more expressive for lower values of Q, as was reported with the experiments based on the *rank sum weight method*. The other conclusions also apply here. The objective Q variation relative to the other objectives are similar to the previously described.



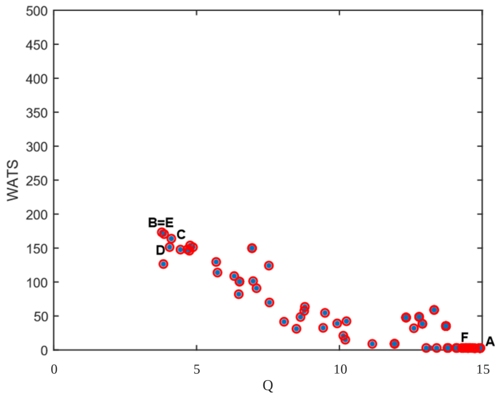
(a) *Q vs. Z_t*



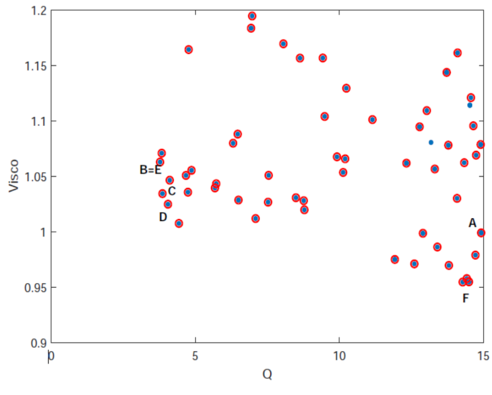
(b) *Q vs. T_{melt}*



(c) *Q vs. Power*

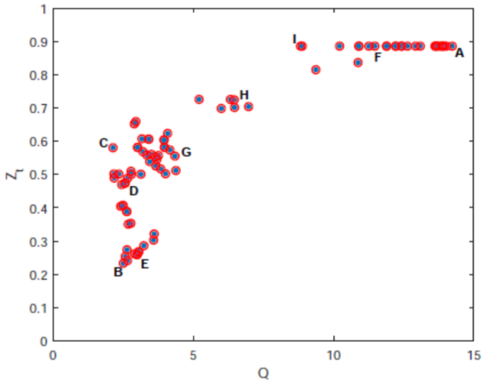


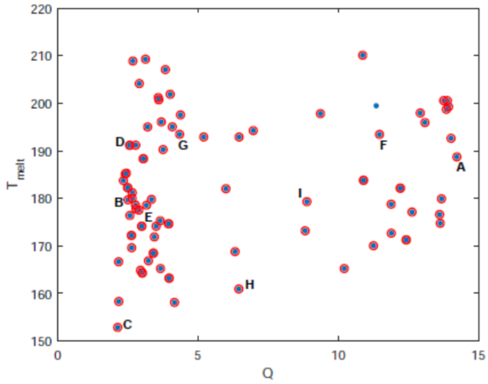
(d) *Q vs. WATS*



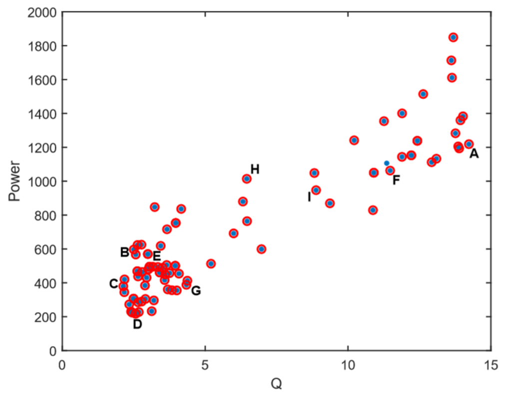
(e) *Q vs. Visco*

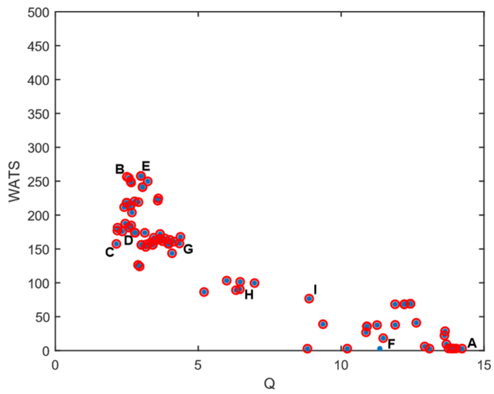
Fig.2. Two-dimensional projections of the Pareto front for the *rank exponential weight method*



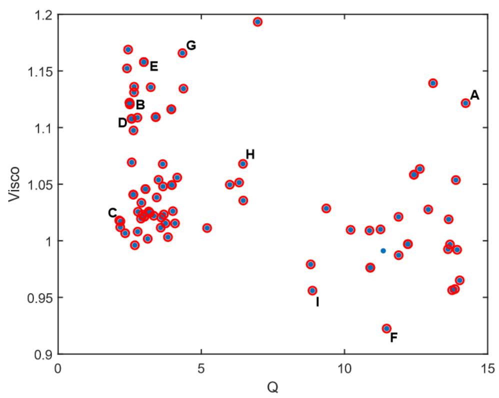


(a) Q *vs.* Z_t (b) Q *vs.* T_{melt}





(b) Q *vs. Power* (d) Q *vs. WATS*



(e) Q *vs. Visco*

Fig.3. Two-dimensional projections of the Pareto front, when the *simplex lattice design* is used

The six extreme solutions, A, B, C, D, E and F from the Pareto front are reported in Table 4 and correspond to the higher value of Q, lower value of Z_t, lower value of T_{melt}, lower value of *Power*, higher value of *WATS* and lower value of *Visco*, respectively. Operating parameter values and objective values from other three solutions, marked with G, H and I in Figure 3, are displayed in last rows of Table 4.

Table 4. Best objective values and other representative solutions using the *simplex lattice design*

	operating parameters				optimized objectives					
	N	Tb_1	Tb_2	Tb_3	Q	Z_t	T_{melt}	$Power$	$WATS$	$Visco$
A	58.4	201	193	168	**14.23**	0.886	189	1219	3	1.12
B	11.8	207	151	200	2.50	**0.233**	180	597	257	1.12
C	10.1	150	150	150	2.13	0.581	**153**	380	157	1.02
D	10.0	160	203	173	2.57	0.474	191	**218**	182	1.11
E	14.8	209	182	150	2.99	0.259	174	570	**258**	1.16
F	48.1	162	187	210	11.47	0.886	193	1063	18	**0.92**
G	17.2	178	208	166	4.34	0.555	193	388	158	1.17
H	30.4	208	150	151	6.46	0.725	161	1014	91	1.07
I	37.8	156	160	203	8.88	0.886	179	947	77	0.96

Analyzing the best values of the objective functions obtained from the three weight generating methods, we may conclude that the *simplex lattice design* technique provides in general slightly better objective values. To assist the decision-maker in his/her decision process, a widely used visualization strategy, known as value path graph, is depicted in Figure 4 in order to give more understanding and insights about the problem. This gives a parallel coordinate plot visualization for the Pareto solutions A, B, C, D, E, F, G, H, I reported in Table 4. The horizontal lines of different colors represent the values of the objectives for different trade-off solutions, i.e., each line is associated with one of the selected solutions. Objective values are normalized to facilitate interpretation and the comparison [29,30,31].

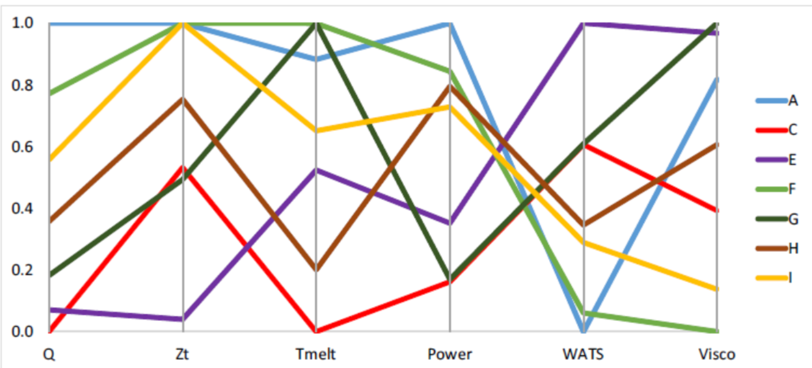


Fig.4. Value path of solutions produced by the *simplex lattice design* weight method

Solutions corresponding to points B and D are not included in the graph because they behave similarly to solutions E and G respectively. The graph highlights the trade-offs and also the similarity of solutions in terms of the objectives. For instance, solutions F and I are very similar. Solution F is better in terms of *Q* and *Visco*, but slightly worse in terms of T_{melt}, *Power* and *WATS*. Solution H is a balanced compromise between all objectives.

A pairwise coordinate plot (with correlation coefficient values) is depicted in Figure 5, which is useful to reveal (positive/negative) correlation or no (linear) correlation between pairs of objectives [32]. Due to its simplicity and completeness, this plot provides relevant information to the decision-maker. The numeric information inside each subplot contains:

“correlation coefficient”[*prob-value*]number of points in the subplot.

A value of *prob-value* less than 0.05 indicates that the correlation between the pair of objectives is considered statistically significant (positive if “correlation coefficient”> 0, negative if “correlation coefficient”< 0).

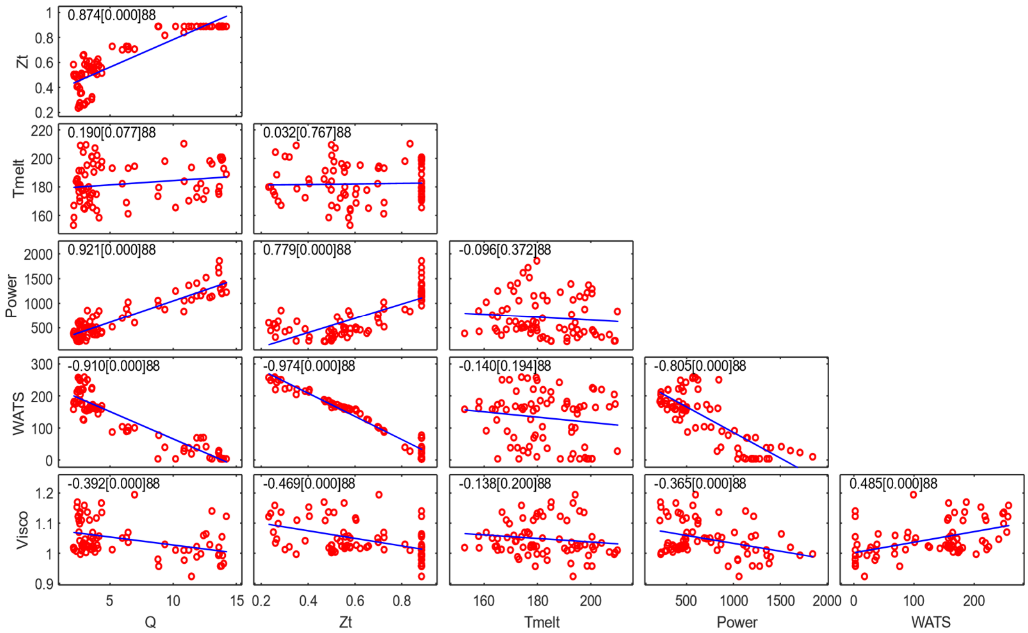


Fig.5. Pairwise coordinate plot of the Pareto front produced by the *simplex lattice design* weight method

6. Conclusions

In this paper, the MOO problem that emanates from the optimal operating conditions of a single screw extrusion is efficiently solved by the weighted Tchebycheff scalarization function and the SA method. Emphasis was given to the weight vectors generating process. Preferences relative to the importance of the objective functions have been also incorporated into the weight process. Experiments were conducted to compare the behavior of the non-dominated solutions provided by the three methods to generate weight vectors. To assist the decision-maker trade-off solutions have been identified from the two-dimensional projections of the Pareto front. The results were analyzed using a path value graph and a pairwise coordinate plot, in terms of the objectives, and show the viability of the weighted Tchebycheff method when solving the MOO single screw extrusion problem.

Acknowledgments. This project has received funding from the European Union’s Horizon 2020 research and innovation programme under the Marie Skłodowska-Curie grant agreement No. 734205-H2020-MSCA-RISE-2017. The work has also been supported by FCT – Fundação para a Ciência e Tecnologia within the R&D Units Project Scope: UIDB/00319/2020, UIDB/00013/2020 and UIDP/00013/2020 of CMAT-UM.

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