CHAPTER 8

THE USE OF EVOLUTIONARY ALGORITHMS TO SOLVE PRACTICAL PROBLEMS IN POLYMER EXTRUSION

António Gaspar-Cunha, José A. Covas

IPC - Institute for Polymers and Composites, Dept. of Polymer Engineering University of Minho, 4800-058 Guimarães, Portugal E-mail: gaspar,jcovas@dep.uminho.pt

This work aims at selecting the operating conditions and designing screws that optimize the performance of single-screw and co-rotating twin-screw extruders, which are machines widely used by the polymer processing industry. A special MOEA, denoted as Reduced Pareto Set Genetic Algorithm, RPSGAe, is presented and used to solve these multiobjective combinatorial problems. Twin screw design is formulated as a Travelling Salesman Problem, TSP, given its discrete nature. Various case studies are analyzed and their validity is discussed, thus demonstrating the potential practical usefulness of this approach.

1. Introduction

Polymer extrusion is a major plastics processing technology used for the manufacture of a wide range of plastics products (such as pipes and profiles, film, sheet, filaments, fibers, electrical wires and cables) and also for the production of raw materials $(e.g., \text{modified polymers, polymer blends, fiber/polymer matrix composites, biodegradable systems)^{1,2}$. The essential unit of an extrusion line is the extruder, which is composed of one (single screw extruder) or more screws (the most common being the co-rotating twin screw extruder) rotating at constant speed inside a heated barrel. Solid polymer (in pellets or powder form) is supplied to the screw channel either by gravity flow from a hopper or by a feeder set at a prescribed rate. The solid progresses along the screw and melts due to the combined effect of conducted and dissipated heat. This (highly viscous non-Newtonian) melt is subsequently homogenized (via both dispersive and distributive mixing), pressurized and forced to pass through the die, where it is shaped into the

 $\mathbf{2}$

A. Gaspar-Cunha, J.A. Covas

required cross-section, before being quenched¹⁻³. Mathematical modelling of the global process involves coupling a sequence of numerical routines, each valid for a process stage where specific physical/rheological phenomena develop (namely solids conveying, melting, melt conveying, dispersivedistributive mixing, devolatilization)¹⁻³. In other words, each zone is described by the relevant governing equations (mass conservation, momentum and energy), together with constitutive equations describing the rheological and thermal responses of the material, linked to the adjacent zones through the appropriate boundary conditions.

The relative simplicity of the screw extruder geometry masks the complexity of the flow developed. In practice, setting the operating conditions and/or designing screws for new applications are usually carried out by a trial-and-error procedure, where tentative extrusion experiments, or machining of screws, are performed until satisfactory results (*i.e.*, the desirable performance) are obtained. Since the above targets correspond to multiobjective problems, and given their typology, they can instead be solved adopting a scientific methodology based on Multi-Objective Evolutionary Algorithms (MOEA)^{4,5}. The present work focus on the application of this optimization methodology to single and twin-screw polymer extrusion. For this purpose, a special MOEA, denoted as Reduced Pareto Set Genetic Algorithm with elitism (RPSGAe), is proposed^{6,7}. This algorithm uses a clustering technique to reduce the number of solutions on the efficient frontier. Fitness is determined through a ranking function, the individuals being sorted using the same clustering technique.

Thus, section 2 presents the main functional process features and discusses the characteristics of the optimization problems. The RPSGAe is presented and described in detail in section 3, where a specific screw design methodology is also proposed. Evolutionary algorithms are then used in section 4 to set the operating conditions and to design screws for single and twin-screw extruders.

2. Polymer Extrusion

2.1. Single screw extrusion

A conventional plasticating single-screw extrusion unit uses an Archimedestype screw (with at least three distinct geometrical zones in terms of channel depth), rotating at constant speed, inside a heated barrel. As illustrated in Fig. 1.A, intensive experimental research demonstrated that the material deposited in the hopper passes through various sequential functional zones

The Use of EAs to Solve Practical Problems in Polymer Extrusion

which will induce a certain thermo-mechanical environment^{1,7}. Flow in the hopper is due to gravity, while that in the first screw turns results from friction dragging (solids conveying). Soon, a melt film will form near to the inner barrel wall (delay zone), followed by the creation and growth of a melt pool (melting zone). Eventually, all fluid elements will progress along the screw channel following an helicoidal path (melt conveying) and pressure flow will take place in the die.

Figure 2 shows the physical assumptions underlying the mathematical model of the global process. Calculations are performed in small screw channel increments, a detailed description being available elsewhere^{7–9}. For a given polymer / system geometry / operating conditions set, the program not only predicts the evolution of important process variables along the screw (as shown in Fig. 1.B for pressure and melting rate), but also yields the values of parameters which, altogether, describe the overall process performance (these include - see Fig. 1.C - mass output, mechanical power consumption, length of screw required for melting, melt temperature, degree of mixing - WATS and viscous dissipation, which is quantified by the ratio maximum temperature / barrel temperature)⁷.

The process is quite sensitive to changes in geometry and/or operating conditions. As can be observed in the example of Fig. 1.C, an increase in screw speed produces an increase in mass output, but at the cost of more power consumption, higher melt temperatures - due to viscous dissipation - and lower mixing quality. In fact, WATS generally decreases with increasing screw speed, as there is less channel length available for mixing (due to lower melting rates) and shorter residence times. Therefore, setting the operating conditions requires establishing a compromise between the relative satisfaction of the above parameters. The same reasoning could be applied to screw design.

2.2. Co-rotating twin-screw extrusion

The limitations of single screw extruders in terms of the interdependence between output, die resistance and mixing quality, as well as in the capability of producing effective random distributive and dispersive mixing stimulated the use of co-rotating twin-screw extruders for compounding operations^{1,2}. In these machines two parallel intermeshing screws rotate in the same direction, inside a cavity with a cross-section with a format-of-8. Since the screws are generally of modular construction, it is possible to build profiles where the location of melting, mixing intensity and average

3

A. Gaspar-Cunha, J.A. Covas



Fig. 1. Single-screw extruder: A) geometry; B) melt pressure and melting profiles; C) performance measures.

residence time can be estimated a priori. Also, the barrel can contain apertures for secondary feeding (e.g., additives, fillers), devolatilization (e.g., additit), devolatilization (e.g., additives, fille





Fig. 2. Physical models for single-screw extrusion.

removal of water vapor or of reaction volatiles), etc. In the case of the extruder of Fig. 3.A, the material is supplied at a prescribed rate, so that conveying sections are only partially fed. Melting will occur at the staggering kneading block upstream (by the combined effect of heat conducted and dissipated from the mechanical smearing of the solid pellets), while the third kneading block will provide the adequate seal for devolatilization.

Although these extruders have also attracted a significant amount of experimental and theoretical work in the last decades^{10–13}, the understanding of certain process stages, such as melting, is still far from complete^{14–16}. Consequently, for modelling purposes melting is often considered as instantaneous and taking place before the first restrictive element upstream. From the melting location to the die exit computations of melt flow are performed separately for each type of screw element (right-handed or left-handed screw elements, staggered kneading disks) - as illustrated in Fig. 4. This is also the concept of the LUDOVIC software¹⁷, whose predictions have been shown to be within 10% of the experimental values^{17,18}. As for single screw extrusion, for a given polymer / system geometry / operating conditions set, the software predicts the evolution along the screw of variables such as

livroCC

 $\mathbf{6}$

A. Gaspar-Cunha, J.A. Covas



Fig. 3. Twin-screw extruder: A) geometry; B) pressure and cumulative residence time; C) performance measures.

temperature, melt pressure, shear rate, viscosity, residence time, specific energy and filling ratio (Fig. 3.B) and the values of global performance parameters (*e.g.*, average residence time, average strain, mechanical power consumption, maximum melt temperature, outlet temperature, as in Fig. 3.C).

April 5, 2004

8:57

7

The Use of EAs to Solve Practical Problems in Polymer Extrusion

The response of these machines is also sensitive to the operating conditions, in this case output, screw rotation speed and temperature. The effect of output is illustrated in Fig. 3. Output influences mainly the number of fully filled channels, hence mechanical power consumption, average residence time and strain. However, the level of shear stresses at kneading disks remains the same, hence the maximum temperatures attained are not affected.



Fig. 4. Physical models for co-rotating twin-screw extrusion.

2.3. Optimization characteristics

As discussed above, for each application the performance of single and twin screw extruders is determined by the operating conditions and machine geometry. The former include screw speed (N) and barrel temperature profiles (T_{bi}) , and mass output (Q) in the case of twin-screw extruders. As illustrated in Fig. 5, which identifies the parameters to be optimized for each type of machine, N, T_{bi} , and Q can vary continuously within a prescribed range, which is dictated by the characteristics of the motor and the thermal stability of the polymer. In the case of the twin-screw machine N and Q

A. Gaspar-Cunha, J.A. Covas

are not independent, since for each N there is a maximum attainable Q (as the screws become fully filled along their axis). This limit is detected by the LUDOVIC¹⁷, which does not converge if the two values are incompatible.

The geometric parameters of single-screw extruders can also vary continuously within a preset interval. As shown in Fig. 5, if one is aiming at designing a new screw for an existing extruder, then consideration should be given to the definition of the screw length of the feed (L_1) and compression (L_2) zones, their corresponding internal diameters $(D_1 \text{ and } D_3,$ respectively), the flight thickness (e) and the screw pitch (P). The variation intervals are defined by a number of reasons, such as excessive mechanical work on the polymer (maximum D_1/D_3 ratio), mechanical resistance of the screw (minimum D_1), polymer conveying characteristics (minimum L_1).

Conversely, screws for twin screw extruders are built by selecting the required number of elements from a set of available geometries and then defining their relative position. As Fig. 5 shows, if a screw is made of 14 elements and the aim is to define the relative position of 10 (of which 5 are transport elements, 4 are kneading blocks and 1 is a reverse element), there are 10! possible combinations, *i.e.*, a complex discrete combinatorial problem must be solved. Although less common, one could also envisage to optimize the geometry of individual elements, which would entail the continuous variation of parameters within a prescribed interval.

Despite the obvious practical importance of the topic, there is limited experience on the use of an optimization approach to define the operating conditions or to design screws for polymer extrusion. Most effort has been concentrated on single screw extrusion^{19,20}, although Potente *et al.*²¹ has recently suggested the use of a quality function to optimize the geometry of specific screw elements for twin screw extruders.

3. Optimization algorithm

3.1. Multi-objective optimization

As most real-world optimization problems, optimization of polymer extrusion is multi-objective. This can be dealt with in two ways, depending on the moment when the decision about the relative importance of the various criteria is to be taken. If it is feasible to establish that importance before the search takes place, then the various individual objectives can be congregated into a unique function, yielding a single objective optimization problem. However, if the relative weight of each criterion is changed, a new optimization run needs to be carried out.



livroCC



Fig. 5. Parameters to be optimized.

When the relative value of the criteria is not known a *priori*, it is possible to take advantage of the fact that Genetic Algorithms work with a population of points to optimize all criteria simultaneously. This is performed with a Multi-Objective Evolutionary Algorithm (MOEA). The result will be a

A. Gaspar-Cunha, J.A. Covas

set of non-dominated vectors, denoted as Pareto-optimal solutions, evidencing the trade-off between the criteria and the parameters to be optimized. Thus, the decision maker can choose a solution resulting from a specific compromise between the relative satisfaction of the individual criteria.

3.2. Reduced Pareto Set Genetic Algorithm with Elitism (RPSGAe)

In MOEAs the selection phase of a traditional Evolutionary Algorithm is replaced by a routine able to deal with multiple objectives. Usually, this is made applying the fitness assignment, density estimation and archiving operators, various methods being available for this $purpose^{4,5}$. In this work, the Reduced Pareto Set Genetic Algorithm with Elitism (RPSGAe)⁶ is adopted, which involves the application of a clustering technique to reduce the number of solutions on the efficient frontier, while maintaining intact its characteristics. The clustering technique, proposed by Roseman and Gero²² and known as complete-linkage method, compares the proximity of solutions on the hyper-space using a measure of the distance between them. Solutions closer to a pre-defined distance are aggregated. Fitness is determined through a ranking function, the individuals being sorted with the same clustering technique. In order to incorporate these techniques in the EA, Algorithm 1 was developed. The RPSGAe follows the steps of a traditional EA, except it defines an external (elitist) population and uses a specific fitness evaluation. It starts with the random definition of an internal population of size N and with the creation of an empty external population. At each generation, the following operations are carried out:

- The internal population is evaluated using the modelling package;
- Fitness is calculated using the clustering technique (see Algorithm 2 below⁶);
- A fixed number of best individuals are copied to the external population until this becomes full;
- Algorithm 2 is applied again, to sort the individuals of the external population;
- A pre-defined number of the best individuals is incorporated in the internal population, by replacing the lowest fitness individuals;
- Reproduction, crossover and mutation operators are applied.

Algorithm 2 starts with the definition of the number of ranks, N_{Ranks} , and the rank of each individual, Rank[i], is set to 0. For each rank, r,

The Use of EAs to Solve Practical Problems in Polymer Extrusion

Algorithm 1 (RPSGAe):

Random initial population (internal) Empty external population while not Stop-Condition do

> Evaluate internal population Calculate the Fitness of all the individuals using *Algorithm 2* Copy the best individuals to the external population **if** the external population becomes full

Apply Algorithm 2 to this population Copy the best individuals to the internal population

end if Select the individuals for reproduction

Crossover

Mutation

end while

the population is reduced to NR individuals (where NR is the number of individuals of each rank), using the clustering technique. Then, rank r is attributed to these NR individuals. The algorithm ends when the number of pre-defined ranks is reached. Finally, the fitness of individual i (F_i) is calculated using the following linear ranking function:

$$F_i = 2 - SP + \frac{2\left(SP - 1\right)\left(N_{Ranks} + 1 - Rank\left[i\right]\right)}{N_{Ranks}} \tag{1}$$

where SP is the selection pressure $(1 < SP \le 2)$. Detailed information on these algorithms can be found elsewhere^{6,7}.

3.3. Travelling Salesman Problem

The above RPSGAe can be easily adapted to the various extrusion optimization problems involving continuous variables, *i.e.*, setting the operating conditions for both single and twin-screw extruders and designing screws for single-screw extruders. When the aim is to optimize the screw configuration of twin-screw extruders, a discrete combinatorial problem must be solved (Twin-Screw Configuration Problem, TSCP). However, TSCP can be formulated as a Travelling Salesman Problem (TSP), as illustrated in Fig. 6. In the TSP the salesman needs to visit n cities, the aim being to se-

livroCC

A. Gaspar-Cunha, J.A. Covas

Algorithm 2 (Clustering):

Definition of N_{Ranks} Rank[i]=0 r = 1 **do** $NR = r(N/N_{Ranks})$ Reduce the population down to NR individuals r = r + 1 **while** $(r < N_{Ranks})$ Calculate fitness **End**

lect the visiting sequence that minimizes the distance travelled and/or the total cost (two alternative routes are suggested). In the TSCP the polymer is the Travelling Salesman and the screw elements are the cities. In this case, the polymer must flow through the different elements, whose location in the screw has to be determined in order to maximize the global process performance.



Fig. 6. Twin-screw configuration problem (TSCP) formulated as a TSP.

Formulating TSCP as a TSP yields the possibility of using the vast number of algorithms available to solve the latter. In fact, single objective TSPs have been solved using $EAs^{23,24}$ but, apparently, only Zhenyu²⁵ approached multi-objective TSPs. The difficulty of using MOEA arises from

April 5, 2004

8:57

The Use of EAs to Solve Practical Problems in Polymer Extrusion 13

the fact that the traditional crossover and mutation operators are not sufficiently capable of granting a positive and rapid evolution of the population along the various generations²⁶. Thus, a specific TSP reproduction operator, incorporating crossover and mutation, and able to make full use of the heuristic information contained in the population, the inver-over, has been suggested. It has been shown to out-perform other evolutionary operators in the resolution of single objective TSPs²⁶.

Consequently, a MOEA for solving multi-objective TSP (or, equivalently, TSCP) was developed (Algorithm 3). It starts with the random generation of the N individuals of the internal population and an empty external population of size 2 * N. After evaluating the former using the LUDOVIC routine, the following actions are taken for each generation:

- The individuals are ranked using Algorithm 2;
- The entire internal population is copied to the elitist population;
- The inver-over operator is applied in order to generate the remaining N individuals of the elitist population;
- The new individuals are evaluated;
- The non-domination test and Algorithm 2 are applied to the elitist population to rank its 2N individuals;
- The best N individuals of the elitist population are copied to the main population.

The algorithm is concluded when the number of generations is reached. The solutions are the non-dominated individuals of the last internal population.

4. Results and discussion

The optimization algorithms discussed in the previous section will now be used to solve the situations depicted in Fig. 5. Single and twin screw extrusion will be studied separately and, for each, the operating conditions and the screw geometry will be optimized.

4.1. Single screw extrusion

Operating conditions

The aim is to determine the operating conditions, *i.e.*, screw speed (N) and barrel temperature profile $(T_1, T_2 \text{ and } T_3)$, which may vary continuously within the range defined between square brackets in Fig. 5, that will maximize the performance described by the six criteria presented in Table

A. Gaspar-Cunha, J.A. Covas

Algorithm 3 (MOEA for TSP):

Random initial population (internal) Empty external population Evaluate internal population while not Stop-Condition do

> Calculate the Fitness of all the individuals using Algorithm 2 Copy the N individuals to the external population Apply the inver-over operator to generate new N individuals Evaluate the new N individuals Apply Algorithm 2 to the external population Copy the best N individuals to the internal population

end while

1. Thus, the global objective is to maximize mass output and degree of mixing (WATS), while minimizing the length of screw required for melting, melt temperature, power consumption and viscous dissipation, which is obviously conflicting. The prescribed range of variation of each criterion is also stated in Table 1. The polymer properties (a commercial high density polyethylene extrusion grade) and the extruder geometry (a Leistritz LSM 36, a laboratorial machine) are known⁷. The following GA parameters were used: 50 generations, crossover rate of 0.8, mutation rate of 0.05, internal and external populations having 100 individuals, limit of the clustering algorithm set at 0.2 and N_{Ranks} equal to 30.

Criteria	Aim	Range of variation
C1 - Output (kg/hr) C2 - Length of screw required for melting (m) C3 - Melt temperature (°C) C4 - Power consumption (W) C5 - WATS	Maximize Minimize Minimize Maximize	$ \begin{array}{r} 1 - 20 \\ 0.2 - 0.9 \\ 150 - 210 \\ 0 - 9200 \\ 0 - 1300 \\ \end{array} $

Table 1. Criteria for optimizing single screw operating conditions and corresponding range of variation.

Figure 7 shows some of the optimal Pareto plots obtained for the simultaneous optimization of all the six criteria, both in the criteria's (Fig.

The Use of EAs to Solve Practical Problems in Polymer Extrusion 15

7.A) and parameters to optimize domain (Fig. 7.B). As expected, in this six-dimensional space distinction between dominated and non-dominated solutions is difficult, since points that appear to be dominated in one Pareto frontier are probably non-dominated in another, i.e., selecting a solution is not easy. One alternative consists in quantifying the relative importance of the criteria using a conventional quality function, such as the weighted sum, applied to the final population:

$$F_i = \sum_{j=1}^q w_j f_j \tag{2}$$

Here, F_i is the fitness of individual i, q is the number of criteria, f_j is the objective function of criterion j and w_j is the corresponding weight $(0 \le w_j \le 1)$. The decision maker defines the weight of each criterion and applies this function to the non-dominated solutions, thus finding the best result. Using output (C1 in Table 1) as a basis of comparison, Table 2 shows the operating conditions proposed when its weight (w_1) varies between 0.1 and 0.5. As output becomes more relevant to the global performance, N increases due to their direct relationship. However, as illustrated in Fig. 1, the remaining criteria will be progressively less assured. The results of this methodology have been validated experimentally⁷.

W	/eights	Operatio	ng Conditions
w_1	w_2 to w_5	$N \ (\mathrm{rpm})$	$T_1/T_2/T_3$ (°C)
0.1	0.9/4	13.1	207/155/150
0.2	0.8/4	23.0	185/183/153
0.3	0.7/4	23.0	185/183/153
0.4	0.6/4	48.5	161/199/195
0.5	0.5/4	48.5	161/199/195

 Table 2.
 Best operating conditions for single-screw extrusion.

Screw design

As identified in Fig. 5, the aim is to define the values of L_1 , L_2 , D_1 , D_3 , P and e that, for the same polymer and for fixed operating conditions (N = 50rpm and $T_i = 170$ °C), will again optimize the criteria identified in Table 1. Since this involves, as above, a six-dimensional space in the criteria's or in the parameters to optimize domains, following the same procedure yields the results shown in Table 3. As illustrated in Fig. 8, two quite different

livroCC





Fig. 7. Optimal Pareto plots: A) Criteria's domain; B) Parameters to optimize domain.

screw profiles are proposed (see Fig. 8), one when output is not relevant, the other when it is at least as important as the remaining criteria. The former has a high D_3/D_1 ratio and a shallow pumping section (L_3) , favoring melting and mixing, but opposing high throughputs. Conversely, the second screw profile possesses a higher channel cross-section, inducing higher flows.

Veights	Screw geometry (mm)						
w_2 to w_5	L_1	L_2	D_1	D_3	P	e	
0.9/4	6.3D	8.4D	22.6	31.9	38.9	3.2	
0.8/4	$7.5\mathrm{D}$	7.1D	25.1	26.9	36.2	3.7	
0.7/4	$7.5\mathrm{D}$	7.1D	25.1	26.9	36.2	3.7	
0.6/4	$7.5\mathrm{D}$	7.1D	25.1	26.9	36.2	3.7	
0.5/4	$7.5\mathrm{D}$	7.1D	25.1	26.9	36.2	3.7	
	w2 to w_5 0.9/4 0.8/4 0.7/4 0.6/4 0.5/4	Weights L_1 w_2 to w_5 L_1 $0.9/4$ $6.3D$ $0.8/4$ $7.5D$ $0.7/4$ $7.5D$ $0.6/4$ $7.5D$ $0.5/4$ $7.5D$	Veights Screw w_2 to w_5 L_1 L_2 $0.9/4$ $6.3D$ $8.4D$ $0.8/4$ $7.5D$ $7.1D$ $0.7/4$ $7.5D$ $7.1D$ $0.6/4$ $7.5D$ $7.1D$ $0.6/4$ $7.5D$ $7.1D$ $0.5/4$ $7.5D$ $7.1D$	Veights Screw geometry w_2 to w_5 L_1 L_2 D_1 $0.9/4$ $6.3D$ $8.4D$ 22.6 $0.8/4$ $7.5D$ $7.1D$ 25.1 $0.7/4$ $7.5D$ $7.1D$ 25.1 $0.6/4$ $7.5D$ $7.1D$ 25.1 $0.5/4$ $7.5D$ $7.1D$ 25.1	Veights Screw geometry (m w_2 to w_5 L_1 L_2 D_1 D_3 0.9/4 6.3D 8.4D 22.6 31.9 0.8/4 7.5D 7.1D 25.1 26.9 0.7/4 7.5D 7.1D 25.1 26.9 0.6/4 7.5D 7.1D 25.1 26.9 0.5/4 7.5D 7.1D 25.1 26.9	Veights Screw geometry (mm) w_2 to w_5 L_1 L_2 D_1 D_3 P $0.9/4$ $6.3D$ $8.4D$ 22.6 31.9 38.9 $0.8/4$ $7.5D$ $7.1D$ 25.1 26.9 36.2 $0.7/4$ $7.5D$ $7.1D$ 25.1 26.9 36.2 $0.6/4$ $7.5D$ $7.1D$ 25.1 26.9 36.2 $0.5/4$ $7.5D$ $7.1D$ 25.1 26.9 36.2	

Table 3. Best screw geometries for single-screw extrusion.

In industrial practice screws must be flexible, *i.e.*, they must exhibit good performance for a range of materials and operating conditions. This

April 5, 2004

8:57





Fig. 8. Best screw profiles: A) $w_1=0.1$; B) $(0.2 \le w_1 \le 0.5 \text{ (see Table 3)})$.

requirement may be included in the design routine by studying the sensitivity of designs proposed by the optimization algorithm to limited changes in relevant parameters, such as polymer rheology, operating conditions and even the relative importance of the weights⁹. More specifically, assuming w_i = 0.2, the five best screws proposed by the optimization algorithm are those of Table 4. When these are subjected to a sensitivity analysis, the data of Fig. 9 is obtained, where the black bars represent the average global performance, and the white bars the respective standard deviation. Thus, screw 1 can be chosen if global performance is of paramount importance; or screw 2 may be selected when process stability has priority.

Table 4. Best screws considered for a sensitivity analysis $(w_i=0.2)$.

	L_1	L_2	L_3	$D_1 \ (\mathrm{mm})$	$D_3 \ (\mathrm{mm})$
Screw 1	7.5D	7.1D	11.4D	26.9	36.2
Screw 2	6.3D	8.4D	11.3D	31.9	38.9
Screw 3	6.3D	8.4D	11.3D	31.9	39.4
Screw 4	6.3D	8.4D	11.4D	31.8	40.6
Screw 5	5.9D	8.4D	11.6D	30.8	32.3

4.2. Twin-screw extrusion

Operating conditions

livroCC

18

A. Gaspar-Cunha, J.A. Covas



Fig. 9. Global sensitivity to small changes in operating conditions, rheological properties and criteria importance of the 5 best screws of table 4.

As shown in Fig. 5, this problem involves determining screw speed (N), barrel temperature profile $(T_1, T_2 \text{ and } T_3)$ and flow rate (Q). The detailed screw geometry is given in Table 5, while Table 6 presents the criteria and their corresponding aim and range of variation. Since Q is imposed by a volumetric/gravimetric feeder but, simultaneously, it is convenient to maximize it, it is taken both as parameter and optimization criterion. The RPS-GAe was applied using the following parameters: 50 generations, crossover rate of 0.8, mutation rate of 0.05, internal and external populations with 100 individuals, limits of the clustering algorithm set at 0.2 and $N_{Ranks} =$ 30.

Table 5. Screw configuration: L - Length (mm); P - Pitch (mm).

	1	2	3	4	5	6	7	8	9	10	11	12	13
 L	97.5	150	60	60	30	120	45	60	60	37.5	120	90	30
Ρ	45	30	20	KB90	-30	30	KB-60	45	30	KB-30	60	30	20

Figure 10 shows the Pareto frontiers in the criteria's domain, plotted against output, while Table 7 presents the results obtained when the set of weights of Table 2 is used upon application of equation (1). As the importance of Q increases, the best solutions (represented in Fig. 10 from 1 to 5) change radically. Therefore, the decision depends entirely on the (somewhat subjective) definition on the relative importance of the criteria.

The Use of EAs to Solve Practical Problems in Polymer Extrusion

Table 6. Criteria for optimizing twin-screw operating conditions and corresponding range of variation.

Criteria	Aim	Range o	of variation
C1 - Output (kg/hr)	Maximize	3	20
C2 - Average strain	Maximize	1000	15000
C3 - Melt temp. at die exit (°C)	Stay within range	180-210	220-240
C4 - Power consumption (W)	Minimize	0	9200
C5 - Average residence time (s)	Minimize	10	300



Fig. 10. Pareto frontiers on the criterias domain after the optimization of the operating conditions.

Screw configuration

Finally, Algorithm 3 will be used to optimize screw configuration, *i.e.*, to define the best location of 10 screw elements (comprising 5 transport elements, 4 kneading blocks and 1 reverse element), as illustrated in Fig. 5. Two criteria, melt temperature and mechanical power consumption - which are particularly dependent on screw geometry - should be minimized. Output, screw speed and barrel temperature are kept constant at 10 kg/hr, 100 rpm and 200 °C, respectively. The same genetic parameters were used, with the exception of the population size (200 external and 100 internal

8:57

April 5, 2004

A. Gaspar-Cunha, J.A. Covas

W	/eights	Operating Conditions					
w_1	w_2 to w_5	$N \ (\mathrm{rpm})$	$Q^* \; (\mathrm{kg/hr})$	T_1 (°C)	$T_2 (^{\circ}\mathrm{C})$	$T_3 (^{\circ}C)$	
0.1	0.9/4	184	3	200	167	194	
0.2	0.8/4	184	3	200	167	194	
0.3	0.7/4	193	25	205	172	205	
0.4	0.6/4	193	25	205	172	205	
0.5	0.5/4	193	25	205	172	205	
0.6	0.4/4	193	25	205	172	205	

Table 7. Best operating conditions for twin-screw extrusion.

individuals).

Figure 11 (top) shows the Pareto-curves in the criteria's domain for the initial and final populations. The improvement provided by MOEA is relevant. Since the two criteria are conflicting, solutions 1, 2 and 3, corresponding to relative degrees of satisfaction of each criterion, are considered, the corresponding screw profiles being represented in Fig. 11 (bottom). Screw 1 produces the highest power consumption, but the lowest outlet temperature. The kneading and reverse elements are located more upstream, therefore this screw is less restrictive downstream. Thus, the polymer melts earlier (increasing energy consumption, as melt flow requires more power than solids flow) and the melt has time to recover from the early viscous dissipation (low melt temperature). The profile - and thus the behavior of screw 3 is the opposite, while screw 3 exhibits a geometry that is a compromise between the other two, although more similar to that of screw 1. These results are in general agreement with practical experience, although a formal experimental validation needs to be carried out.

5. Conclusions

An elitist multi-objective genetic algorithm, denoted as RPSGAe, was used to select the operating conditions and to design screws that optimize the performance of single-screw and co-rotating twin-screw extrusion, which are important industrial processing technologies. These correspond to complex multi-objective, combinatorial, not always continuous problems. The examples studied demonstrated that MOEA is sensitive to the type and relative importance of the individual criteria, that the method proposed yields solutions with physical meaning and that it is possible to incorporate important empirical knowledge through constraints/prescribed variation range of both criteria and process parameters.





Fig. 11. Twin-screw configuration results: Top - Pareto curve; Bottom - optimal screws.

Acknowledgments

This work was supported by the Portuguese Fundação para a Ciência e Tecnologia under grant POCTI/34569/CTM/2000.

References

- 1. C. Rauwendaal, Polymer Extrusion (Hanser Publishers, Munich 1986).
- J.F. Agassant, P. Avenas and J. Sergent, La Mise en Forme des Matires Plastiques (Lavoisier, 3rd edition, Paris, 1996).
- 3. Z. Tadmor and I. Klein, *Engineering Principles of Plasticating Extrusion* (Van Nostrand Reinhold, Ney York, 1970).
- 4. C.A. Coello Coello, D.A. Van Veldhuizen and G.B Lamont, *Evolutionary* Algorithms for Solving Multi-Objective Problems (Kluwer, 2002).
- 5. K. Deb, Multi-Objective Optimization using Evolutionary Algorithms (Wiley, 2001).
- 6. A. Gaspar-Cunha and J.A. Covas, *RPSGAe A Multiobjective Genetic Algorithm with Elitism: Application to Polymer Extrusion*, in *Metaheuristics*

A. Gaspar-Cunha, J.A. Covas

for Multiobjective Optimisation, Lecture Notes in Economics and Mathematical Systems, Eds. X. Gandibleux, M. Sevaux, K. Sörensen, V. T'kindt (Springer, 2004).

- 7. A. Gaspar-Cunha, *Modelling and Optimisation of Single Screw Extrusion* (Ph. D. Thesis, University of Minho, Braga, 2000).
- J.A. Covas, A. Gaspar-Cunha and P. Oliveira, An Optimization Approach to Practical Problems in Plasticating Single Screw Extrusion, Polym. Eng. and Sci. 39, 3, p. 443 (1999).
- A. Gaspar-Cunha and J.A. Covas, The Design of Extrusion Screws: An Optimisation Approach, Intern. Polym. Process. 16, p. 229 (2001).
- J.L. White, Twin Screw Extrusion; Technology and Principles (Hanser, Munich, 1990).
- 11. J.L. White, A.Y. Coran and A. Moet, *Polymer Mixing; Technology and Engineering* (Hanser, Munich, 2001).
- H. Potente, J. Ansahl and R. Wittemeier, *Throughput characteristics of Tightly Intermeshing Co-rotating Twin Screw Extruders*, Intern. Polym. Proc. 5, p. 208 (1990).
- H. Potente, J. Ansahl and B. Klarholtz, *Design of Tightly Intermesing Co-*Rotating Twin Screw Extruders, Intern. Polym. Proc. 9, p. 11 (1994).
- B. Vergnes, G. Souveton, M.L. Delacour and A. Ainser, Experimental and Theorectical Study of Polymer Melting in a Co-rotating Twin Screw Extruder, Intern. Polym. Proc. 16, p. 351 (2001).
- H. Potente and U. Melish, A Physico-Mathematical Model for Solids Conveying in Co-rotating Twin Screw Extruders, Intern. Polym. Proc. 11, p. 101 (1996).
- S. Bawiskar and J.L. White, A Composite Model for Solid Conveying, Melting, Pressure and Fill Factor Profiles in Modular Co-Rotating Twin Screw Extruders, Intern. Polym. Proc. 12, p. 331 (1997).
- B. Vergnes, G. Della Valle and L. Delamare, A Global Computer Software for Polymer Flows in Corotating Twin Screw Extruders, Polym. Eng. Sci. 38, p. 1781 (1998).
- O.S. Carneiro, J.A. Covas and B. Vergnes, *Experimental and Theorectical Study of Twin-Screw Extrusion of Polypropylene*, J. Appl. Polym. Sci. 78, p. 1419 (2000).
- F. Fassihi-Tash and N. Sherkat, In-exact Decision Support for the Design of Plasticating Extruder Screws, Proceedings of Polymat'94, p. 434 (1994).
- 20. C.A. Thibodeau and P.G. Lafleur, *Computer Design and Screw Optimization*, Proceedings of the PPS Annual Meeting, Shangai, China, p. 15 (2000).
- H. Potente, A. Mller and K. Kretschmer, Development and Verification of a Method to Optimize Individual Screw Elements for Co-rotating Twin Screw Extruders, Proceeding of ANTEC2003 conference, USA (2003).
- M.A. Roseman and J.S. Gero, *Reducing the Pareto Optimal Set in Multi*criteria Optimization, Eng. Optim. 8, p. 189 (1985).
- Y. Nagata and S. Kobayashi, Edge Assembly Crossover: A High-power GA for the TSP, Seventh Int. Conf. on Genetic Algorithms, Michigan, USA, p. 450 (1997).

The Use of EAs to Solve Practical Problems in Polymer Extrusion

- 24. C.L. Valenzuela and L.P. Williams, *Improving Simple Heuristic Algorithms for the TSP using a GA*, Seventh Int. Conf. on Genetic Algorithms, Michigan, USA, p. 458 (1997).
- Y. Zhenyu, L. Zhang, K. Lishan and L. Guangming, A New MOEA for Multi-objective TSP and Its Convergence Property Analysis, Proceedings of the Second Int. Conf. On Evol. Multi-Objective Optimization (EMO'2003), Faro, Portugal, p. 342 (2003).
- 26. G. Tao and Z. Michalewicz, *Inver-over Operator for the TSP*, Proceedings of the 5th Parallel Problem Solving from Nature, Amsterdam, p. 803 (1998).