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OPTIMIZATION OF SINGLE SCREW EXTRUSION

Abstract: *Multi-objective evolutionary optimization algorithms (MOEA) are used for the optimization of plasticating single screw extrusion. For this purpose, a specific MOEA is linked to available process modelling routines. The methodology is used to set the operating conditions and identify the screw geometry for a specific case study, thus demonstrating the practical utility of this approach.*
Keywords: *extrusion process, optimization, Pareto chart*

1. Introduction

The optimization of single screw extrusion is a difficult task as it involves taking into attention several conflicting objectives [1-3]. Two major practical challenges are the definition of the optimal operating conditions and/or the identification of the geometrical parameters yielding the best process performance. Traditionally, a trial-and-error approach combined with empirical knowledge has been used for this purpose. Also, some attempts based on mathematical models coupled to statistical analysis have been applied [4-6]. Nevertheless, a more efficient approach is to handle single screw extrusion as an optimization problem where different conflicting objectives are to be considered simultaneously [1, 3, 7]. In such a case, Multi-objective Evolutionary algorithms (MOEA), such as the Reduced Pareto Set Genetic Algorithm (RPSGA) [1, 2], can be used. Generally, the outcome of these methodologies is a group of solutions approaching the set of Pareto optimal solutions, which represents different trade-offs between the objectives. Decision making strategies can be implemented to assist the decision maker to select, from the Pareto optimal set, the more suitable solutions for the single screw extrusion process.

This chapter discusses the application of a multi-objective optimization methodology based on evolutionary algorithms for the definition of the operating conditions and/or the geometry of a single screw extruder for a representative case study.

2. Optimization problem formulation

The optimization of the single screw extrusion requires coupling different tools that will create a comprehensive system being able to consider the response of the extruder to the appropriate set of input parameters. Thus, the MOEA is

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coupled to a modelling routine of plasticating extrusion, which must be able to compute the values of the relevant objectives for a given set of equipment geometry and dimensions, operating conditions and polymer properties. The modelling routine is presented in more detail in chapter 1 and in references [1, 2]. It describes mathematically the plasticating sequence by a set of balance equations that are coupled to a rheological constitutive law and a set of boundary conditions [2].

The most relevant objectives (extruder performance) are generally considered to be the mass output (Q), the length of screw required for melting the polymer (Z_t), the melt temperature at the die exit (T_{exit}), the mechanical power consumption (*Power*) and the degree of mixing. The latter may be quantified by the weighted-average total strain (*WATS*), a measure of distributive mixing. Usually, the aim is to maximize Q and *WATS* and minimize Z_t, T_{exit} and *Power*. The values attained by these objectives depend on the values of the decision variables. There are two groups of variables (Figure 1). One corresponds to the operating conditions of the extruder, specifically the screw speed (N), and the temperature profile of the heater bands in the barrel (T_{b1}, T_{b2}, T_{b3}). The range of variation of the former depends on the mechanical power system (motor and reduction gear) of the extruder. The lower and upper bounds for the range of temperatures of the heater bands are the polymer melting temperature and the onset of degradation, respectively. The other group of variables comprises the geometrical parameters,

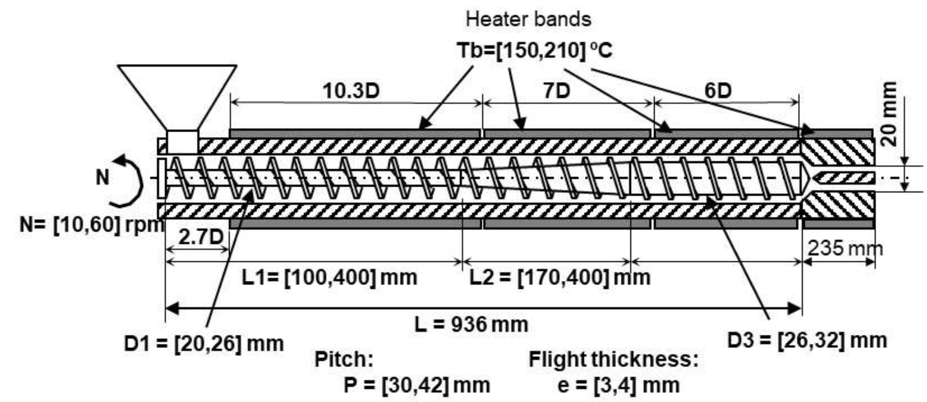

Fig. 1. Operational and geometrical variables to be optimized

which encompass the internal screw diameter of the feed (D_1) and metering zones (D_3), the axial lengths of the feed (L_1), compression (L_2), and metering zones (L_3), the flight thickness (e) and the screw pitch (p). The ranges of variation of the geometrical parameters are usually defined based on empirical knowledge. For example, if the compression zone is too short, the rate of decreasing channel depth downstream could become higher than the melting rate, resulting in material clogging. Conversely, since the shallower the screw channel the higher the melting rate, a very long compression zone will result in an unnecessarily long melting stage. It should be noted that all these decision variables are continuous.

As noted above, the aim is to optimize several conflicting criteria simultaneously. This implies, for example, increasing the screw speed which will bring out higher outputs, but also lower quality of mixing and greater energy consumption. Therefore, there is no single solution that optimizes all criteria, but instead a set of solutions that represents different trade-offs between them. This type of problems can be formulated as a multi-objective optimization problem (MOP). A general mathematical formulation of a MOP can be written as follows:

$$\begin{aligned} \underset{x \in R^n}{\text{minimize}} \quad & f(x) \equiv (f_1(x), \dots, f_m(x)) \\ \text{subject to} \quad & c_i(x) \geq 0, i \in I \\ & c_i(x) = 0, i \in E \\ & lb \leq x \leq ub \end{aligned} \tag{1}$$

where, $f: R^n \rightarrow R^m$ are the m objective functions, $c_i: R^n \rightarrow R$ are the constraint functions and I and E are two finite sets of indices. For $i \in I$, c_i are the *inequality constraints* and for $i \in E$, c_i are the *equality constraints*. lb and ub are the vectors of the lower and upper bounds on the decision variables, respectively.

A point x that satisfies the constraints is called a *feasible point*. The set of feasible points is defined by:

$$\Omega = \{x \in R^n: c_i(x) \geq 0, i \in I; c_i(x) = 0, i \in E; lb \leq x \leq ub\}.$$

Thus, the multi-objective optimization problem (1) can be rewritten more compactly as:

$$\underset{x \in \Omega}{\text{minimize}} \ (f_1(x), \dots, f_m(x)) \tag{2}$$

In multi-objective optimization, the solutions are compared in terms of dominance. The following definitions are used [8].

Definition 1 (Pareto dominance): Given $x, y \in \Omega$, the point x is said to dominate point y, denoted by $x \prec y$, if and only if

$f_i(x) \leq f_i(y)$, for all $i \in \{1, \dots, m\}$ and $f_j(x) < f_j(y)$ for at least one $j \in \{1, \dots, m\}$.

Definition 2 (Pareto optimality): Let $x^* \in \Omega$ be a feasible point; x^* is Pareto optimal if there is no vector the point $y \in \Omega, y \neq x^*$ that

$f_i(y) \leq f_i(x^*)$, for all $i \in \{1, \dots, m\}$ and $f_j(y) < f_j(x^*)$ for at least one $j \in \{1, \dots, m\}$.

The set of the images of the Pareto optimal set is called the *Pareto optimal front*. Mathematically, any maximization objective can be converted as a minimization one since $\max f_i(x)$ is equivalent to $-\min -f_i(x)$. Hence, in this chapter any maximization objective will be reformulated as a minimization one.

In the context of the optimization of a specific single screw extrusion process, the objective functions f_i, for $i \in \{1, \dots, m\}$, can be normalized taking into consideration reference values for them in the search space of the real problem. Thus, the objective functions can be re-scaled to the same order of magnitude in the interval [0,1], the normalized objectives being computed for all $i \in \{1, \dots, m\}$ by:

$$F_i(x) = \begin{cases} \dfrac{f_i(x) - f_i^{min}}{f_i^{max} - f_i^{min}} & \text{if } f_i^{min} \leq f_i(x) \leq f_i^{max} \\ 1 & \end{cases} \qquad (3)$$

where $f_i^{min} = \min_{x \in \Omega} f_i(x)$ and $(f_1^{min}, \dots, f_m^{min})$ is called the *objective ideal vector*, and each component f_i^{max} of the vector $(f_1^{max}, \dots, f_m^{max})$ is an estimation of the *nadir objective vector* obtained from a payoff table [10]. For normalized objectives, a maximization objective can also be reformulated as a minimization objective as follows:

$$\max_{x \in \Omega} F_i(x) = \min_{x \in \Omega} \left(1 - \frac{f_i(x) - f_i^{min}}{f_i^{max} - f_i^{min}}\right) \qquad (4)$$

This reformulation is adopted in this work. The single screw optimization problem is a bound constrained multi-objective optimization problem. To simplify the formulation, the decision variables are denoted by $x = (N, T_{b1}, T_{b2}, T_{b3}, D_1, D_3, L_1, L_2, e, p)$. For the extruder size range and layout illustrated in Figure 1 and assuming the processing of a typical thermoplastic polyolefin (High Density Polyethylene (HDPE), the lower and upper bounds vectors are $lb = (10,\ 150,\ 150,\ 150,\ 20,\ 26,\ 100,\ 170,\ 3,\ 30)$ and $ub = (60,\ 210,\ 210,\ 210,\ 26,\ 32,\ 400,\ 40,\ 4,\ 42)$, respectively. The minimum and maximum values of the objective functions are defined based on the practical experience with this equipment and material. Table 1 presents normalized objective functions, for generic values of f^{min} and f^{max}.

Table 1. Objective functions to be optimized

Description	Aim	f^{min}	f^{max}	Normalization
Mass output - Q (kg/hr)	maximize	1.0	20.0	$F_1(x) = 1 - \frac{f_1(x) - f_1^{min}}{f_1^{max} - f_1^{min}}$
Length – Z_t (m)	minimize	0.2	0.9	$F_2(x) = \frac{f_2(x) - f_2^{min}}{f_2^{max} - f_2^{min}}$
Melt temperature - T_{melt} (ºC)	minimize	150.0	210.0	$F_3(x) = \frac{f_3(x) - f_3^{min}}{f_3^{max} - f_3^{min}}$
Power consumption - *Power* (W)	minimize	0.0	9200	$F_4(x) = \frac{f_4(x) - f_4^{min}}{f_4^{max} - f_4^{min}}$
Mixing degree - *WATS*	maximize	0.0	1300	$F_5(x) = 1 - \frac{f_5(x) - f_5^{min}}{f_5^{max} - f_5^{min}}$

Thus, the mathematical formulation of the single screw multi-objective optimization problem is given by

$$\begin{aligned} \underset{x \in R^{10}}{\text{minimize}} \quad & (F_1(x), F_2(x), F_3(x), F_4(x), F_5(x)) \\ \text{subject to} \quad & lb \leq x \leq ub \end{aligned} \qquad (5)$$

where the $F_i(x)$, for $i \in \{1,2,3,4,5\}$, are given in Table 1.

3. Multi-objective Optimization Methods

Different approaches for solving multi-objective optimization problems are reported in the literature [8, 10]. One approach includes the use of scalarization methods. In these methods, the multi-objective optimization problems are reformulated as single objective optimization using a scalarized function that depends on the set of parameters, such as weights or reference points. Different sets of parameters must be used to obtain different approximations to the Pareto optimal solutions. Thus, in this type of approach several single optimization problems must be solved.

For example, in the weighted sum scalarization method, the MOP in equation (3) is reformulated using an aggregated function, as follows:

$$\begin{aligned} \underset{x \in R^{10}}{\text{minimize}} \quad & \textstyle\sum_{i=1}^{5} w_i F_i(x) \\ \text{subject to} \quad & lb \leq x \leq ub \end{aligned} \qquad (6)$$

where $w_i \geq 0$ are the weights, and $\sum w_i = 1$. One advantage of these methods is the possibility of being solved using the simpler single objective optimization algorithms available in the literature. Nevertheless, these methods have some drawbacks. They require the definition of appropriate sets of values for the parameters that depend on the problem. Additionally, to approximate the Pareto optimal front of the multi-objective problem, solving several single objective optimization problems can be computationally expensive.

Alternatively, Evolutionary Algorithms (EAs) can be used instead [9, 10]. EAs are particularly suited to deal with the multi-objective nature of real problems since they work with a population of candidate solutions (or vectors), rather than with a single solution point. Moreover, EAs have the ability to seek the global optimum, avoiding being trapped in local optima. In Multi-objective Evolutionary algorithms (MOEAs), some mechanisms are used to promote the convergence towards the Pareto front. It is also possible to implement diversity preserving techniques during the search, to obtain a representative and diverse set of compromise solutions. Thus, MOEAs can provide, in a single run, approximations to several Pareto optimal solutions, representing different trade-offs between the objectives.

The Reduced Pareto Set Genetic Algorithm (RPSGA) is a MOEA that has been used successfully to optimize single screw extrusion [1-3, 7, 11]. RPSGA uses a clustering technique to reduce the number of solutions and to guarantee their good distribution along the Pareto front during the search procedure. Initially, a population of points is generated randomly. At each generation, several operations are performed. First, the solutions of the population are evaluated (*i.e.,* the values of the objectives are computed). Next, a clustering technique is applied to reduce the number of non-dominated solutions (*i.e.*, approximations to the Pareto front) based on ranks. Then, a linear ranking function is used to compute the fitness value of the solutions. This value depends on the rank of each solution in the population, which is related to its performance, location and non-domination condition. The best individuals are selected for reproduction using a roulette wheel selection. For the reproduction, a SBX recombination operator and polynomial mutation are used [11]. The iterative process stops when a pre-defined maximum number of generations is reached. Details about RPSGA can be found in [11].

MOEAs are easy to implement, explore the entire search space and, consequently, are able to escape from local optimal solutions and can be easily adapted to work in the optimization in different conditions.

4. Numerical Results

In this section, the RPSGA is used to optimize the single screw extrusion problem defined in Figure 1 and Table 1. Seven different scenarios, identified in Table 2, are considered to optimize the operating conditions and the screw geometry. In scenarios 1 to 4, the operating conditions of the extruder are optimized using only two objectives. These correspond to bi-objective optimization problems, that are relevant to check if the solutions produced by the

RPSGA are suitable for the extrusion process. Moreover, the results obtained are simpler to analyze, enable an easier visualization of the trade-offs between the solutions, as well as easier selection of the best solution to use from the set of the dominated solutions obtained. In the case of the scenarios 5 to 7, all five objectives were considered. Concerning the decision variables, in scenarios 1 to 5 only the operating conditions are considered, in scenario 6 only the geometrical parameters are optimized, whilst scenario 7 includes both types of decision variables are used.

Table 2. Scenarios for single screw extrusion optimization

Scenarios	Objectives	Decision variables
1	(Q, Z_t)	$x = (N, T_{b1}, T_{b2}, T_{b3})$
2	(Q, T_{melt})	$x = (N, T_{b1}, T_{b2}, T_{b3})$
3	(Q, *Power*)	$x = (N, T_{b1}, T_{b2}, T_{b3})$
4	(Q, *WATS*)	$x = (N, T_{b1}, T_{b2}, T_{b3})$
5	(Q, Z_t, T_{melt}, *Power*, *WATS*)	$x = (N, T_{b1}, T_{b2}, T_{b3})$
6	(Q, Z_t, T_{melt}, *Power*, *WATS*)	$x = (D_1, D_3, L_1, L_2, e, p)$
7	(Q, Z_t, T_{melt}, *Power*, *WATS*)	$x = (N, T_{b1}, T_{b2}, T_{b3}, D_1, D_3, L_1, L_2, e, p)$

The thermal, physical and rheological characteristics (the shear rate and temperature dependence of the viscosity are modelled by the Carreau-Yasuda equation) for a High Density Polyethylene, HDPE (grade ALCUDIA TR-135, manufactured by Repsol) are presented in Table 3:

$$\eta = \eta_0[1 + (\lambda\dot{\gamma})^{\alpha}]^{(n-1)/\alpha} \tag{7}$$

The values chosen for the parameters of the RPSGA used resulted from previous empirical studies [1, 3, 11]: 50 generations; crossover probability of 0.8; mutation probability of 0.05; internal and external populations with 100 individuals; limits of the clustering algorithm set at 0.2; and number of ranks set at 30.

Table 3. Properties of the HDPE ALCUDIA TR-135, manufactured by Repsol

Density	Solids	ρ_s	495.0	$kg\ m^{-3}$
	Melt	ρ	854.4	
Thermal Conductivity	Solids	k_s	0.186	$W\ m^{-1}\ °C^{-1}$
	Melt	k_m	0.097	
Specific Heat	Solids	C_s	2350	$J\ kg^{-1}$
	Melt	C_m	2535	
Melting	Heat	H	167x10^3	$J\ kg^{-1}$
	Temperature	T_m	119.9	°C
Carreau-Yasuda equation	Viscosity	η_0	18000	$Pa\ s$
		E/R	10000	K
		$\hat{\lambda}$	0.70	s
		a	1.70	
		n	0.30	
		T_0	463.15	K

Figure 2 shows the Pareto fronts obtained for scenarios 1 to 4 (left column in Figure 2) and the two-dimensional projections of the Pareto front for scenario 5 (right column in Figure 2). In the first case, since only two objectives are optimized simultaneously, the algorithm converges to a curve, the Pareto front, that defines the trade-offs between the objectives in a two-dimensional space. For example, in scenario 2 the higher the output the higher is the melt temperature, as the viscous dissipation becomes more important. In scenario 5, the algorithm works in a 5-dimensional objective space. To visualize the trade-offs among the objectives, four two-dimensional projections of the Pareto front are drawn (right column in Figure 2). In such a case, it is important to note that some points that seem to be dominated in a given two-dimensional representation are non-dominated in another two-dimensional projection. In Figure 2, points P1 to P5 identify the best values for each objective, respectively. For example, point P1 identifies the maximum value of the output, while point P2 is the minimum value of the length of the screw required for melting.

Tables 4 and 5 show the decision variables and the corresponding objective functions values for these solutions. For instance, the maximum output for scenarios 1 to 4 is 8.57 kg/h, whilst for scenario 5 it attains just 7.69 kg/h, a reduction of 10.2%. This shows that the existence of several objectives (in scenario 5) may hinder attaining better/higher values of the individual objectives. Table 6 presents the relative difference between the values of the objectives for scenario 5 and scenarios 1 to 4 (in percentage). As it can be seen, for some objectives, in scenario 5 it was actually possible to improve some values (melt temperature and mechanical power consumption objectives).

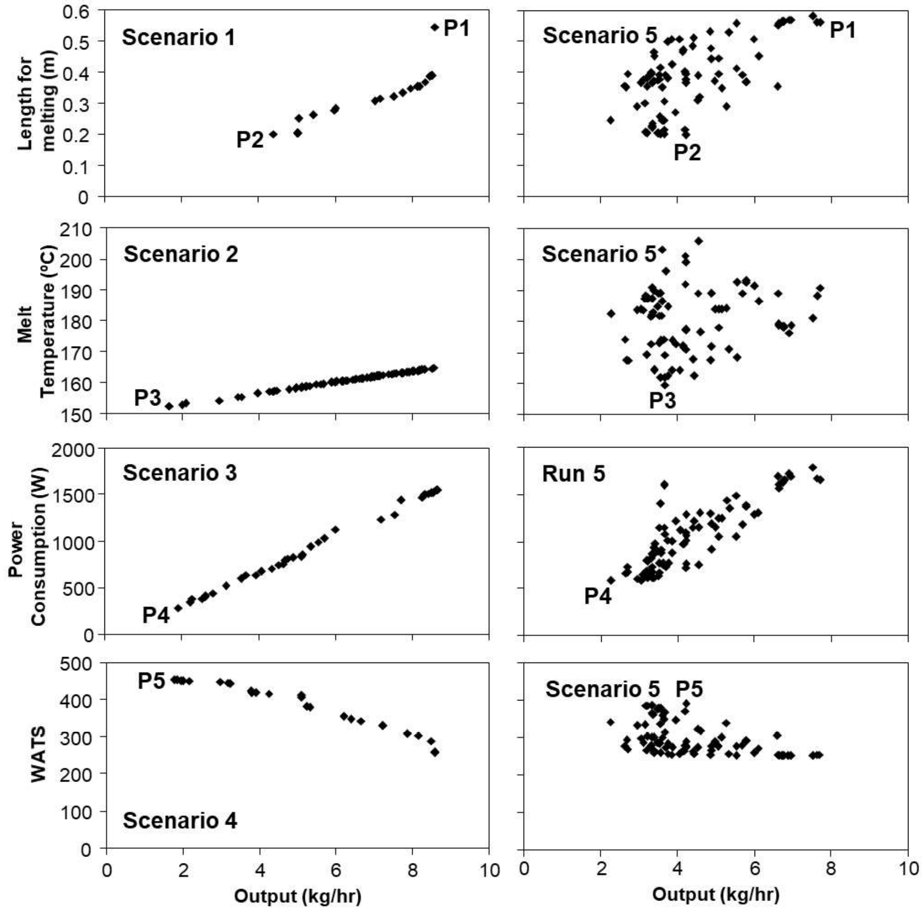

Fig. 2. Comparison between the Pareto fronts for scenarios 1 to 4 (left column) and the two-dimensional projections of the Pareto front for scenario 5 (right column)

Table 4. Solutions with the best values for each objective function for scenarios 1 to 4

	Operating conditions				Objectives				
	N (rpm)	T_{b1} (°C)	T_{b2} (°C)	T_{b3} (°C)	Q (kg/h)	Z_t (m)	T_{melt} (°C)	*Power* (W)	*WATS*
P1	59.4	210	196	199	**8.57**	0.544	206	1694	256
P2	28.8	203	200	197	4.37	**0.200**	202	1051	406
P3	10.7	150	202	150	1.64	0.323	**152**	296	297
P4	11.6	204	201	207	1.91	0.198	205	**276**	398
P5	12.3	209	154	150	1.77	0.145	157	524	**454**

Table 5. Solutions with the best values for each objective function for scenario 5

	Operating conditions				Objectives				
	N (rpm)	T_{b1} (°C)	T_{b2} (°C)	T_{b3} (°C)	Q (kg/h)	Z_t (m)	T_{melt} (°C)	*Power* (W)	*WATS*
P1	54.2	188	170	177	**7.69**	0.562	191	1654	254
P2	29.5	185	184	162	4.22	**0.201**	177	1292	392
P3	25.4	151	188	157	3.66	0.215	**160**	1598	369
P4	14.7	170	178	189	2.26	0.246	183	**586**	342
P5	29.5	185	184	162	4.22	0.200	177	1292	**392**

Table 6. Relative differences between the values of the objectives of scenario 5 and those of scenarios 1 to 4 (in %)

	Objectives				
	Q (kg/h)	Z_t (m)	T_{melt} (°C)	*Power* (W)	*WATS*
P1	**-10.2**	-3.2	7.2	2.3	-1.1
P2	-3.5	**-0.5**	12.5	-22.9	-3.5
P3	123.0	33.4	**-4.8**	-439.5	24.4
P4	18.5	-24.7	11.1	**-112.3**	-14.2
P5	138.5	-38.7	-12.7	-146.7	**-13.7**

A similar analysis of the results can be done for scenarios 6 and 7. Figure 3 shows the two-dimensional projections of the Pareto front for scenario 6. The clouds of non-dominated solutions indicate the existence of a compromise between all the objectives. Table 7 presents the geometrical parameters corresponding to the best values for each objective function. Table 8 identifies the operating conditions and geometrical parameters corresponding to the best values for each objective function for scenario 7. Finally, Table 9 shows the relative difference between the values of the objectives for scenario 7 and scenarios 1 to 4 (in percentage). In scenario 7, all the objectives were improved, except the length of screw required for melting.

Table 7. Optimal point corresponding to the best values for each objective function for scenario 6

	Geometrical parameters					
	L_1 (mm)	L_2 (mm)	D_1 (mm)	D_3 (mm)	p (mm)	e (mm)
P1	131	259	22.1	27.9	38.7	3.1
P2	101	183	22.0	31.7	32.2	3.3
P3	168	301	21.8	32.0	37.0	3.5
P4	390	365	21.7	30.9	40.7	3.1
P5	101	181	21.9	31.9	31.1	3.4

Table 8. Optimal point corresponding to the best values for each objective function for scenario 7

	Operating conditions				Geometrical parameters					
	N (rpm)	T_{b1} (ºC)	T_{b2} (ºC)	T_{b3} (ºC)	L_1 (mm)	L_2 (mm)	D_1 (mm)	D_3 (mm)	p (mm)	e (mm)
P1	58.1	189	198	172	174	266	23.3	27.3	38.1	3.5
P2	24.1	207	195	177	143	305	24.2	26.8	37.6	3.3
P3	19.7	152	180	156	204	248	25.0	31.1	36.2	3.1
P4	10.9	161	196	152	270	290	25.1	29.4	37.9	3.3
P5	46.8	183	179	173	138	220	25.0	31.2	41.4	3.5

Table 9. Relative differences between the values of the objectives of scenario 7 and those of scenarios 1 to 4 (in %)

	Objectives				
	Q (kg/h)	Z_t (m)	T_{melt} (°C)	*Power* (W)	*WATS*
P1	61.9	-9.2	-0.9	-18.0	-39.8
P2	32.2	-27.9	-12.7	46.8	-23.1
P3	-5.3	-77.4	1.0	49.6	0.6
P4	8.5	-54.6	12.6	36.1	-22.2
P5	63.6	-66.0	-5.8	-35.8	20.5

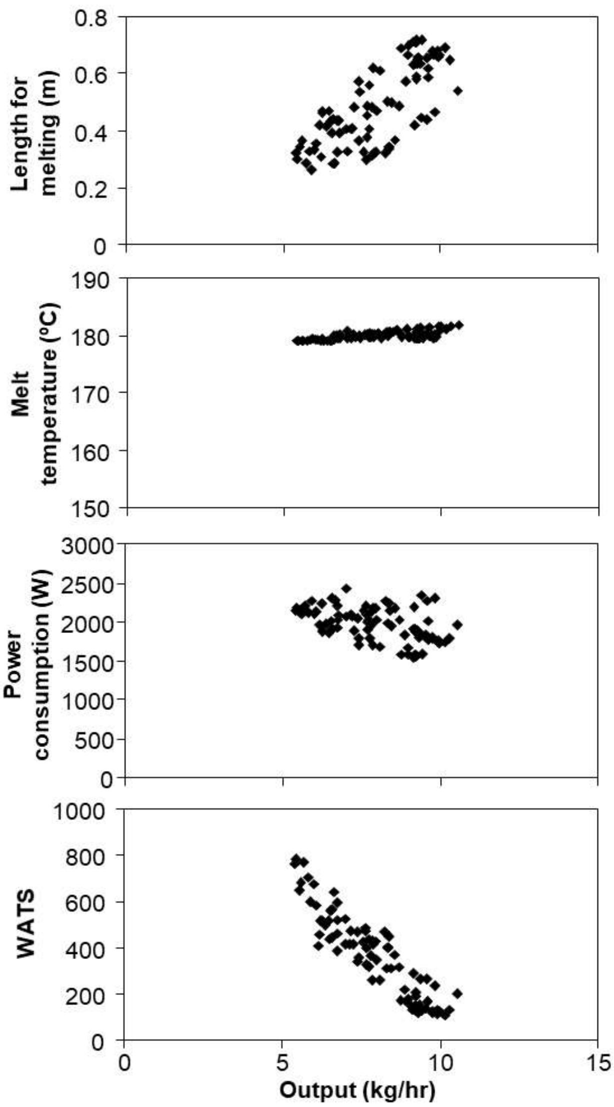

Fig. 3. Two-dimensional projections of the Pareto front for scenario 6

5. Decision Making

The decision maker (DM) must select the most suitable solution for the single screw extrusion problem from the Pareto optimal set. In this context, decision making strategies can be used to assist the DM [11]. In this work, the weighted sum method is used with different sets of weights to identify solutions according to the DM preferences. In practice, it is possible to define a tolerance (ϵ) that allows to reduce the region of the solutions.

For each scenario studied in the previous section, different sets of weights were used and an $\epsilon = 0.1$. For instance, Figure 4 top shows the original Pareto front for scenario 1 (upper left side in Figure 2) and Figure 4 bottom presents the solutions obtained for three sets of weights, considering the DM preferences. The set of weights are $w_1 = (0.8, 0.1)$, $w_2 = (0.5, 0.5)$, and $w_3 = (0.2, 0.8)$, the corresponding solutions being denoted in the graph as a), b) and c), respectively. As it can be seen, the method is sensitive to the preferences of the DM. For example, as the output weight is decreased, the lower is the output of the solutions.

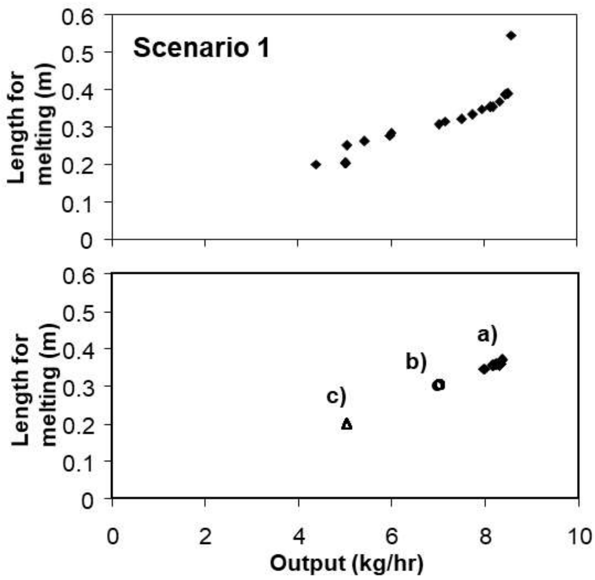

Fig. 4. Pareto front for scenario 1 (top) and the solutions obtained for three sets of weights (bottom)

Figure 5 presents the two-dimensional projections of the solutions obtained using the weighted sum method for scenario 5, considering two sets of weights: $w_1 = (0.8, 0.05, 0.05, 0.05, 0.05)$ and $w_2 = (0.2, 0.2, 0.2, 0.2, 0.2)$. Again, when the output weight decreases, the lower is the output of the solutions. Furthermore, the Pareto solutions are concentrated in smaller regions when compared with those obtained initially for scenario 5 (see Figure 2).

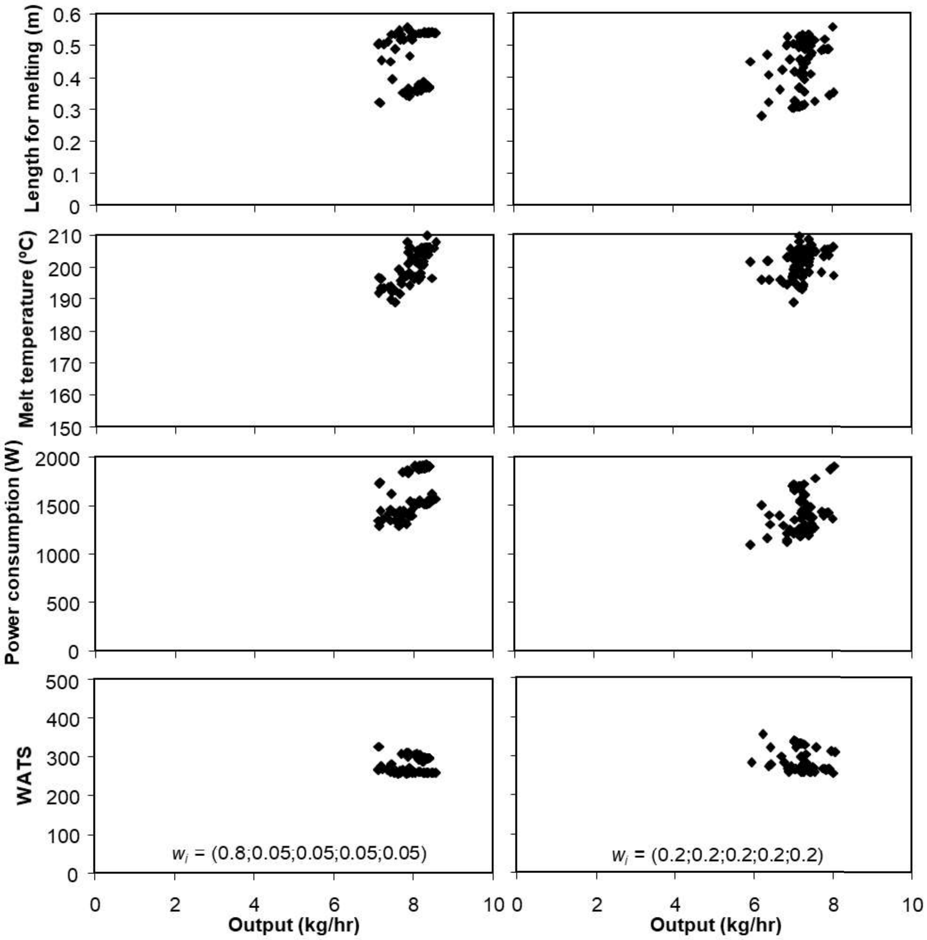

Fig. 5. Two-dimensional projections of the solutions obtained for two sets of weights for scenario 5

6. Conclusions

Traditionally, the optimization of single screw extrusion is performed based on empirical knowledge, often combined with trial-and-error procedures. Tentative extrusion experiments, or machining of screws, are performed until a desirable performance is obtained. This is costly and inefficient. Instead, setting the adequate operating conditions, or defining the screw geometry, can be assumed as an optimization problem. This chapter introduced a scientific approach to solve correctly and efficiently an important class of practical technological problems, including single screw extrusion.

Single screw extrusion was modelled as a multi-objective optimization problem, where the aim is to optimize its performance, as measured by several relevant objectives. This problem involves different conflicting objectives, that depend on the operating conditions, or geometrical parameters, or both. The optimization method proposed was able to solve satisfactorily the problem and the solutions are viable and in agreement with current process knowledge (experimental validation is difficult and costly for obvious reasons). Finally, a decision making strategy incorporating the DM preferences was applied to assist the selection of solutions in the Pareto front.

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