Multiobjective Optimization of Polymer Extrusion: Decision Making and Robustness

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ABSTRACT: A Multi-Objective Evolutionary Algorithm (MOEA) is used to optimize polymer single screw extrusion. In this approach, the MOEA is linked to a modelling routine that quantifies the objectives as a function of the decision variables (*i.e.*, operating conditions and/or screw geometry). Due to the conflicting nature of some objectives, the optimization algorithm uses a set of possible solutions to the problem that evolves during successive generations to a set of optimal solutions denoted as Pareto set. Since practical process optimization should yield a single solution, it is convenient to implement also a Decision Making (DM) strategy. Two methodologies were followed. In one case, the solutions were selected based on the preferences of a decision maker. Alternatively, the sensitivity of the solutions to small changes in the design variables was taken into account through a robustness analysis. The analysis of various case studies and the comparison with experimental data validated the method and demonstrates its potential.

1 INTRODUCTION

Single screw extrusion is a major processing technology in the plastics industry. It is also an important unit operation of other key polymer processing techniques such as injection molding and blow molding. The process consists in converting solid pellets at the inlet into a homogeneous melt that is forced at the highest possible rate through a shaping die, yielding an extrudate with the required cross-section. In daily practice, process designers and engineers must define the best screw profile and/or the most adequate set of operating conditions for a given product/polymer system. This is a challenging task due to two major reasons. First, the thermomechanical environment developing inside an extruder is complex, including non-isothermal flow of solids, melting, mixing (both distributive and dispersive) and non-isothermal melt flow in the screw and die channels. Secondly, the performance of the system is described by a number of objectives (mass throughput, degree of mixing, melt temperature at the die exit, etc.) that must be satisfied simultaneously, albeit some of them being conflicting (*e.g.*, mass throughput and mechanical energy consumption).

Trial-and-error procedures for defining the screw profile and the operating conditions to yield the best performance are still commonly used in practice. Automatization of this process can be achieved through optimization methodologies (Covas et al. 1999; Potente and Zelleröhr 1996). Such an approach entails coupling an optimization algorithm with a process modelling routine that computes the performance objectives for a given set of operating conditions and/or system geometry.

Approaching the optimization of screw extrusion from a multiobjective optimization perspective gives rise to a set of optimal solutions known as Pareto set. In order to come up with a unique solution, the Decision Maker (DM) must express his/her preferences at some point of the optimization. These preferences can be articulated before, after or during the run of the optimization algorithm.

In this work, multiobjective optimization of screw extrusion is addressed with MOEA and incorporating two decision making support methods. The first is based on the relative importance of the objectives, which is relatively straightforward. The second is concerned with the ability of the solutions to tolerate small perturbations in the design variables, an issue that is particularly relevant to extrusion.

2 POLYMER EXTRUSION

In order to achieve the ultimate goal of forcing a melt at high rate through a shaping die, the extruder must efficiently fulfill a number of tasks including being able to receive raw materials in different physical forms and convey them forward, melting the material in a relatively short screw length, ensuring sufficient dispersive and distributive mixing, generating the pressure required for the melt to flow through the die at the desired output, etc.

Most extruders consist of an Archimedes-type screw, with diameter *D,* rotating inside a hollow barrel with length *L*. A lateral opening in the barrel allows the inlet of material through the hopper, while the shaping die is coupled to the opposite end. Both barrel and die contain heater bands. Often, the screw has three geometrically distinct sections with lengths L_1, L_2 and L_3, respectively. The feed section upstream has constant channel depth (H_1). The channel depth of the next section compression) decreases linearly (between H_1 and H_3). The metering section downstream has a shallower channel (constant depth H_3). The screw helix is defined by its pitch (P) and flight thickness (e). The operating conditions set by the operator include screw rotation speed (*N*) and barrel/die temperature profile (T_b). The relevant material data include physical (friction coefficients, solids and melt density, etc.), thermal (heat conduction coefficients, melting temperature, heat capacity, etc.) and rheological properties (non-Newtonian viscosity).

As the solid material progresses from the hopper until it emerges from the die, it experiences a sequence of distinct thermomechanical environments:1) gravity flow of particles in the; 2) friction dragging of the particles along the screw together with conduction heating from the barrel; 3) melting of a thin layer of material near to the inner barrel wall; 4) progressive melting of the remaining material, following a mechanism involving segregation of the melt and surviving solids; 5) viscous dragging of the molten material with pressure generation; 6) pressure flow through the die (Rauwendaal 1986). Each of these steps can be treated mathematically by constitutive equations relating to mass, momentum and energy conservation, together with a rheological law, coupled to the relevant boundary conditions. A global process description is obtained by linking adjacent steps with appropriate boundary conditions. Then, for a given set of inputs, the model predicts mass output, Q, average melt temperature at die exit, T_{melt}, mechanical power consumption, $Power$, length of screw required to melt the polymer, L_{melt}, degree of distributive mixing (in terms of the average deformation induced, $WATS$), etc. Details of the modeling routine and of its experimental validation can be found elsewhere (Gaspar-Cunha 2000).

Process optimization will be discussed using the case studies presented in Table 1 (polymer properties and die geometry will remain constant). As indicated, optimization concerns finding the best operating condition and/or the best screw geometry. For each case study, the table indicates the decision variables (process parameters) and the objectives (process responses) taken in. The aim is to maximize mass output, $Q \in [1,20]$ kg/hr and the degree of mixing, $WATS \in [0,1300]$, whilst minimizing the length of screw required for melting, $L_{melt} \in [0.2,0.9]$ m, melt temperature at die exit, $T_{melt} \in [150,210]$ °C and the mechanical power consumption, $Power \in [0,9200]$ W. The range of variation of the decision variables is given in Table 2.

Table 1 Optimization case studies.

Case	Decision Variable						Objectives
	Operating conditions						
1							Q, L_{melt}
2							Q, T_{melt}
3		N	T_{b1}	T_{b2}	T_{b3}		$Q, Power$
4							$Q, WATS$
5							All
	Screw geometry						
6							$Q, Power$
7	L_1	L_2	H_1	H_3	P	e	$Q, WATS$
8							All
	Both						
9		N	T_{b1}	T_{b2}	T_{b3}		$Q, Power$
10	L_1	L_2	H_1	H_3	P	e	$Q, WATS$
11							All

Table 2 Decision variables: operating conditions and screw geometry.

	Variable	Range	Units
Operating conditions	N	[10, 60]	rpm
	T_{b1}	[150, 210]	°C
	T_{b2}	[150, 210]	°C
	T_{b3}	[150, 210]	°C
Screw geometry	L_1	[100, 400]	mm
	L_2	[170, 400]	mm
	H_1	[5, 8]	mm
	H_3	[2, 5]	mm
	P	[30, 42]	mm
	e	[3, 4]	mm

3 MULTIOBJECTIVE OPTIMIZATION

To search Pareto optimal solutions, the present study relies on the Non-dominated Sorting Genetic Algorithm (NSGA–II), which is a well-established state-of-the-art MOEA (see Deb *et al.* (2002)). Modifications were necessary to the calculation of the fitness values. During the search, population members are sorted according to these values.

3.1 *Relative importance of objectives*

This preference information is expressed by defining the weight vector whose components sum up to 1, with each component w_i expressing how the i-th objective is important to the DM. The solution that best meets the DM preferences is determined by the

Weighted Stress Function Method (WSFM) (Ferreira et al. 2007). The weighted stress function can be defined as:

$$\sigma_i(f_i, w_i) = \begin{cases} \omega \tan\left(-\frac{\pi}{\psi(w_i)}(f_i - w_i)\right) + \xi(w_i), & f_i \le w_i \\ \omega \tan\left(-\frac{\pi}{\varphi(w_i)}(f_i - w_i)\right) + \xi(w_i), & f_i > w_i \end{cases} \quad (1)$$

Where:

$$\omega = \begin{cases} \frac{-\xi(w_i)\psi(w_i)}{\tan\left(\frac{\pi}{\varphi(w_i)}(w_i - 1 + \delta_1)\right)\varphi(w_i)}, & f_i \le w_i \\ \frac{-\xi(w_i)}{\tan\left(\frac{\pi}{\varphi(w_i)}(w_i - 1)\right)}, & f_i > w_i \end{cases} \quad (2)$$

$$\varphi(w_i) = \frac{3}{4}(1 - w_i)^2 + 2(1 - w_i) + \delta_1 \quad (3)$$

$$\psi(w_i) = \varphi(w_i) + 4w_i - 2 \quad (4)$$

$$\xi(w_i) = -\frac{1}{\tan\left(-\frac{\pi}{2 + 2\delta_2}\right)}\tan\left(-\frac{\pi}{1 + \delta_2}\left(w_i - \frac{1}{2}\right)\right) + 1 \quad (5)$$

WSFM can be used for both minimization and maximization problems, though Equation (1) assumes maximization of the objectives. All objectives must be normalized, so that their values are in the range $[0, 1]$ and all components of the ideal objective vector are equal to 1. Given the weight vector $\boldsymbol{w} = (w_1, \ldots, w_m)$ specifying the relative importance of the objectives and the set of solutions $X = \{x^1, \ldots, x^N\}$, the solution that best meets the preferences can be found by solving:

$$\text{minimize}_{x \in X}: \; T(x) = \max_{1 \le i \le m} \sigma_i(f(x), w) \quad (6)$$

Thus, the fitness of the i-th population member can be formulated as:

$$F(i) = Rank(i) + \frac{T(i)}{T(i) + 1} \quad (7)$$

where $Rank(i)$ is the rank based on the Pareto dominance. Smaller fitness values are preferred.

3.2 *Robustness of solutions*

The robustness issue is addressed by the following steps (Gaspar-Cunha *et al.* 2014):

(i) Calculation of a variance-based measure of the i-th individual with respect to the m-th objectives, R_m:

$$R_m(i) = \frac{1}{N'}\sum_{j=1}^{N'} \frac{|f_m(x_i) - f_m(x_j)|}{|x_i - x_j|} \quad (8)$$

where N' is the number of neighbors, j, whose distance in the decision space, d'_{ij}, in not greater than d'_{max}. This distance can be calculated as:

$$d'_{ij} = \sqrt{\sum_{k=1}^{L}(x_{ki} - x_{kj})^2} \quad (9)$$

Since multiple objectives are considered, the robustness measures of individual objectives are combined:

$$R(i) = \frac{1}{M}\sum_{m=1}^{M} R_m(i) \quad (10)$$

(ii) Calculation of the distance metric for diversity preservation:

$$I(i) = \sum_{i=1}^{N} sh(d_{ij}) \quad (31)$$

where $sh(d_{ij})$ is a sharing function that takes into account the distance in the objective space, d_{ij}, between the i-th population member and all its neighbors, j. This sharing function it can be calculated as:

$$sh(d_{ij}) = \begin{cases} 1 - \left(\frac{d_{ij}}{\sigma_{share}}\right)^2, & d_{ij} \le \sigma_{share} \\ 0, & \text{otherwise} \end{cases} \quad (12)$$

where σ_{share} is a constant to be determined experimentally.

(iii) Calculation of the global fitness value of the i-th population individual, $F(i)$:

$$F(i) = \text{Rank}(i) + \varepsilon\frac{I(i)}{I(i) + 1} + (1 - \varepsilon)\frac{R(i)}{R(i) + 1} \quad (43)$$

where $\text{Rank}(i)$ is the rank based on the Pareto dominance relation and ε is the dispersion parameter that determines the degree to which robustness influences global fitness (Gaspar-Cunha *et al.* 2014). Smaller fitness values correspond to a better performance.

4 RESULTS AND DISCUSSION

4.1 *DM based on importance of objectives*

To examine the influence of the relative importance of the objectives on the optimization results, various combinations of weights were considered, namely $w_1, w_2 \in \{0.1, 0.2, 0.5, 0.8, 0.9 | \ w_1 + w_1 = 1\}$. For three representative combinations of weights, Figures 1-3 display the results considering output and power consumption as objectives.
As expected, Figure 1 (constant screw geometry) shows that, for a fixed weight vector, solutions converge to a specific Pareto optimal region whose location depends on the settings of w_1, w_2. For $w_1 = 0.9$, the focus of the search is mainly on maximizing the output, whereas for $w_2 = 0.9$ this criterion is somewhat neglected and NSGA-II aims mostly at finding solutions that minimize power consumption.

As shown in Figure 2 (constant operating conditions), NSGA–II fails to identify solutions along a Pareto front. Instead, they converge to the same region. This suggests that it is difficult to control output and power only by means of screw geometry. In 4fact, these objectives are not only conflicting, but mostly dependent on screw speed and barrel temperature.

Figure 3 concerns the simultaneous optimization of all variables to obtain the most adequate screw geometry and operating set point. NSGA-II is able to locate distinct Pareto optimal regions for Q and $Power$, depending on the relative importance attributed to each objective. Higher *Q* and lower *Power* are obtained when comparing with the results for the preceding case studies (approximately 50% and 10%, with respect to Figure 1, 20% and 90%, respectively, in relation to Figure 2). This is consistent with expectations, as handling more parameters offers more control over the process.

Although not shown here, similar trends were observed for the remaining case studies.

4.2 *DM based on robustness of solutions*

This section focuses the robustness of solutions rather than their relative importance. This is crucial when defining the operating conditions for extrusion, since in industrial practice the control system of a typical extruder cannot avoid small fluctuations of the barrel temperatures during operation. These affect the underlying thermal phenomena, namely conducted and dissipated heat, which in turn may induce output instabilities such as surging.

In the following, the influence of the dispersion parameter, ε, in equation 13 is investigated. Figure 4 shows the solutions generated by NSGA-II for case study 3. The various plots correspond to different ε values. As ε increases, the solutions become better

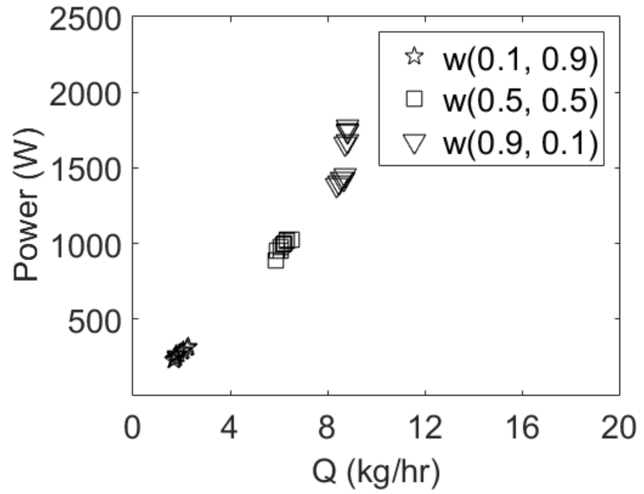

Figure 1 Case studies involving operating conditions.

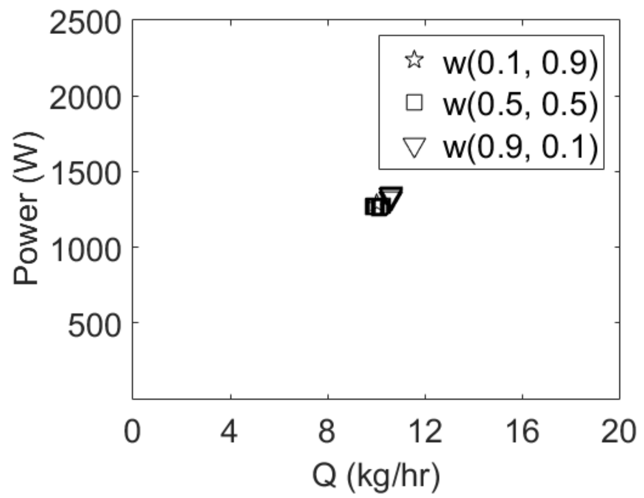

Figure 2 Case studies involving screw geometry.

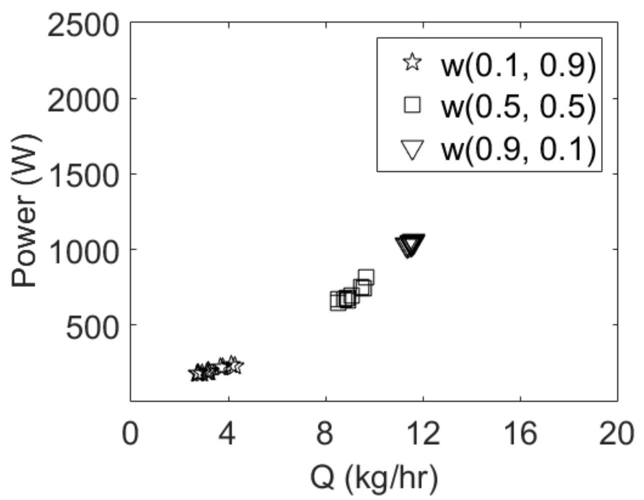

Figure 3 Case studies involving both operating conditions and screw geometry.

distributed along the Pareto optimal region. These results evidence response patterns that are useful to the process engineer. Mass output of robust solutions does not exceed 9 kg/hr, but most robust solutions are located in regions with high *Q*. In turn, this corresponds to power consumption. In such circumstances, the requirements in terms of robustness can

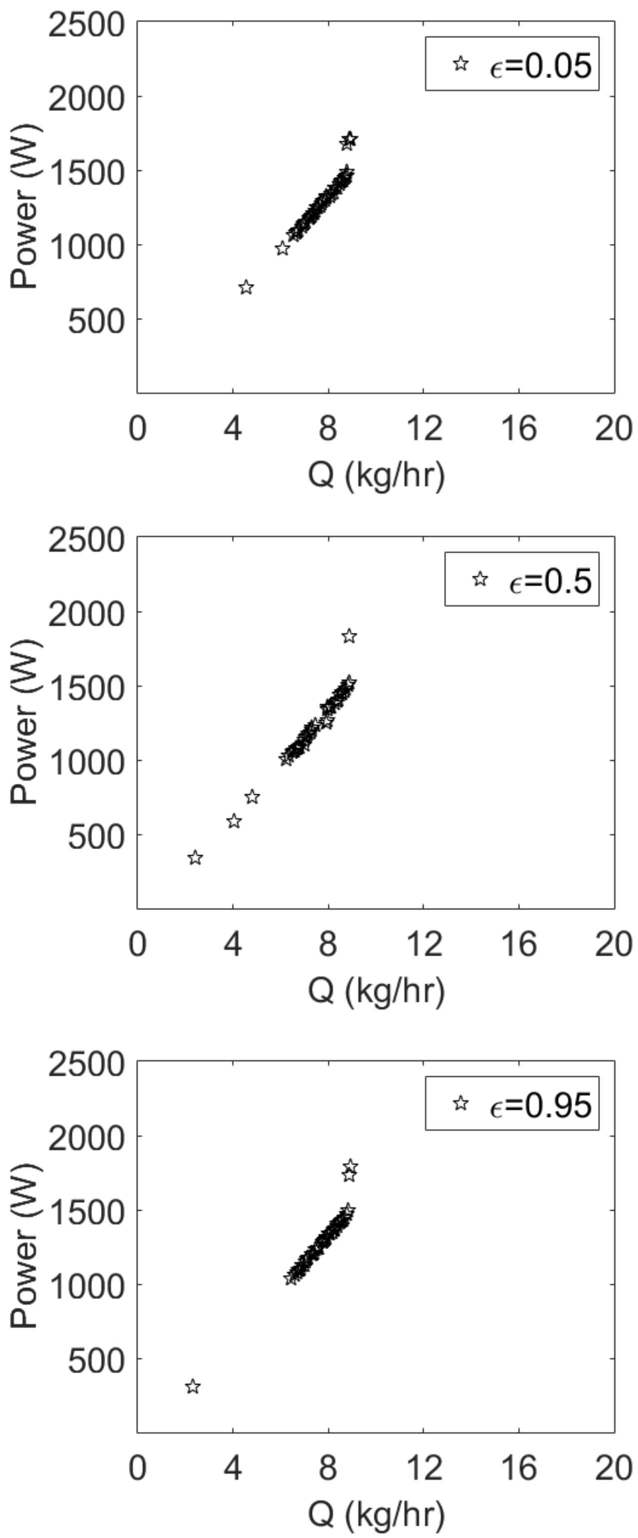

Figure 4 Robustness for case studies involving operating conditions.

be reduced, which can be readily achieved increasing ε. In principle, a higher grained resolution of a wider region of the Pareto front is accessed. Therefore, ε controls the extent of solutions depending on the degree of robustness. This can be particularly useful when the DM preferences are incomplete or lack precise, which is often the case.

It should be noted that the location of the Pareto front remained unchanged when comparing results obtained in the present and previous sections. What changed was the focus of the search, which was determined either by the importance of the objectives or the robustness of the solutions.

4.3 *Best solutions*

Considering the case studies dealing with operating conditions, Table 3 presents the values of the variables and of the objectives for the solutions having the best fitness values for different preferences and for robustness. In each case, various solutions meet the DM preferences in terms of the relative importance of the objectives, as opposed to the selection based on robustness, which results in a unique solution. This is because in a set of Pareto optimal solutions, there is a single best solution with respect to robustness, whilst various solutions are the best compromise for different set of weights. Moreover, the most robust solution is very similar to the one where output is most important (weights (0.9 0.1)).

Table 3 Solutions for case studies concerning operating conditions.

DM	Decision variables				Objectives	
	N	T_{b1}	T_{b2}	T_{b3}	Q	L_{melt}
(0.1 0.9)	21.1	209.6	167.2	203.5	3.2	0.1
(0.5 0.5)	48.2	209.2	182.0	209.3	7.0	0.3
(0.9 0.1)	59.9	170.0	168.0	208.9	8.8	0.6
Rob	57.2	154.2	208.5	194.8	8.5	0.5
	N	T_{b1}	T_{b2}	T_{b3}	Q	T_{melt}
(0.1 0.9)	16.2	161.5	155.2	150.2	2.3	154.6
(0.5 0.5)	56.1	175.7	150.5	150.1	7.8	164.1
(0.9 0.1)	59.9	150.8	158.5	209.8	8.9	202.9
Rob	59.9	152.5	156.2	150.6	8.5	166.0
	N	T_{b1}	T_{b2}	T_{b3}	Q	$Power$
(0.1 0.9)	10.5	168.5	201.9	201.0	1.8	243.3
(0.5 0.5)	39.5	198.1	208.9	206.4	6.1	949.7
(0.9 0.1)	59.7	162.7	178.0	209.8	8.8	1770.0
Rob	49.6	193.4	209.9	209.7	7.3	1182.3
	N	T_{b1}	T_{b2}	T_{b3}	Q	$WATS$
(0.1 0.9)	44.9	151.0	171.2	209.8	6.8	235.3
(0.5 0.5)	42.3	150.6	161.6	209.9	6.4	235.0
(0.9 0.1)	59.9	151.3	203.1	206.4	9.1	235.0
Rob	59.5	151.3	203.5	208.9	9.0	238.8

5 CONCLUSIONS

A design optimization approach was proposed for the optimization of plasticating single screw extrusion. The aim is to support the process engineer in the identification of the solutions with the most desirable characteristics. The proposed methodology couples a MOEA with decision maker preferences and robustness approaches. First, preference information was quantified by attributing weights expressing the relative importance of individual objectives. Secondly, the robustness of solutions upon small perturbations in the decision variables was taken into consideration. The DM can express his/her preferences by means of a dispersion parameter controlling the extent of the solution in terms robustness. The smaller the dispersion parameter, the more robust solutions are obtained.

Various case studies involving the definition of extrusion operating conditions, extruder screw design and the two together were tackled by the methodology proposed. The results obtained demonstrated that the outcome is greatly affected by the choice of the design variables, thus highlighting the importance of using effective tools to support technical decisions concerning extrusion. Simultaneously, the trade-offs between objectives provide scientific knowledge on major process responses and can also contribute to achieving higher extrusion performance.

ACKNOWLEDGMENTS

This work was supported by the Portuguese Fundação para a Ciência e Tecnologia under grant PEst-C/CTM/LA0025/2013 (Projecto Estratégico - LA 25 - 2013-2014 - Strategic Project - LA 25 - 2013-2014).

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