Use of Multi-Objective Evolutionary Algorithms in Extrusion Scale-up

José António Covas[1] and António Gaspar-Cunha[1]

[1] IPC- Institute for Polymers and Composites / I3N,
University of Minho, Campus de Azurém
4800-058 Guimarães, Portugal
{jcovas, agc}@dep.uminho.pt

Abstract. Extrusion scale-up consists in ensuring identical thermo-mechanical environments in machines of different dimensions, but processing the same material. Given a reference extruder with a certain geometry and operating point, the aim is to define the geometry and operating conditions of a target extruder (of a different magnitude), in order to subject the material being processed to the same flow and heat transfer conditions, thus yielding products with the same characteristics. Scale-up is widely used in industry and academia, for example to extrapolate the results obtained from studies performed in laboratorial machines to the production plant. Since existing scale-up rules are very crude, as they consider a single performance measure and produce unsatisfactory results, this work approaches scale-up as a multi-criteria optimization problem, which seeks to define the geometry/operating conditions of the target extruder that minimize the differences between the values of the criteria for the reference and target extruders. Some case studies are discussed in order to validate the concept.

Keywords: Multi-Objective Evolutionary Algorithms, Extrusion, Scale-Up.

1 Introduction

Scale-up is very often the action of defining the geometry and operating conditions of a machine that reproduce the working conditions of another of the same type and of different size, but processing the same material. This is a procedure of great practical importance. For example, in the case of polymer extrusion, scale-up rules are used to design large extruders using the results of studies performed on laboratory-scale machines. Extrapolating know-how instead of performing research on large-output machines allows for significant time savings [1-3].

Scale-up rules were proposed over several decades by different researchers, namely Carley and McKelvey (1953), Maddock (1959), Pearson (1976), Yi and Fenner (1976), Schenkel (1978), Chung (1984) and Rauwendaal (1986) [1-3]. These studies used analytical process descriptions to correlate large and small primary scaling variables (diameter, channel depth, screw length and screw speed) simply in terms of an exponent of their diameter ratio. However, since plasticating extrusion is a complex process involving solids conveying, melting of these solids and melt conveying, as well as other related phenomena such as mixing, such correlations only hold when a single process criterion is kept constant, e.g. constant melt flow shear rate, or constant melting rate. This was recognized in the reviews prepared by Rauwendaal (1987) and Potente (1991) [2, 3], who anticipated unbalanced solids and melt conveying rates when applying most of the rules available.

A more performing scaling-up methodology is therefore needed. It is important to consider simultaneously several process criteria and, since they are often conflicting, to know the degree of satisfaction eventually attained. Flexibility in terms of the criteria selected is also important, in contrast with the available methods that provide relations for specific performance measures. Thus, it makes sense to consider extrusion scale-up as a multi-objective optimization problem, where the purpose is to define the geometry/operating conditions of the target extruder that minimize the differences between the values of the criteria for the reference and target extruders. This work applies a Multi-Objective Evolutionary Algorithm (MOEA) methodology, previously developed by the authors, to perform that task. Rather than selecting the best optimization method, the aim here is to characterize the problem and ascertain the level of success of the solutions proposed.

The text is organized as follows. In section 2 we present the optimization methodology (which uses a MOEA) and the process modelling routine, both developed by the authors. Section 3 discusses one scale-up example, which is presented and solved. Finally, section 4 proposes some conclusions.

2 Multi-Objective Scale-Up

2.1 Optimization Methodology

As stated above, extrusion scale-up consists in extrapolating the behaviour of a reference extruder to another of the same type, but of different size (denoted as target extruder). Thus, we know the geometry and processing conditions of the reference extruder and wish to define either the operating conditions (if the machine exists), or the geometry and operating conditions (if it is to be built/purchased) of the target extruder, in such a way that the major performance measures of both machines are as similar as possible. This is seen here as an optimization problem where we seek to determine the geometry/operating conditions of the target extruder that minimize the differences in performance in relation to the reference extruder.

The multi-objective scale-up optimization methodology proposed includes the following steps:

1- Use the process flow modelling routine to predict the responses of the reference extruder under a specific set of operating conditions and polymer system;

2- Analyse the results and define the most important parameters to be used for scale-up;
3- Organize known information on target extruder (geometry: screw external diameter and length/diameter ratio; operating range: screw speed, set temperatures);
4- Perform scale-up via minimization of the differences in performance between the two extruders (optimization criteria).

The method requires three basic routines: a modelling package, a multi-objective optimization algorithm and a criteria quantification routine (see Figure 1). The algorithm defines automatically the (increasingly more performing) solutions to be used by the modelling routine. The parameter values obtained from the latter serve as input data to the criteria quantification routine, which compares them with the equivalent ones for the reference extruder. This information is supplied to the optimization routine, which defines new improved solutions to be evaluated, the process being repeated until a stop criterion is reached.

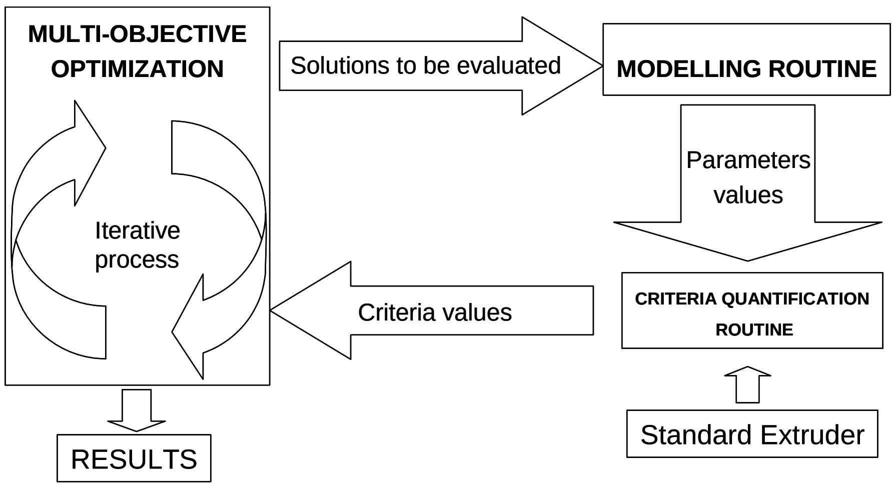

Fig. 1. Scale-up optimization methodology.

2.2 Multi-Objective Evolutionary Algorithms

During the last decade Multi-Objective Evolutionary Algorithms (MOEA) have been recognized as a powerful tool to explore and find out approximations to Pareto-optimal fronts in optimization problems [4, 5]. This is essentially due to their capacity to explore and combine various solutions to find the Pareto front in a single run and the evident difficulty of the traditional exact methods to solve this type of problems.

In a multi-objective algorithm the solution space is seen as sets of dominated and non-dominated points. These are solutions at least as good as the remaining with respect to all objectives, but strictly better with respect to at least one objective, *i.e.*, one solution point dominates another when it is equally good in every objective and formally better in at least one objective [4]. Since in MOEA the various criteria (or objectives) are optimized simultaneously, each individual solution belonging to the Pareto set establishes a compromise between all criteria. An efficient MOEA must distribute homogeneously the population along the Pareto frontier and improve the solutions along successive generations.

In this work, the Reduced Pareto Set Genetic Algorithm with elitism (RPSGAe) is adopted [6,7]. Initially, RPSGAe sorts the population individuals in a number of pre-defined ranks using a clustering technique, in order to decrease the number of solutions on the efficient frontier, while maintaining its characteristics intact. Then, the individuals' fitness is calculated through a ranking function. To incorporate this technique, the algorithm follows the steps of a traditional GA, except that it takes on an external (elitist) population and a specific fitness evaluation. Initially, the internal population is randomly defined and an empty external population is formed. At each generation, a fixed number of the best individuals, obtained by reducing the internal population with the clustering algorithm [6], is copied to the external population. This process is repeated until the number of individuals of the external population is complete. Then, the clustering technique is applied to sort the individuals of the external population, and a pre-defined number of the best ones is incorporated in the internal population, replacing the less fit individuals. Detailed information on this algorithm can be found elsewhere [6, 7].

2.3 Single Screw Extrusion Modelling Routine

Extrusion is a process whereby a molten polymer is forced to flow continuously through a die of a given shape, thus yielding a product with a constant cross-section (Figure 2). Despite the apparent simplicity of both machine and procedure, some basic functions must be accomplished if the product is to exhibit good performance. Process continuity is ensured by using an Archimedes-type screw, rotating inside the heated barrel at constant speed. Some screw geometric features and proper selection of barrel temperatures determine the most appropriate sequence of solid polymer conveying in the initial screw turns, progressive melting of this material, melt conveying with pressure generation and flow through the die [1, 7]. These individual stages are also illustrated in Figure 2. Their characteristics are described mathematically by a set of differential flow equations, which are coupled by appropriate boundary conditions to provide a global plasticating model that is solved numerically.

The vertical pressure profile in the hopper is computed to set an initial condition at the extruder entrance. In the initial screw turns, we assume the linear displacement of an elastic solid plug subjected to increasing temperature due to the combined contribution of friction dissipation and heat conduction from the surrounding metallic surfaces. Delay (i.e., beginning of melting) is sub-divided into the initial existence of a melt film separating the solids from the barrel, followed by encapsulation of the solids by melt films. Melting follows a mechanism involving 5 distinct regions, one being the melt pool, another the solid plug and the remaining melt films near to the channel walls. Melt pumping and die flow were modelled considering the non-isothermal flow of a non-Newtonian fluid. Calculations are performed in small screw channel increments, a detailed description being given elsewhere [7, 8].

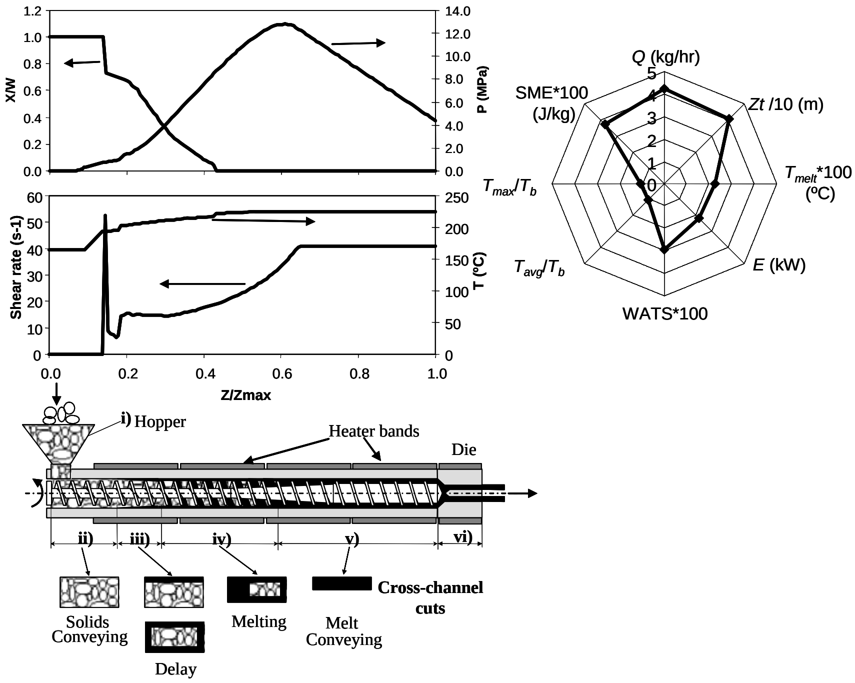

Fig. 2. Single screw extrusion: the machine, physical models and results of the modelling routine.

2.4 Scale-Up Criteria

For scale-up purposes, it makes sense to define two types of criteria. The first deals with single value parameters such as power consumption (*E*), specific mechanical energy (energy consumption per unit output, *SME*), output (*Q*) or degree of mixing (weight average total strain, *WATS*), which are illustrated in the radar plot of Figure 2 and provide an overview of the extruder behaviour under a specific set of input conditions. Within the same type, other criteria could be selected, such as well-known adimensional numbers like Cameron, Peclet or Brinkman, which account for temperature development, relative importance of convection and conduction and extent of viscous dissipation, respectively, thus estimating complementary aspects of the thermo-mechanical environment. The second type of criteria deals with the evolution of certain parameters along the screw, such as melting (solid bed, *X/W*), pressure (*P*), shear rate ($\dot{\gamma}$) and temperature (*T*) axial profiles. The following equations are used to define the objective functions for single values and profile parameters, respectively (see Figure 3):

$$F_j = \frac{\left|C_j - C_j^r\right|}{C_j^r} \;. \tag{1}$$

$$F_j = \frac{\displaystyle\sum_{k=1}^{K} \frac{\left|C_{j,k} - C_{j,k}^r\right|}{C_{j,k}^r}}{K} \;. \tag{2}$$

where F_j is the fitness of criterion j, C_j and C_j^r are the values of criterion j (single values) for the target and reference extruders, respectively, and $C_{j,k}$ and $C_{j,k}^r$ are the values of criterion j on location k (along the extruder) for the target and reference extruders, respectively.

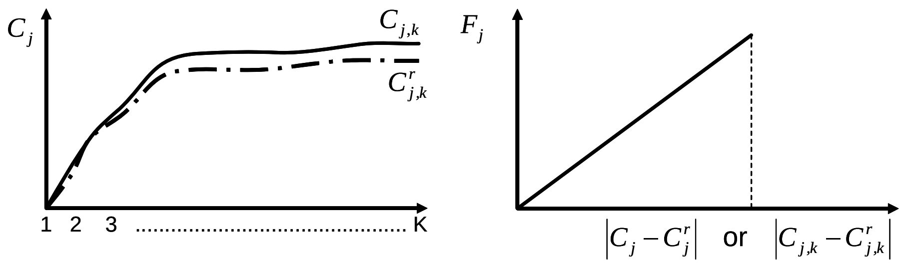

Fig. 3. Definition of the fitness of a criterion.

3 Scaling-Up Single Screw Extruders

3.1 Example

Using as reference a laboratorial extruder with a diameter of 30 mm and as target an extruder with a diameter of 75 mm (see table 1 and Figure 4), we wish to perform scale-up in terms of operating conditions. Data for the reference extruder was obtained using a screw speed (N) of 50 rpm and a uniform barrel temperature profile (T_i) of 190 ºC. The range of variation of the target extruder parameters is: N [10-200]

rpm; T_i [170-230] ºC. Data from polypropylene (NOVOLEN PHP 2150 from BASF) is adopted for the computational work.

Table 1. Geometry of the extruders used for scale-up.

D (mm)	L/D	L_1/D	L_2/D	L_3/D	Compression ratio
75	30.0	10.0	10.0	10.0	3.3
30	30.0	10.0	10.0	10.0	2.5

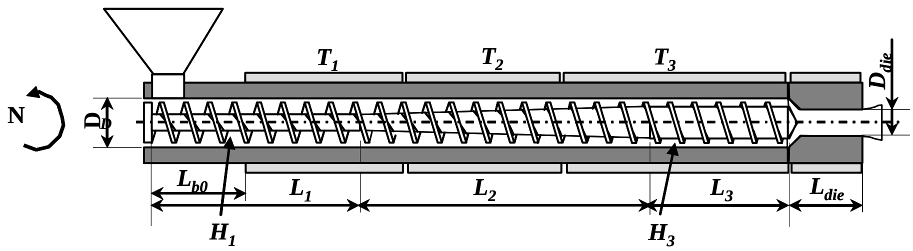

Fig. 4. Parameters required to describe the extruder geometry and operating conditions.

3.2 Results and Discussion

Figure 5 shows the results of the optimization when the various criteria were considered individually. A distinct set of operating conditions is proposed for each criterion. The smaller the value of the objective function the more successful the scale-up is. As expected, scaling-up using criteria related to machine size (output, power consumption) becomes difficult for considerable diameter ratios (in this case, 2.5). However, the use of constant values or functions related to flow characteristics (e.g., relative melting rate, average shear rate, average shear stress, viscous dissipation and adimensional numbers) is quite successful.

Figure 6 assesses the degree of satisfaction of the remaining criteria, when a specific single criterion is analysed. Shear rate, shear rate profile and Cameron number were selected for this purpose. Not surprisingly, optimization of a single criterion is feasible, but has little value in terms satisfying simultaneously other important performance measures which, in many cases, are conflicting.

The advantages of multi-criteria optimization were tested with three examples. The first considers three criteria, average shear rate, *C1*, WATS, *C2*, and viscous dissipation, *C3*. The second example deals with the simultaneous optimization of *C1*, Cameron number, *C4*, and melting profile, *C5*. Finally, the third example includes all criteria *C1* to *C5*.

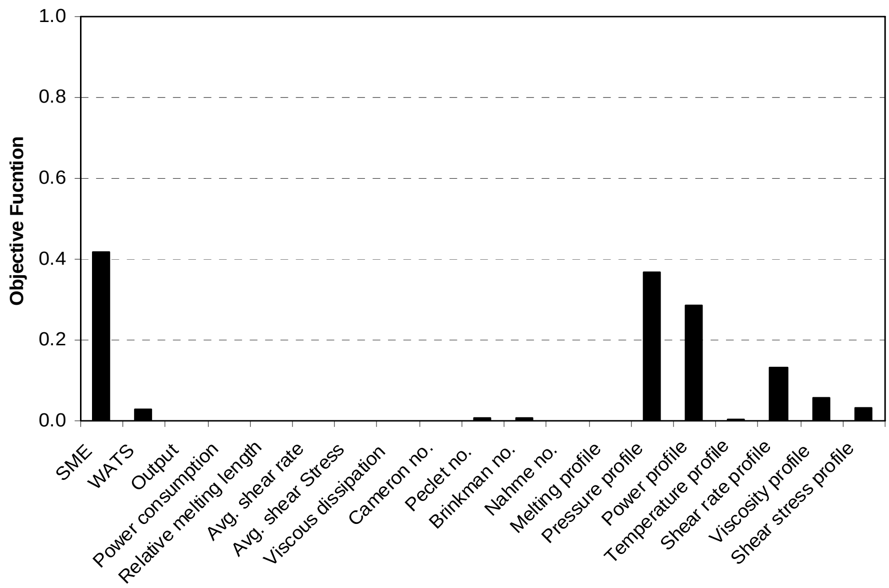

Fig. 5. Scaling-up for operating conditions using individual criteria.

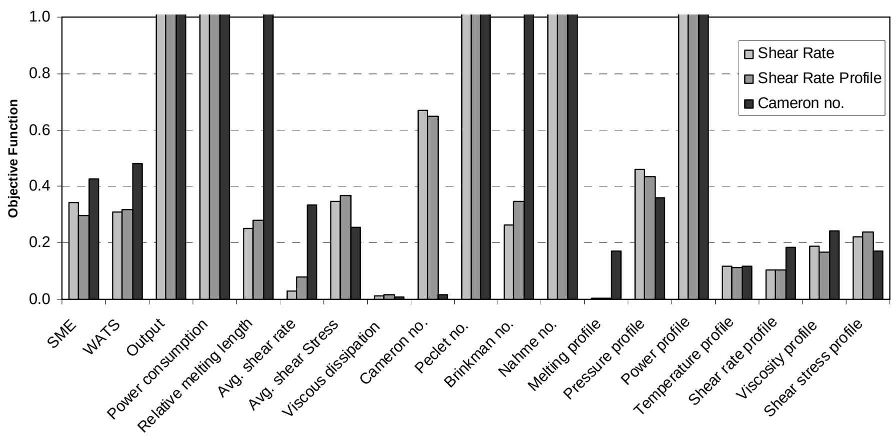

Fig. 6. Influence of the optimal operating conditions for shear rate, shear rate profile and Cameron no. on the satisfaction of the remaining criteria.

The results are shown in Figure 7 and Table 2. The figure presents the 3-dimensional Pareto surface for example 1, where criteria *C1*, *C2* and *C3* were optimized concurrently. The solutions identified as 1, 2 and 3 represent the best ones to minimize *C1*, *C2* and *C3*, respectively. Solution *S* minimizes the average of the 3 criteria, i.e., it yields a good compromise between the three criteria. Table 2 shows the operating conditions resulting from the solutions proposed for the three examples, the values of the 5 criteria (columns F1 to F5, but in examples 1 and 2 only three criteria were considered in the optimisation run) and the average F for solution *S*. When 5 criteria are optimised simultaneously a better solution is found, despite of the conflicting nature of some of the extruder responses.

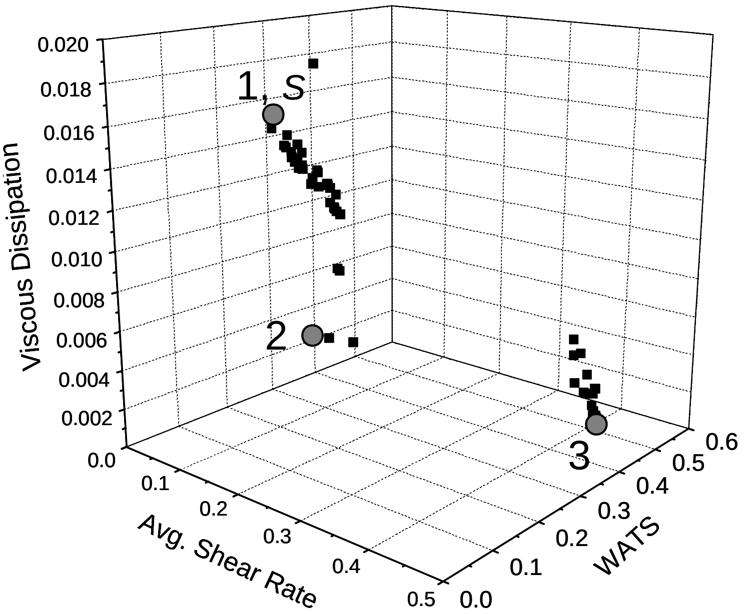

Fig. 7. Pareto frontiers for example 1.

4 Conclusions

The methodology proposed for extrusion scale-up is able to consider simultaneously various criteria and to take into account their relative importance. It can be applied to the scale-up of either operating parameters and/or geometry. Moreover, the efficiency of the scaling-up can be easily assessed by monitoring the implication of the exercise on the satisfaction of other process measures.

This methodology can be easily extended to other polymer processing technologies, as long as sufficiently precise modelling routines are available.

Table 2. Optimization with multiple criteria.

Criteria	Point	*N* (rpm)	T_1 (ºC)	T_2 (ºC)	T_3 (ºC)	F_1	F_2	F_3	F_4	F_5	*F*
C1,C2, C3	1	32.3	202.4	224.6	227.6	0.00	0.31	0.01	0.66	0.01	
	2	39.7	211.6	219.3	213.1	0.25	0.16	0.01	0.06	0.13	
	3	44.1	225.9	201.2	170.6	0.40	0.52	0.00	0.02	0.17	
	S	*32.3*	*202.4*	*224.6*	*227.6*	***0.00***	***0.31***	***0.01***	*0.66*	*0.01*	***0.20***
C1, C4 C5	1	32.3	226.1	200.9	213.5	0.00	0.31	0.01	0.66	0.01	
	2	40.5	224.1	189.5	206.2	0.27	0.43	0.01	0.00	0.16	
	3	34.4	223.2	200.5	199.7	0.06	0.31	0.01	0.68	0.00	
	S	*39.3*	*174.8*	*198.9*	*184.6*	***0.22***	*0.46*	*0.01*	***0.08***	***0.13***	***0.18***
C1 to C5	1	32.3	202.4	220.7	186.4	0.00	0.31	0.01	0.66	0.01	
	2	36.9	190.6	216.3	196.4	0.15	0.10	0.01	0.43	0.15	
	3	44.1	189.8	220.4	181.5	0.40	0.52	0.00	0.02	0.17	
	4	41.8	198.2	194.0	189.0	0.32	0.46	0.01	0.00	0.17	
	5	34.4	184.2	198.7	198.7	0.07	0.31	0.01	0.68	0.00	
	S	*36.9*	*190.6*	*216.3*	*196.4*	***0.15***	***0.10***	***0.01***	***0.43***	***0.15***	***0.17***

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