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Extrusion Scale-up: An Optimization-based Methodology

Given a reference extruder with a certain geometry and operating point, the aim of scale-up is to define the geometry and operating conditions of a target extruder (generally of significantly different size) in order to subject the material being processed to the same flow and heat transfer conditions, thus yielding products with the same characteristics. Since existing scale-up rules are crude, as they usually consider a single performance measure and produce unsatisfactory results, this work approaches scale-up as a multi-criteria optimization problem, where the aim is to define the geometry/operating conditions of the target extruder that minimize the differences between the values of various performance criteria for the reference and target extruders. Some case studies are discussed involving individual and multi-criteria scaling-up in terms of operating conditions, geometry, and both together, the usefulness of the approach being demonstrated. A few experiments are also performed in order to validate the concept.

1 Introduction

Scale-up is the action of defining the geometry and/or the operating conditions of a given machine/manufacturing sequence that replicate the working conditions of a different equipment of the same type but distinct size, processing the same material. This is a procedure of great practical importance. For example, in the case of polymer extrusion, the availability of scale-up rules enables the design of large extruders using the results of studies performed on laboratory scale – often cleverly instrumented – machines, that were developed for the in-depth understanding of the relevant physical, chemical and rheological phenomena developing during operation. Scale-up rules may also be used to extrapolate to laboratorial equipment the occurrence of problems identified in the production plant, whose origin and resolution can then be investigated at lower costs. Subsequently, scale-up rules must be utilized again to apply the solution found in the production equipment.

Scale-up rules for single screw extrusion were proposed over several decades by researchers with paramount contributions to the development of scientific and technical knowledge on plasticating extrusion, such as Carley and McKelvey (1953), Maddock (1959; 1979), Pearson (1976), Fenner and Williams (1971), Schenkel (1978), Chung (1984), Rauwendaal (1986; 1987), Potente (1991) and Elemans and Meijer (1994). Tables with scale-up rules can be found in general extrusion studies (for example, Stevens and Covas (1995)). More recently, scale-up of specific process aspects, such as mixing, have also been investigated (for example, Manas-Zloczower (2001)). Most approaches use analytical process descriptions to correlate the so-called large and small primary scaling variables (diameter, D, channel depth, H, screw length, L, and screw speed, N) in terms of an exponent of the ratio of the reference and target screw diameters:

$$x = x_0 d^{\psi}, \tag{1}$$

where x and x_0 are the large and small scaling variables, respectively, d is the diameter ratio and ψ is the scale-up index for a given process response. Since plasticating extrusion is a complex procedure, involving several steps and variables related to solids conveying, melting of these solids and melt conveying, in general this type of correlations only holds when: i) a single criterion is kept constant (e. g. constant melt shear rate, or constant melting rate), ii) part of the process is analysed (for example, Carley and McKelvey (1953) considered melt conveying, while Yi and Fenner (1976) studied melting and Potente and Fischer (1977) analysed solids and melt conveying) and iii) constant global geometrical features are assumed (generally, constant L/D or L/H).

Rauwendaal (1987) performed an interesting comparative analysis of the effect of the existing scale-up rules on extrusion performance. For each major process variable, relationships of the type of Eq. 1 were derived. For example, if average shear rate in the screw channel is approximated to the equivalent Couette shear rate, the following equation applies:

$$\dot{\gamma} = \frac{\pi N D}{H}, \tag{2}$$

Expressing each of the primary variables D, N and H in the form of equation 1, the exponents l, v and h are defined, respectively, which, upon insertion into Eq. 2, yields:

$$\dot{\gamma} \propto d^{1+v-h}, \tag{3}$$

i. e., shear rate is directly proportional to the right hand term. Similar expressions for other variables were obtained, namely for melt conveying rate, residence time, shear strain, melting

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capacity (conductive and dissipative), solids conveying, power consumption and specific energy consumption. Each of the available scale-up strategies was then assessed in terms of their effect on the process variables that were not covered by the analysis. Unfortunately, in most cases unbalanced solids and melt conveying rates or excessive viscous dissipation, were predicted and attributed to the lack of generality of the scale-up rules. Later, Potente (1991), who also reviewed the existing scale-up rules, confirmed these limitations. Thus, it seems that current scale-up rules:

– can tackle a single criterion (e. g. shear rate, melting rate, melt conveying rate) and only a process step (e. g., melt conveying, melting), which implies that when more than a process characteristic must be considered distinct rules (of the type of expression 1) have to be applied individually and simultaneously, which may lead to contradictory results;
– take into account only a few global geometrical features or operational variables (D, H, L and N). However, if, for example, a larger screw is to be designed based upon available data for a smaller screw, more geometrical features must be defined, such as helix angle, compression ratio, length of each geometrical zone. If the reference and target extruders exist and one attempts to reproduce in one machine the thermomechanical environment developing in the other, the barrel temperature profile should be part of the analysis;
– are based on simplified mathematical process descriptions, which have limited quantitative predictive capability and fail to cover the overall machine behaviour;
– are rigid in terms of the criteria that can be scaled-up, i. e., the user cannot include a new criterion, such as a particular ratio or an dimensionless number.

Therefore, a more performing scaling-up methodology is needed, namely in terms of:

– considering simultaneously several process criteria and, since they are often conflicting, identifying the final relative degree of satisfaction attained;
– selecting as scale-up criteria single values (e. g., average shear rate) as well as functions (e. g., shear rate profile along the screw axis);
– allowing for flexibility in selecting and/or defining the criteria;
– using accurate descriptions of flow and heat transfer in the extruder.

In principle, these requirements can be fulfilled if extrusion scale-up is regarded as a multi-objective optimization problem where the aim is to define the geometry/operating conditions of the target extruder that minimize the differences between the values of the selected process response parameters of the reference and target extruders. Conceptually, similar approaches were used previously to design single (Gaspar-Cunha and Covas (2001, 2004) and twin screw extruders (Gaspar-Cunha et al. (2005)). This work investigates such a possibility. The optimization methodology is first presented, its main building blocks (optimization algorithm, modelling routine and objective function) being discussed. Then, both single and multi-criteria problems are tackled, to evidence the benefits of the latter. Finally, an experimental set of results on scale-up for operating conditions is confronted with the predictions supplied by the method.

2 Multi-objective Scale-up

2.1 *Optimization Methodology*

As discussed above, extrusion scale-up consists in extrapolating the features (in terms of thermo-mechanical environment) of a reference extruder to another of the same kind, but of different dimensions (denoted as target extruder) processing the same material. In practice, the geometry and processing conditions of the reference extruder are known and the aim is to define either the operating conditions (if the target equipment exists), or the geometry and operating conditions (if a machine is to be designed or purchased) of the target extruder in such a way that the major performance measures of both machines are as similar as possible. This can be equated as an optimization problem were the aim is to determine the geometry/operating conditions of the target extruder that minimize the differences in performance in relation to the reference extruder for a given processing situation. Its solution requires the following steps (see illustration in Fig. 1):

1. Use a flow modelling routine to predict the responses of the reference extruder for the polymer system under a specific set of operating conditions;
2. Analyse the results and define the most important parameters to be used for scale-up;
3. Sort out available information on target extruder (geometry – at least screw diameter and length/diameter ratio, L/D, operating range – screw speed, set temperatures);
4. Perform scale-up via minimization of the differences in performance of the two extruders (to be characterized by the optimization criteria selected in step 2).

Thus, the method is based on the interrelationships between three basic routines: a plasticating extrusion modelling package, a criteria quantification routine and a multi-objective optimization algorithm. The algorithm defines automatically the (gradually more performing) solutions to be evaluated via the modelling routine. The values obtained by the latter serve as input data to the criteria quantification subprogram, which compares them with the equivalent ones for the reference extruder and then quantifies the quality of each solution. This information is supplied to the optimization routine, which identifies new improved solutions to be evaluated, the process being repeated until a stop criterion is reached.

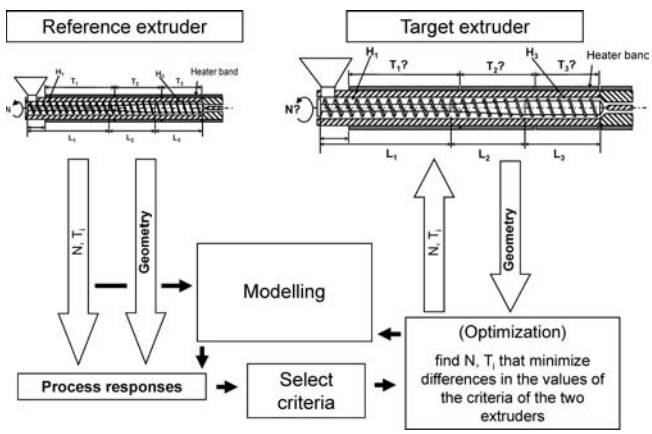

Fig. 1. Scale-up optimization methodology applied to operating conditions

Optimization algorithms are generally expensive from a computational point of view. In this particular problem, during an optimization run the process modelling routine is used hundreds of times. Therefore, in order for the method to have practical value, plasticating extrusion must be described accurately from a physical point of view, but approximate mathematical descriptions, less demanding in terms of computing times, must be adopted. This is an issue that requires careful balancing.

2.2 Modelling of Plasticating Single Screw Extrusion

Within the restrictions discussed at the end of the previous section, plasticating along the screw was sub-divided in the sequence of stages depicted in Fig. 2, encompassing solids conveying, delay, melting and melt conveying. Local flow and heat transfer were described mathematically by a set of governing equations that were coupled to those of adjacent zones by appropriate boundary conditions, to provide a global model that is solved numerically.

In order to set an initial condition at the screw entrance, the vertical pressure profile in the hopper was computed adopting the analysis developed by Walker (1966). In the initial screw turns, the conventional assumption of the linear displacement of an elastic solid plug is adopted, but the plug is also considered to be subjected to increasing temperature due to the combined contribution of friction dissipation and conduction from the surrounding metallic surfaces (Broyer and Tadmor, 1972; Tadmor and Broyer, 1972). When the latter causes the formation of the first melted material prior to the development of a specific melting mechanism, the Delay step develops. This is sub-divided into the initial creation of a melt film separating the solids from the barrel, as heat conduction and dissipation are higher at this interface, followed by encapsulation of these solids by melt films created by the same effects near to the screw root and flights (Kacir and Tadmor, 1972) (these stages are denoted as Delay (1) and Delay (2) in Fig. 2, respectively). Coherently, melting follows a mechanism involving 5 distinct regions as proposed by Elbirli et al. (1984), one being the melt pool, another the solid plug and the remaining three melt films adjacent to the screw root and flights. Finally, melt flow during melting, melt pumping and die pressure flow were modelled considering the 2-D non-isothermal flow of a non-Newtonian fluid.

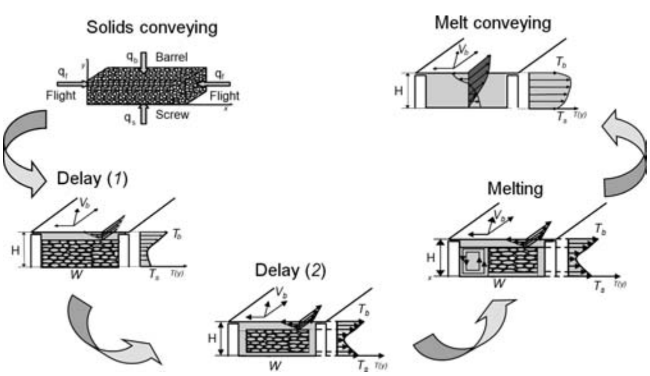

Fig. 2. Plasticating stages along an extruder screw

Calculations were performed in small screw channel increments, a detailed description of the overall sequence being given elsewhere (Gaspar-Cunha, 2000). The limitations of such a description include the following: i) in the initial stages of solids conveying loose pellets are present, not a coherent solid plug, which may cause an overestimation of output, ii) the channel cross-section and shape of individual solids and melted zones are more complicated than simple rectangles, c) melt flow is considerably three-dimensional, d) the conventional kinematic simplification of a rotating barrel and a fixed screw may convey further inaccuracies (Wang et al., 1996).

Fig. 3 exemplifies some of the programme predictions, which are of two types: i) evolution along the screw axis of variables such as melting (quantified in terms of the solids to channel width ratio, X/W), pressure, melt temperature, shear rate, among others; ii) values of key process parameters like output, Q, length of screw required for melting, z_t, melt temperature at die exit, T_{melt}, mechanical energy consumption, E, extent of distributive mixing (quantified via the weight average total strain, WATS, as proposed by Pinto and Tadmor (1970)), specific mechanical energy (energy consumption per unit output), SME and viscous dissipation (measured as average melt temperature to barrel temperature and/or as maximum melt temperature to barrel temperature ratios), T_{avg}/T_b, T_{max}/T_b.

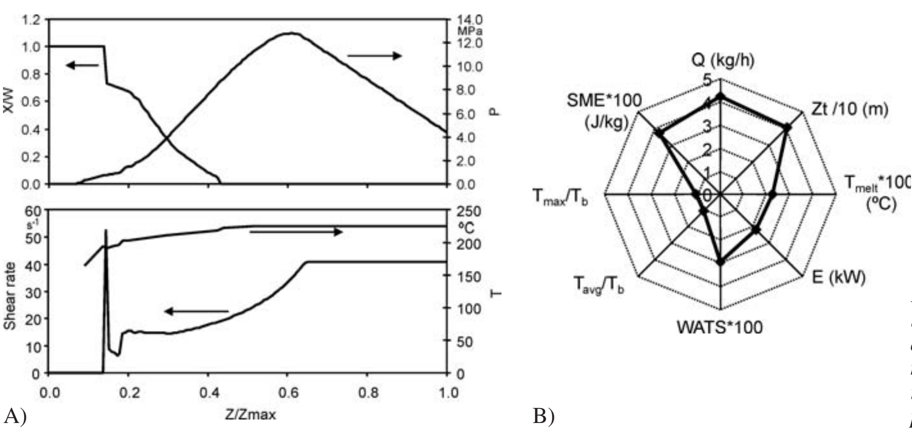

Fig. 3. Example of predictions of the modelling routine for a specific processing condition and material. A) evolution along the screw of melting, pressure, average shear rate and temperature; B) radar lot of various process parameters

2.3 Scale-Up Criteria

The accurate selection of the criteria to be used for a specific scale-up process will condition *ab initio* the success of the operation. Common scale-up factors include shear rate, pumping rate, melting rate, solids conveying rate, residence time, shear strain, power consumption, specific energy consumption, or area/throughput (Rauwendaal, 1987). Potente (1991) considered also throughput, temperature and pressure. Depending on the aim of the scale-up operation (e. g., designing new equipment with higher output, reproducing the flow conditions of the production plant in the laboratory equipment and/or vice-versa) it probably makes sense to pick the most relevant criteria from three groups:

– related directly to machine performance;
– describing specific aspects of flow and heat transfer;
– classical dimensionless numbers that assess the relative magnitude of transfer phenomena.

Output, power consumption and pressure are popular extruder responses, but since their values are inherently related to machine size, it should be difficult to perform an efficient scale-up using them as criteria. It seems more appropriate to adopt ratios such as Q/(WHND) (total flow rate to drag flow rate), specific mechanical energy (energy consumption per unit output, SME) and ΔPL/H (pressure per unit channel). Values of WATS, relative melting length (z_t/Z), average shear rate, average shear stress, overall viscous dissipation (T_{avg}/T_b, T_{max}/T_b) and average residence time reflect major aspects of flow and heat transfer. Finally, Cameron (inverse of Graetz), Peclet, Brinkman and Nhame dimensionless numbers are also good candidates to estimate the intensity of the thermo-mechanical effects inside the extruder. The first two quantities estimate the extent of temperature rise in a confined flow, by balancing convection in the flow direction against conduction in the cross-channel and in the flow directions, respectively. Therefore, they provide information on whether flow is essentially adiabatic, temperature develops, or the thermal regime is fully developed. Brinkman and Nhame assess the importance of viscous dissipation (for example, the Brinkman number is often used to estimate the extent of viscous dissipation in the melt film separating the solid bed from the barrel wall during melting, that is promoted by the local shear rates). The average shear rate, shear stress, and shear viscosity at each channel cross-section are computed from the values at every mesh nodes all over that cross-section. Dimensionless numbers use average values along the channel.

Most of the above criteria can be taken as a single global value, but in some cases it might make sense to attempt to reproduce the evolution along the screw length. Examples would be the melting (solid bed to channel width ratio, X/W), the average shear rate ($\dot{\gamma}$), the average temperature (T) and the cumulative residence time ($\bar{t}$) profiles along the screw axis. The evolution of dimensionless numbers along the barrel could also be envisaged.

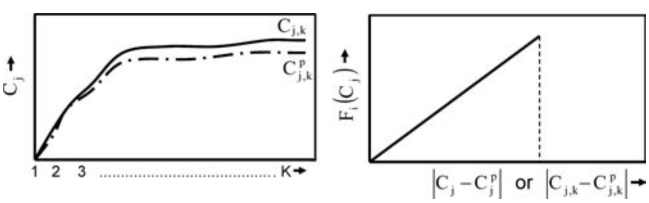

Fig. 4. Defining the fitness of a criterion

Each of the above criteria will be incorporated in the scale-up methodology in terms of an objective function (see Fig. 4 for an identification of variables):

$$F_j = \frac{\left|C_j - C_j^r\right|}{C_j^r}, \tag{4}$$

$$F_j = \frac{\sum_{k=1}^{K} \frac{\left|C_{j,k} - C_{j,k}^r\right|}{C_{j,k}^r}}{K}, \tag{5}$$

for single values and axial profiles, respectively, 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. Obviously, the aim is to minimize F_j.

2.4 Multi-objective Evolutionary Algorithms

The simplest way to perform a multi-objective optimization is to consider a global objective function taking in all individual objectives. One possibility is:

$$F = \sum_{j=1}^{q} w_j F_j, \tag{6}$$

where w_j is a weight reflecting the relative importance of the various individual criteria (with $\Sigma w_j = 1$). Minimization of F can be achieved by different optimization schemes. Evolutionary algorithms were used here because they are able to explore the entire search space, can distinguish between local and absolute minima and are relatively straightforward to implement as they do not require derivatives. The search process uses a population of points (solutions) – which brings about some advantages that will become evident below – but also requires considerable computational resources. In fact, since each point of each iteration step (denoted here as generation) requires a dedicated run of the modelling package, as discussed above the latter must call for modest computation times if solutions are to be proposed within reasonable periods.

Evolutionary Algorithms (EAs) mimic natural evolution, the sequence of calculations being identified in the flowchart of Fig. 5. The calculations start with the random definition of all the individuals composing the population (population initialization step). In the following evaluation step, the values of the criteria for each individual are determined from the data created by the modelling routine. Once these are known, it is possible to determine the fitness of every individual (value F). This is then followed by the reproduction (i. e., selection of the best individuals to define the contents of the next generation), crossover and mutation (these are methods to define the characteristics of the new individuals) steps, in a manner similar to that adopted by nature, as implied by the nomenclature. Calculations finish when all individuals converge to the same solu-

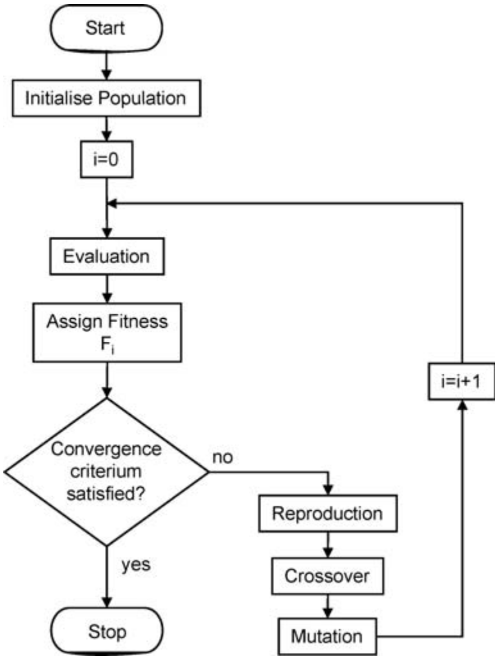

Fig. 5. Flowchart of an evolutionary algorithm

tion, or when a prescribed number of generations have been explored. More details on this method are given in Goldberg (1989).

The above scheme has two important drawbacks: 1) if after an optimization run any adjustments to the parameters of equation 6 are to be made (for example, change the relative importance of two criteria), an entirely new optimization run must be performed; 2) similarly, if equation 6 needs to be modified (changing the relationship between the criteria or, more simply, appending a new criterion), a new run must be performed. A route to overcome these difficulties consists in applying a multi-objective optimization algorithm using the advantage of EAs of working with a population of solutions. In this case, the various criteria are optimized simultaneously and independently in order to find out, in successive generations, the set of the non-dominated solutions (Deb (2001), Coello Coello (2002)).

Pareto plots are graphical representations of the compromise between 2 (2D plots) or 3 (3D plots) criteria. They include non-dominated and dominated and solutions (Deb (2001)). Non-dominated solutions are at least as good as others with respect to one of the criteria, but better with respect to the remaining criteria. The set of non-dominated solutions composes the optimal Pareto front. Dominated solutions are worst than non-dominated solutions, hence, not interesting. Therefore, for a given multi-objective optimization problem, Pareto plots allow the identification of the optimal front by taking into consideration whether each criterion is to be maximized or minimized and the best solution (in this front) will depend on the relative weight/importance attributed to each criterion. This importance can easily be changed, obviously without affecting the plot.

In the case of problems involving n criteria, the n-dimensionality of the representation can be converted in n-1 2D representations. In practice, the best solution may be difficult to find, as a non-dominated solution in one plot may be dominated in another. Research is currently being performed on decision-assisted methods (Ferreira et al. (2007)) this remaining an important open problem related to optimization. In this work, when the use of Pareto representations to locate the best solution becomes difficult, equation 6 is applied to the final population. Thus, changes in the weights do not require a new optimization run, simply the identification of the new location of the solution.

Multi-Objective Evolutionary Algorithms (MOEA) are accepted as a powerful search tool to find out approximations to Pareto-optimal fronts in optimization problems (Deb (2001), Coello Coello et al. (2002)). 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 this work, the Reduced Pareto Set Genetic Algorithm with Elitism (RPSGAe) was adopted (Gaspar-Cunha (2000), Gaspar-Cunha and Covas (2004)). This algorithm sorts the population individuals in a number of pre-defined ranks using a clustering technique, in an attempt to reduce the number of points on the optimal frontier while maintaining its characteristics intact, thus making it easier to select the solution. This is followed by the calculation of the individuals' fitness through a ranking function. In order to accomplish this, the computations follow the steps of a traditional GA (Fig. 5), except that they take on an external (elitist) population and a specific fitness evaluation. Since detailed presentation and discussion about this procedure can be found elsewhere (Gaspar-Cunha (2000), Gaspar-Cunha and Covas (2004)) it seems sufficient to state here the sequence of steps:

i) the internal population is randomly defined and an empty external population is formed;
ii) at each generation, a fixed number of the best individuals, obtained by reducing the internal population with the clustering algorithm, are copied to the external population;
iii) the process is repeated until the number of individuals of the external population is complete;
iv) the clustering technique is applied to sort the individuals of the external population, and
v) a pre-defined number of the best ones is incorporated in the internal population, replacing the lowest fitness individuals.

3 Scaling-up Examples

The methodology proposed in the previous section will be tested in a number of scale-up problems. First, scaling-up between existing extruders (i. e., in terms of operating conditions, as the geometry is pre-fixed) will be studied. Their main characteristics are presented in Table 1 (see also Fig. 6). The three smallest machines are available at the University of Minho. Although the range of diameters is narrow, the geometries are quite distinct. Table 2 identifies the corresponding case studies. They test the capacity of the method to scale-up and scale-down within different dimensional ranges, thus providing an initial appraisal of the methodology pros and cons. Therefore, both single and multi-criteria problems will be solved, in order to ascertain criteria feasibility, implication of a specific criterion on the overall performance, and eventual benefits from assembling several criteria simultaneously. In the problems solved, when any of these extruders is used as reference, it operates with a screw speed (N) of 50 min^{-1} and a flat barrel temperature profile (T_i) of 190 °C. The prescribed range of variation of the target extruder is: N [10–200] min^{-1} and T_i [170–230] °C.

D (mm)	L/D	L_1/D	L_2/D	L_3/D	Compression ratio
10	26	8	10	8	1.4
30	30	10	10	10	2.5
36	24.6	11.6	7	6	2.8
75	30	10	10	10	3.3

Table 1. Extruders used in the study

Case study	Reference extruder diam. mm	Target extruder diam. mm
1	30	36
2	30	75
3	30	10
4	10	75
5	75	10

Table 2. Scale-up case studies

Scaling-up in terms of geometry follows. In this case, both the reference (D = 30 mm) and target (D = 75 mm) extruders operate at 50 min^{-1} and 190 °C, the aim being to define the geometrical features identified in Fig. 6 (L and D are fixed at 2175 and 75 mm, respectively, L_1, L_2 and L_3 may vary between 200 and 1000 mm, and H_1 and H_3 range in the intervals 7.5 to 15 mm and 2.5 to 7.5 mm, respectively).

Finally, scaling-up in terms of both geometry and operating conditions is discussed. The geometry and operating conditions of the 30 mm reference extruder are the same as above, while only the total L (2175 mm) and D for the 75 mm target extruder are prescribed, as scale-up involves the simultaneous identification of the best screw profile and operating conditions.

In all cases, a polyethylene extrusion grade (ALCUDIA T-100 from Repsol) is used, the main properties being collected in Table 3. As indicated in the Table, the effect of pressure and/or temperature on properties, such as solids (Hyun and Spalding, 1990) and melt density, friction coefficients (Spalding and Hyun, 1995) and solids and melt conductivity can be considered, the practical difficulty lying in making such data available.

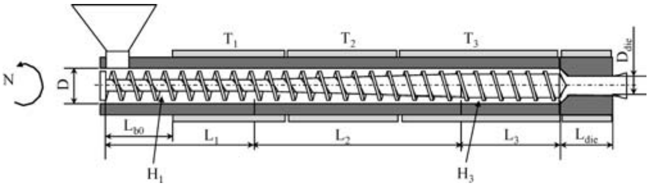

Fig. 6. Configuration of the extruders and operating parameters

Property	Law	Symbol	Value
Solids density	$\rho = \rho_\infty + (\rho_0 - \rho_\infty)e^P$	ρ_∞ (kg/m^3) ρ_0 (kg/m^3)	922.0 495.0
Melt density	$\rho_m = g_0 + g_1T + g_2P + g_3TP$	ρ_0 (kg/m^3) ρ_1 (kg/m^3 °C) ρ_2 (kg/m^3 Pa) ρ_3 (kg/m^3 °C Pa)	840.0 −0.4236 2.18×10^{-7} 3.9×10^{-12}
Friction coefficients: – polymer-barrel – polymer-screw	$f = f_0 + f_1T + f_2P$	f_b f_s	0.45 0.25
Solids thermal conductivity	–	K_s (W/m °C)	0.186
Melt thermal conductivity	$k_m = k_0 + k_1T + k_2P$	K_0 (W/m °C)	0.097
Heat of fusion	–	h (kJ/kg)	167.0
Solids specific heat	–	C_s (J/kg)	2350.0
Melt specific heat	$C_m = C_0 + C_1T + C_2P$	C_0 (J/kg)	2535.0
Melting temperature	–	T_m (°C)	120.0
Viscosity	$\eta = \eta_0 a_T (1 + (\lambda a_T \dot{\gamma})^a)^{\frac{n-1}{a}}$ $a_T = \exp\left(\frac{E}{R}\left(\frac{1}{T} - \frac{1}{T_0}\right)\right)$	E/R (K^{-1}) λ n η_0 a T_0	10000.0 0.7 0.3 18000.0 1.7 190.0

Table 3. Properties of HDPE Alcudia T100

4 Results and Discussion

4.1 Scaling-up in Terms of Operating Conditions

The scale-up criteria discussed in section 2.3 (related to machine performance, to flow and heat transfer and to classical dimensionless numbers) were considered individually for case study 1 of Table 2, yielding the results presented in Figs. 7 and 8. Fig. 7 shows the value of the each objective function when the optimization is completed (the aim being to reach $F_i = 0$, i. e., identical response of the reference and target extruders for a specific parameter). In turn, Fig. 8 presents the operating conditions of the target extruder corresponding to the F_i values of Fig. 7.

As illustrated in Fig. 7, with the exception of those parameters that are readily dependent on machine size (e. g., pressure and power profiles), the majority of the remaining criteria is either zero, or quite small, regardless of being single values or profiles/functions. Fig. 8 demonstrates that the satisfaction of each criterion requires a specific set of operating conditions (screw speed, barrel temperature profile), which implicitly suggests that the fulfilment of one criterion may be obtained at the cost of not suiting many others. This also explains why Specific Mechanical Energy, SME, obtained by dividing the total mechanical power consumption by the volumetric output, could not be scaled-up successfully ($F \approx 0.4$ in Fig. 7). Although the objective functions for power consumption and output could be zeroed (the two machines have similar sizes), each solution was found for a distinct operating condition. It was not possible to find a third operating point where the objective function corresponding to their ratio was nil.

Table 4 contains the numerical data of Figs. 7 and 8 for case study 1 and the equivalent results for the remaining four case studies identified in Table 2. The same general observations remain valid for a wider extruder diameter range, i. e., the values of F_i are high for output, power consumption, pressure profile

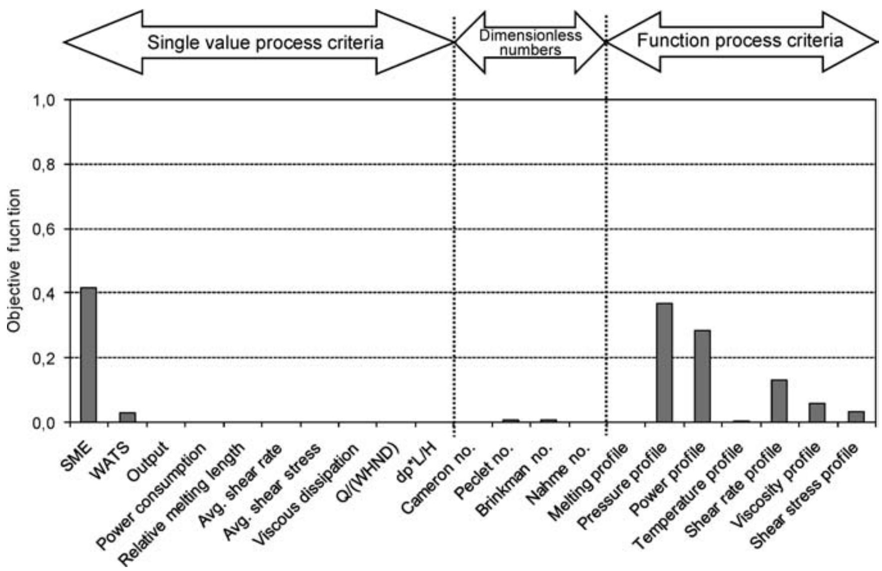

Fig. 7. Scale-up results (operating conditions) for case study 1 in terms of individual objective function values

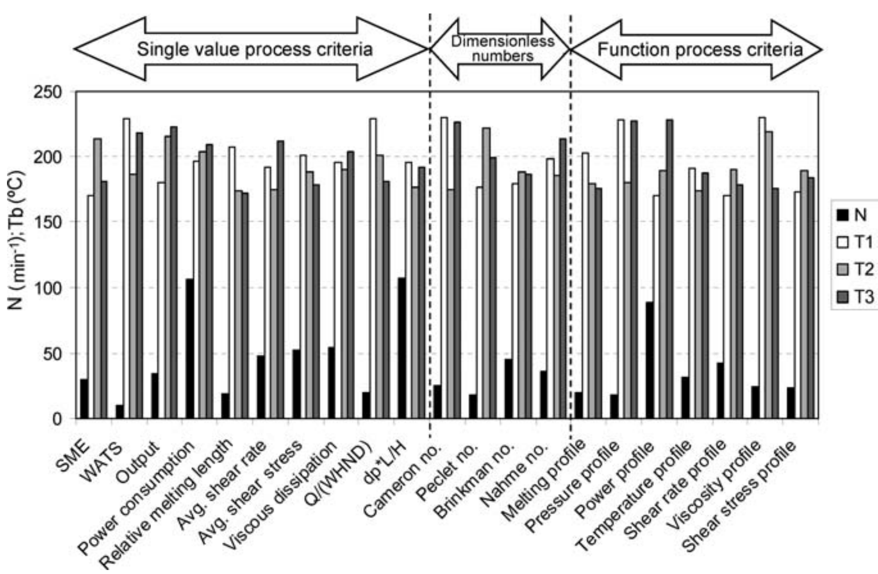

Fig. 8. Scale-up results (operating conditions) for case study 1 in terms of individual operating conditions (screw speed, barrel temperature)

and power consumption profile, may be important in some cases for SME and WATS and are small or nil for the remaining criteria.

A more detailed discussion of some results may offer evidence that the methodology takes the correct actions. For example, case study 2 involves scaling up from 30 mm to 75 mm diameter extruders, the results being poor for output, power consumption and power profile, all related to machine size. Yet, the screw speed proposed by the algorithm for the target extruder is the lowest possible value (10 min^{-1}), in an attempt to match the lower output provided by the smaller reference extruder at 50 min^{-1}. The results in terms of objective function values to scale down from 30 to 10 mm diameters (case study 3), or from 75 to 10 mm diameters (case study 5) are not very different. Now, the suggested screw speed for the smaller target extruder is the highest value prescribed (200 min^{-1}), for obvious reasons. Case studies 4 and 5 are symmetrical (scale-up from 10 to 75 mm diameter screws and vice-versa), but the results are quite diverse. Scaling-up is more difficult than scaling-down in terms of output, power consumption, WATS and SME, which is related to the values of the operating conditions prescribed for the reference extruder, and to the range of variation of the operating conditions defined for the target extruder. In fact, in the case of the output criterion it is easier to scale down from a 75 mm diameter machine operating at 50 min^{-1} to a 10 mm machine working at its top speed, than to scale-up from a 10 mm machine operating at 50 rpm to a much bigger 75 mm machine whose minimum screw speed is set at 10 min^{-1} (the table shows that in most cases the screw cannot rotate as low as it would be required to match outputs – well under 10 min^{-1}).

When a specific single criterion is selected for scale-up, it is important to estimate the degree of satisfaction of the remaining criteria. In order to investigate this aspect, the following procedure was adopted, the results being summarized in Fig. 9: i) choose case study 2 for this assessment, as it involves machines of sufficiently different sizes; ii) select average shear rate, shear rate profile and Cameron number as pertinent criteria; iii) separately for each of these, use their optimal operating conditions (i. e., the operating conditions obtained from scaling-up using them as criteria) as input to compute the value of the objective functions for the remaining criteria. For example, in the case of average shear rate, the corresponding objective value is small (0.07 in Table 4) but the values of the remaining criteria may become important (medium grey bars in Fig. 9), namely for output, power consumption, Cameron, Peclet and Nahme numbers and power consumption profile. A similar situation is verified for shear rate profile and Cameron number (dark grey and light grey bars, respectively), i. e., when their optimal operating conditions for scale-up are used, many

Criterion	Case study 1					Case study 2					Case study 3					Case study 4					Case study 5				
	F	Operating conditions				F	Operating conditions				F	Operating conditions				F	Operating conditions				F	Operating conditions			
		N	T1	T2	T3		N	T1	T2	T3		N	T1	T2	T3		N	T1	T2	T3		N	T1	T2	T3
SME	0.42	30.2	171	214	182	0.00	15.7	215	190	173	0.43	133.9	172	174	213	1.24	34.5	207	210	227	0.03	133.9	172	174	213
WATS	0.03	10.1	229	187	219	0.10	37.0	211	223	209	0.26	10.1	225	178	203	1.17	36.8	191	221	213	0.54	10.1	225	178	203
Output	0.00	34.5	180	216	223	1.24	10.1	221	203	191	0.69	199.6	174	177	212	*	*	*	*	*	0.97	199.6	174	177	212
Power consumption	0.00	106.0	197	204	210	0.77	10.1	224	203	190	0.90	197.0	171	216	182	*	*	*	*	*	0.99	198.1	175	172	213
Relative melting length	0.00	19.4	208	175	173	0.07	36.9	217	210	211	0.01	10.1	227	196	191	0.25	38.6	217	213	216	0.00	159.2	206	208	204
Avg. shear rate	0.00	47.8	192	176	212	0.07	32.4	217	205	203	0.01	61.7	176	214	223	0.25	21.2	204	190	224	0.00	106.5	224	193	207
Avg. shear Stress	0.00	52.3	202	189	178	0.08	134.2	183	228	208	0.01	153.1	228	226	227	0.11	134.3	213	173	221	0.01	34.5	199	224	212
Viscous dissipation	0.00	54.8	196	191	204	0.00	44.6	193	190	206	0.00	192.9	173	214	189	0.00	12.6	216	190	192	0.00	192.1	171	215	200
Cameron no.	0.00	25.5	230	175	227	0.00	42.4	195	220	220	0.00	199.7	229	202	185	0.00	36.9	224	176	226	0.00	199.6	218	216	216
Peclet no.	0.01	18.4	177	223	200	0.00	15.7	196	226	195	0.01	111.5	191	200	213	0.01	196.3	200	198	185	0.01	196.7	171	202	219
Brinkman no.	0.01	45.3	180	189	187	0.00	45.3	180	189	187	0.01	121.2	214	228	225	0.01	148.3	181	191	174	0.01	162.6	178	171	176
Nahme no.	0.00	36.4	199	187	214	0.00	18.8	173	213	207	0.01	122.3	205	225	205	0.01	10.1	224	203	190	0.01	183.2	175	212	187
Melting profile	0.00	20.0	203	180	177	0.00	34.5	201	212	200	0.01	31.9	215	180	193	0.11	38.7	223	216	199	0.04	162.6	192	181	200
Pressure profile	0.37	17.8	229	180	227	0.26	95.4	214	219	213	0.48	23.9	227	182	213	1.04	141.5	188	220	179	1.43	10.1	230	204	189
Power profile	0.29	88.9	171	190	229	0.87	10.1	224	203	190	0.71	195.3	186	191	230	*	*	*	*	*	0.76	27.2	183	196	228
Temperature profile	0.01	31.9	192	174	188	0.11	12.2	196	206	189	0.02	16.9	198	208	185	0.13	12.2	172	207	191	0.06	189.1	230	173	229
Shear rate profile	0.13	42.6	171	191	179	0.10	29.8	229	221	208	0.23	62.4	229	194	179	0.23	13.9	220	184	204	0.27	65.1	227	228	185
Viscosity profile	0.06	24.6	230	220	177	0.15	21.0	176	213	208	0.10	63.7	220	217	223	0.25	18.4	178	203	205	0.24	189.2	230	212	229
Shear stress profile	0.03	23.2	174	190	185	0.09	161.1	176	222	184	0.04	29.0	174	172	181	0.09	161.3	182	201	175	0.08	28.1	203	212	206

* scale-up not feasible (see text).

Table 4. Scale-up results (operating conditions) for all case studies

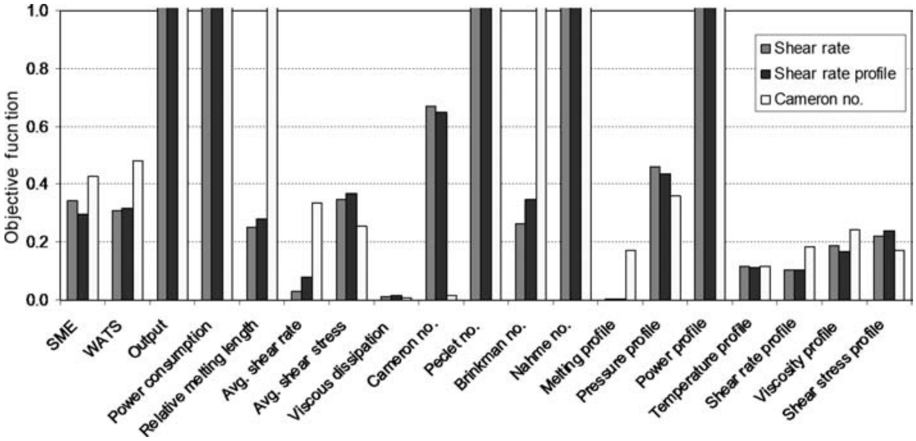

Fig. 9. Effect of the individual scale-up of 3 criteria (shear rate, shear rate profile and Cameron number) on the value of the objective function of the remaining individual criteria (case study 2)

Criteria	Solution	N min^{-1}	T_1 °C	T_2 °C	T_3 °C	F_1 ASR	F_2 WATS	F_3 VD	F_4 Ca	F_5 X/W	F
Avg. shear rate WATS	1	32.3	174.7	204.4	183.4	0.00	0.31	0.01	0.66	0.01	
	2	36.8	215.1	222.0	208.3	0.15	0.22	0.01	0.59	0.14	
	Gobal	36.4	192.9	226.0	202.7	**0.13**	**0.30**	0.01	0.69	0.00	**0.23**
Avg. shear rate Viscous dissipation	1	32.3	221.5	218.2	199.6	0.00	0.31	0.01	0.66	0.01	
	3	44.1	208.4	186.8	214.7	0.40	0.52	0.00	0.02	0.17	
	Global	34.4	172.8	206.0	207.3	**0.06**	0.31	**0.01**	0.68	0.00	**0.21**
Avg. shear rate Cameron no.	1	32.3	204.9	212.8	204.7	0.00	0.31	0.01	0.66	0.01	
	4	40.5	206.1	216.3	224.2	0.27	0.44	0.01	0.01	0.16	
	Global	36.8	208.7	198.7	209.1	**0.15**	0.44	0.01	**0.14**	0.14	**0.18**
Avg. shear rate Melting profile	1	32.3	208.9	188.4	224.7	0.00	0.31	0.01	0.66	0.01	
	5	34.4	192.3	210.0	204.4	0.07	0.31	0.01	0.68	0.00	
	Global	33.5	193.4	218.4	183.2	**0.04**	0.31	0.01	0.67	**0.00**	**0.21**
Avg. shear rate WATS Viscous dissipation	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	
	Global	32.3	202.4	224.6	227.6	**0.00**	**0.31**	**0.01**	0.66	0.01	**0.20**
Avg. shear rate Cameron no. Melting profile	1	32.3	226.1	200.9	213.5	0.00	0.31	0.01	0.66	0.01	
	4	40.5	224.1	189.5	206.2	0.27	0.43	0.01	0.00	0.16	
	5	34.4	223.2	200.5	199.7	0.06	0.31	0.01	0.68	0.00	
	Global	39.3	174.8	198.9	184.6	**0.22**	0.46	0.01	**0.08**	**0.13**	**0.18**
Avg. shear rate WATS Viscous dissipation Cameron no. Melting profile	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	
	Global	36.9	190.6	216.3	196.4	**0.15**	**0.10**	**0.01**	**0.43**	**0.15**	**0.17**

Table 5. Multi-criteria scale-up results (operating conditions) for case study 2

of the remaining criteria will remain unsatisfied, which means that the thermo-mechanical environments inside the reference and target extruders will be distinct and that the behaviour of the latter may turn out to be unbalanced. This result is not surprising, not only because Fig. 8 and Table 4 had already shown that the satisfaction of each individual criterion requires a specific operating point, but also because many of the criteria used in this work are conflicting. In principle their simultaneous consideration should yield better results, as some performance compromises could be found.

In order to explore multi-criteria scale-up, but keeping the analysis as uncomplicated as possible, the following criteria will be selected from the series considered in Table 4 (and denoted as criterion 1 to 5, C_1 to C_5, respectively): average shear rate, WATS (i. e., distributive mixing), viscous dissipation, Cameron number and melting profile. They encompass single values and functions, and include quantities related to flow and heat transfer and one dimensionless number. Table 5 collects the data generated. The first column identifies the group of criteria that are being considered simultaneously for scale-up (again, case study 2). The table contains results for four combinations of pairs of two of the above 5 criteria, two groups of three and all 5 criteria together. The second column (entitled "solution") identifies if the information of the following rows refers to the individual optimization of criterion 1, …, 5, or if it is the global solution for that particular combination. Columns N, T_1, T_2 and T_3 refer to the optimal operating conditions of each proposed solution, whereas columns F_1 to F_5 and F contain the values of the individual objective functions, and the global value, respectively. If the values of F_1 to F_5 have been printed in bold, this means that they were selected as objectives for scale-up, otherwise they represent the impact on that criterion from selecting other criteria for scale-up. For example, consider simultaneously average shear rate, C_1, and Cameron number, C_4 (third combination using pairs of two criteria). If C_1 is taken as a single criterion, objective value F_1 would be zero, but the remaining four would take the values of 0.31, 0.01, 0.66 and 0.01, respectively (i. e., $F_4 = 0.66$); when C_4 is considered by itself, its objective value becomes 0.14 (F_4), and the remaining turn into 0.27, 0.44, 0.01 and 0.16, respectively (thus, $F_1 = 0.27$). When both C_1 and C_4 are scaled-up simultaneously (row "global"), $F_1 = 0.15$, $F_4 = 0.14$ (now printed in bold), and the global F for the five criteria is 0.18. In other words, performing simultaneously a scale-up for C_1 and C_4 enables finding a better solution than doing it separately. This behaviour is generally observed, i. e., both Table 4 (for the single objective examples) and Fig. 9 show that when a specific criterion is used for scale-up its F value is minimised, but it can become significant when other criteria are considered. However, when multicriteria scale-up is performed, the F values of the objective functions included tend to assume intermediate values in relation to the minimum obtained for individual scale-up and the maximum calculated

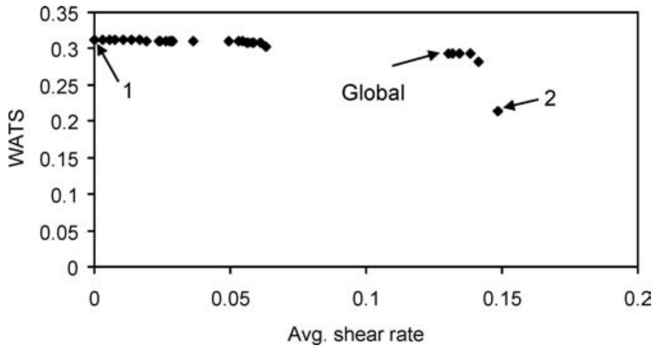

Fig. 10. Pareto frontier for a two criteria (average shear rate, C_1, and WATS, C_2) scale-up example from Table 5

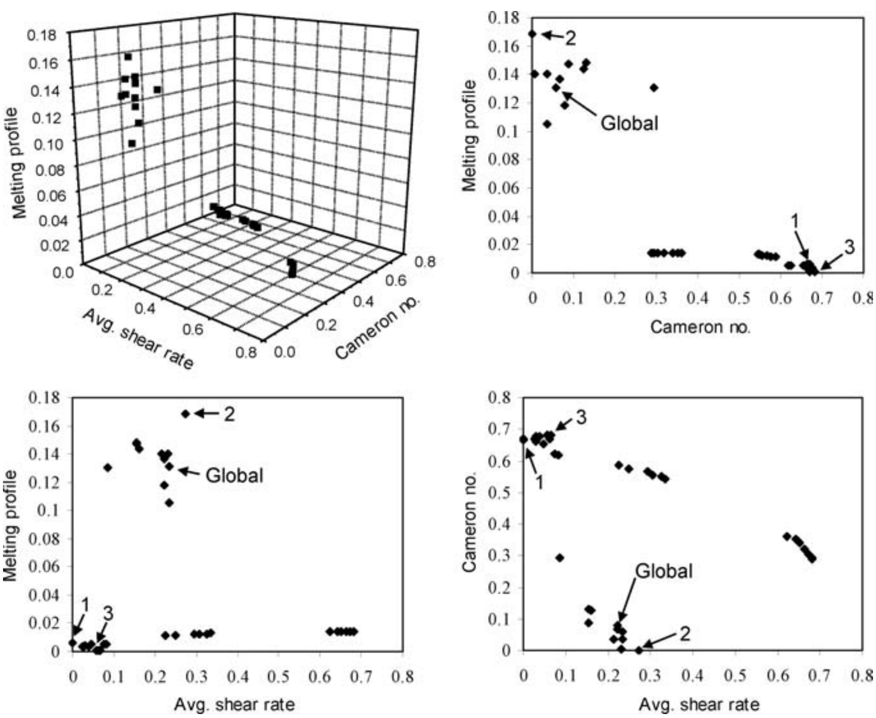

Fig. 11. Pareto frontier for a three criteria (average shear rate, C_1, Cameron number, C_4, Melting profile, C_5) scale-up example from Table 5: 3D plot and corresponding 2D projections

when other criteria are taken. The advantages of multicriteria scale-up are more evident from the analysis of the global F values in Table 5. For the two criteria exercises, the F values obtained were 0.23, 0.21, 0.18 and 0.21, which corresponds to an average F = 0.21. If three criteria are treated at one time, the F values are 0.20 and 0.18, i. e., an average 0.19. If the 5 criteria are tackled simultaneously, F = 0.17. Thus, although more scale-up criteria are taken on, thus making the exercise more complete/adequate, the global F values can still decrease. Simultaneously, the degree of satisfaction of all individual criteria is known, so that the user may eventually undertake further actions.

Figs. 10 and 11 plot the Pareto frontiers for two criteria (C_1, C_2) and three criteria (C_1, C_4, C_5) scale-up examples from Table 5, respectively. Given the correlation between C_1 and C_2 and the requirement to minimize the values of objectives, the location of solutions 1 and 2 in Fig. 10 is obvious, while the coordinates of the global solution correspond to a good compromise between both. In the case of the 3D graph (Fig. 11), the same reasoning applies. When dealing with 5 criteria, the choice of solutions becomes much more complicated, as the 5-dimensional correlation can only be visualized by several 2D or 3D representations. In doing this, solutions that are non-dominated in one representation may be dominated in another, further complicating the analysis. As stated above, the solutions for problems with n > 3 dimensions were found by applying equation 6 to the final data, with all weights being assumed as identical.

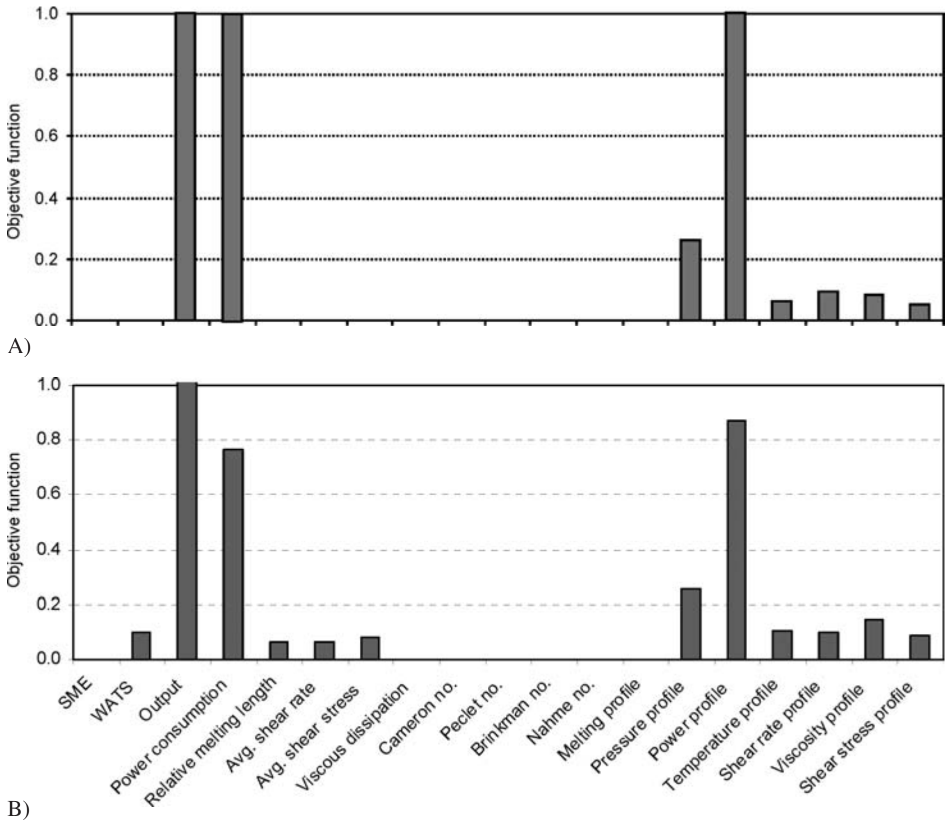

Fig. 12. Scale-up results for case study 2 in terms of individual objective function values; top: geometry; bottom: operating conditions

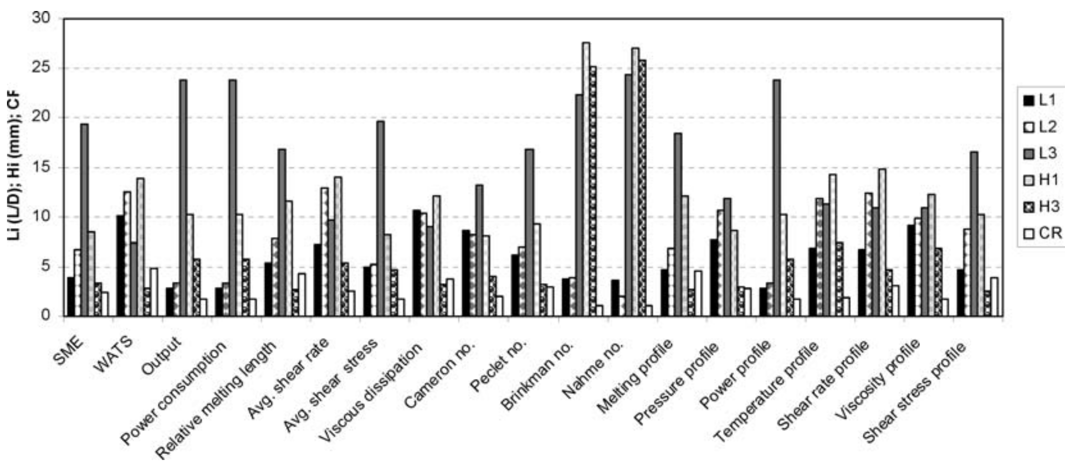

Fig. 13. Scale-up results (geometry) for case study 2 in terms of individual geometrical parameters (L_1, L_2, L_3, H_1, H_3, CR)

4.2 Scaling-up in Terms of Geometry

This section tackles scaling-up from the 30 mm to the 75 mm extruder, keeping the same set of operating conditions. Fig. 12 compares the values of the individual functions obtained for scale-up for operating conditions reported in Table 4 and for geometry for case study 2. With the exception of output and power consumption, most of the objective functions are now either nil or a bit smaller than those for the case of scaling-up based only in operating conditions. This is not surprising, since scale-up in terms of geometry has more degrees of freedom (five geometrical parameters against four operational variables). Fig. 13 confirms that the satisfaction of the individual criteria requires distinct geometries. This should again imply that if scale-up is performed only on the basis of the fulfilment of a single criterion, many other process features will not be scaled-up appropriately and the target extruder will show signs of unbalanced solids conveying, melting, melting rate, or mixing.

The same multicriteria approach was applied to average shear rate, WATS, Viscous dissipation, Cameron number and melting profile criteria (C_1 to C_5, as before), the corresponding results being listed in Table 6 (the differences to Table 5 being the fact that the optimal operating conditions of the latter are replaced by the optimal geometrical features in the former).

The benefits of performing a multicriteria scale-up are again distinguishable. For example, in the first two-criteria combination (C_1 and C_2), if C_1 is taken as a single criterion, its objective value F_1 becomes zero and the corresponding value of F_2 (WATS) is 0.18; when C_2 is considered by itself, $F_2 = 0$ and $F_1 = 0.07$. When both C_1 and C_2 are scaled-up simultaneously, $F_1 = 0.02$ and $F_2 = 0$, while the global F for the

Criteria	Solution	L_1 L/D	L_2 L/D	L_3 L/D	H_1 mm	H_3 mm	F_1 ASR	F_2 WATS	F_3 VD	F_4 Ca	F_5 X/W	F
Avg. shear rate WATS	1	8.1	12.2	8.7	14.7	5.3	0.00	0.18	0.02	0.60	0.18	
	2	7.2	12.4	9.4	13.9	5.0	0.07	0.00	0.02	0.54	0.17	
	Global	8.7	12.1	8.2	15.0	4.8	**0.02**	**0.00**	0.02	0.61	0.17	**0.16**
Avg. shear rate Viscous dissipation	1	11.0	11.6	6.4	12.5	5.5	0.00	0.59	0.00	0.55	0.18	
	3	10.8	11.8	6.4	12.5	5.5	0.00	0.63	0.00	0.54	0.18	
	Global	11.0	11.8	6.2	12.5	5.5	**0.00**	0.63	**0.00**	0.55	0.18	**0.27**
Avg. shear rate Cameron no.	1	10.5	11.8	6.7	13.0	5.3	0.00	0.54	0.01	0.55	0.18	
	4	11.7	8.6	8.7	8.0	3.6	0.53	0.37	0.03	0.01	0.18	
	Global	8.8	11.1	9.1	9.3	5.0	**0.25**	0.20	0.02	**0.27**	0.18	**0.18**
Avg. shear rate Melting profile	1	12.2	12.1	4.7	14.9	3.9	0.00	0.32	0.01	0.64	0.17	
	5	7.6	7.7	13.7	14.3	2.5	0.91	0.10	0.03	0.83	0.01	
	Global	33.5	12.1	4.7	14.9	3.9	**0.00**	0.32	0.01	0.64	**0.17**	**0.23**
Avg. shear rate WATS Viscous dissipation	1	10.4	12.7	5.9	12.2	5.5	0.00	0.32	0.00	0.61	0.18	
	2	8.1	13.1	7.8	11.7	4.5	0.17	0.01	0.00	0.39	0.18	
	3	10.5	12.9	5.6	12.3	5.4	0.01	0.62	0.00	0.53	0.18	
	Global	8.2	12.7	8.1	14.7	4.8	**0.03**	**0.01**	**0.02**	0.58	0.17	**0.16**
Avg. shear rate Cameron no. Melting profile	1	11.7	10.9	6.4	12.2	5.6	0.00	0.62	0.00	0.55	0.18	
	4	8.6	10.3	10.2	9.2	3.0	0.67	0.68	0.05	0.00	0.17	
	5	6.1	8.8	14.1	13.0	2.5	0.99	0.00	0.03	0.77	0.01	
	Global	8.4	11.0	9.6	8.7	4.0	**0.44**	0.32	0.02	**0.07**	**0.18**	**0.21**
Avg. shear rate WATS Viscous dissipation Cameron no. Melting profile	1	8.3	11.2	9.5	13.7	5.7	0.00	0.35	0.01	0.57	0.18	
	2	11.5	12.2	5.3	9.3	3.2	0.39	0.00	0.02	0.20	0.18	
	3	8.9	13.2	6.9	11.6	4.5	0.15	0.19	0.00	0.40	0.18	
	4	11.2	12.6	5.2	7.6	3.4	0.55	0.10	0.03	0.00	0.18	
	5	4.9	12.3	11.8	11.4	2.5	0.95	0.74	0.04	0.07	0.11	
	Global	7.1	12.2	9.7	10.8	4.9	**0.19**	**0.01**	**0.00**	**0.35**	**0.18**	**0.15**

Table 6. Multi-criteria scale-up results (geometry) for case study 2

five criteria rates at 0.16. If average shear rate and viscous dissipation are paired (C_1 and C_3), the global F = 0.27. However, if the three criteria C_1, C_2 and C_3 are taken simultaneously, F = 0.16. When the 5 criteria (C_1 to C_5) are studied jointly, F = 0.15. The average value of the global objective function in Table 5 is 0.20, whereas that of Table 6 is 0.19, which shows again that scale-up of geometrical features may be slightly more precise than doing it exclusively on the basis of operating conditions.

4.3 Full Scale-up

For the case studies selected in Table 2, full scale-up consists in defining simultaneously the four operational parameters (N, T_1, T_2 and T_3) and the five geometrical variables (L_1, L_2, L_3, H_1, H_3) of the target extruder that induce identical values for the criterion/criteria taken as relevant. When each individual criterion is taken separately, F_i is nil in all cases, which did not happen for scale-up for operating conditions (Fig. 7, Table 4) and geometry (Fig. 12) and should be due to the fact that the problem has now many more degrees of freedom. As shown in Fig. 14 for the same five criteria that have been studied in more detail, each solution requires a specific screw profile and operating condition. Globally, the results seem to make sense. The screw speed of the 75 mm machine is lower than the 50 rpm at which the 30 mm equipment is operating. The average shear rates of both extruders are approximated by increasing the compression ratio of the bigger machine (3.2 versus 2.5); WATS requires a longer metering zone; viscous dissipation and Cameron number are controlled via a smaller compression ratio; the melting profile of the bigger machine can be made more efficient (hence, similar to that developing in the smaller machine) by shortening the compression zone and increasing the rate at which channel depth decreases (this being equivalent to increasing the compression ratio).

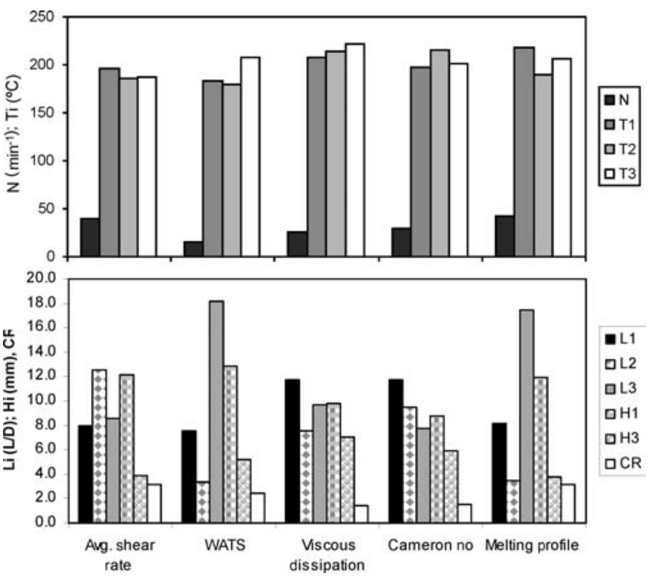

Fig. 14. Full scale-up for case study 2 assuming individual criteria. Top: operating conditions of the target extruder; bottom: geometry of the target extruder

As shown in Fig. 15, again for the same criteria, when the optimal operating conditions used for the scale-up of a particular criterion are adopted, most of the remaining criteria will remain unsatisfied, thus encouraging the application of the multi-criteria approach, as before. Table 7 presents data equivalent to that of Tables 5 and 6 but, for the sake of reading simplicity, the values of the 9 solutions were not included, neither were the objective function values for the individual criteria. Two observations are striking: i) the global F values are lower than before: as seen above, the average value of the global objective functions for operating conditions (Table 5) is 0.20, for geometry (Table 6) is 0.19 and for full-scale-up reduces to 0.15; ii) when the five criteria (C_1 to C_5) are studied together, the corresponding F values become 0.17, 0.15 and 0.11, respectively. This is an encouraging result, since it implies that it is possible to perform extrusion scale-up taking simultaneously into account at least five relevant performance measures without generating significant differences in their thermomechanical behaviour. In principle, the more criteria are incorporated, the more complete the exercise will be, although the success will always be dependent on the nature and eventual conflicting character of the criteria chosen.

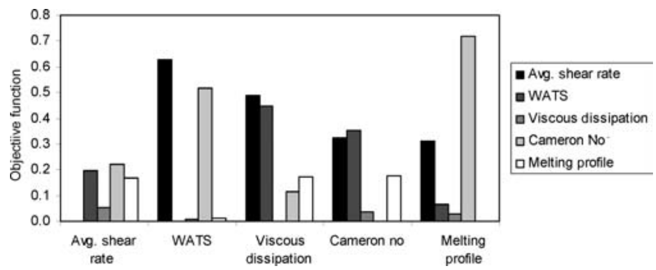

Fig. 15. Effect of individual scale-up on the value of the objective function of the remaining individual criteria (full scale-up, case study 2)

Criteria	F_1 ASR	F_2 WATS	F_3 VD	F_4 Ca	F_5 X/W	F
Avg. shear rate WATS	**0.00**	**0.00**	0.10	0.23	0.17	**0.10**
Avg. shear rate Viscous dissipation	**0.00**	0.01	**0.00**	0.67	0.01	**0.14**
Avg. shear rate Cameron no.	**0.00**	0.17	0.04	**0.00**	0.18	**0.08**
Avg. shear rate Melting profile	**0.00**	0.05	0.01	0.81	**0.00**	**0.17**
Avg. shear rate WATS Viscous dissipation	**0.00**	**0.00**	**0.00**	0.65	0.01	**0.13**
Avg. shear rate Cameron no. Melting profile	**0.00**	0.99	0.04	**0.00**	**0.00**	**0.19**
Avg. shear rate WATS Viscous dissipation Cameron no. Melting profile	**0.26**	**0.04**	**0.03**	**0.05**	**0.17**	**0.11**

Table 7. Multi-criteria scale-up results (full scale-up) for case study 2

5 Experimental Scale-up

Confirming the promising results reported above requires the experimental validation of the methodology developed. This is not at all an easy task, since it requires:

i) the availability of a target extruder having geometrical flexibility, i.e., with many available screw profiles, so that it can be proved that a particular geometry is more adequate for scale-up than the remaining;
ii) the possibility to measure experimentally the variables that are required to quantify the scale-up criteria of the various types considered above (namely, constant values and functions). This would necessitate the availability of two very well instrumented extruders of different sizes.

An extra difficulty lies in the fact that when a direct comparison between theoretical and experimental scale-up is performed, it is not evident which are the contributions of the process modelling routine and of the scale-up methodology to the differences that will certainly be observed between the two sets of data.

Thus, this section reports a preliminary assessment of the scale-up methodology proposed, with an exclusive focus on operating conditions (as it is performed between two existing extruders) and making use of a limited number of criteria. The reference extruder was the 10 mm machine presented in Table 1, while the target extruder is the 30 mm extruder included in the same table. The threefold increase in diameter that the problem involves seems sufficiently significant for validation purposes. Nevertheless, three comments seem relevant:

– it should be emphasized that previous use of the miniature extruder has shown that its small size favours heat transfer in the radial direction, which is not always accounted for correctly by the conventional plasticating models adopted for extrusion modelling;
– the small extruder requires raw material to be fed in powder form. Again, this could affect the predicting capacities of the modelling routine (which takes the solids as a consistent elastic solid), especially in what concerns output and pressure generation.
– The good processability of HDPE does not challenge the predictive capacities of the method (on the other hand, differences between predictions and observations should be little dependent on material characteristics).

The machines selected are prototypes with some interesting capabilities, namely that of collecting quickly material samples along the barrel at predefined locations (see Machado et al. (1999) for details on these devices). Since these samples are approximately spherical in shape, i.e., with a low surface to volume ratio, and polymers have low thermal diffusivity, sticking a fast response thermocouple into their core provides a reasonably accurate measurement of average material temperature (this procedure has been validated by Carneiro et al. (2000)). Therefore, one possible criterion for scale-up can be the axial average material temperature profile, i.e., a function-type objective. Differences between experimental and predicted values are anticipated, as the temperature profile will be measured in a limited number of locations, i.e., the latter will be much cruder than the predicted temperature evolution along the barrel. Despite of the comments above, the second criterion selected was the Q/(WHND) ratio, which normalizes the output to the size and operating conditions of the extruder, as it is easy and accurate to measure.

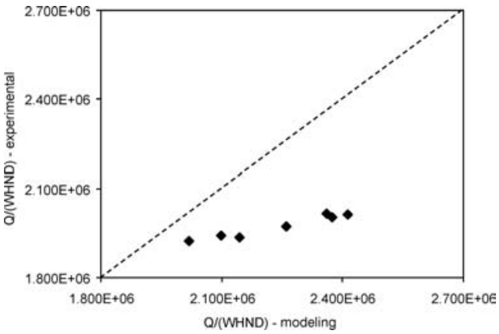

Fig. 16. Experimental versus calculated Q/(WHND)

Fig. 16 compares the values of the predicted and calculated from experimental data Q/(WHND) ratios for the 30 mm extruder. The machine processed the HDPE extrusion grade identified previously at different screw speeds and barrel temperature profiles. It is important to recall the difficulty in obtaining reliable material data, especially when it relates with machine size and materials of construction. For example, although solids conveying is strongly affected by friction coefficients and these depend on the characteristics of the reference and target extruders, the values in Table 3 were used for both machines. The die L_{die} and D_{die} (as defined in Fig. 6) were 130 and 20 mm, respectively. As screw speed ranges between 20 and 70 min^{-1}, differences increase from 4 to 15 %. Experimental data are less sensitive to changes in screw speed than the theoretical predictions.

Having in mind this magnitude of the differences, the procedure was the following:

1. Solve the scale-up problem as in section 4.1 and obtain the corresponding Pareto plot (Fig. 17A depicts both the initial population and the non-dominated solutions of the final population).
2. In this representation, identify the optimal front (shaded area in Fig. 17A). Since both criteria are to be minimized, the optimal front joins solutions 1 to 3. Points 4 to 7, which were picked up to represent the general features of the population, correspond to non-optimal solutions;
3. Identify the set of operating conditions corresponding to these solutions;
4. Carry out extrusion runs using these operating points and, for each one, acquire data on Q, N and on the axial average melt temperature profile;
5. Compute the values of the two objective functions for each run and represent the "experimental" Pareto plot – open points in Fig. 17B.

The detailed analysis of Fig. 17B brings about the following conclusions:

1. The relative coordinates of most of the theoretical and experimental points is comparable;
2. The configuration of the experimental and theoretical optimal front is approximately the same;
3. There is an obvious vertical shift of the experimental data relative to the computational values (about 0.1 in terms of absolute F values).

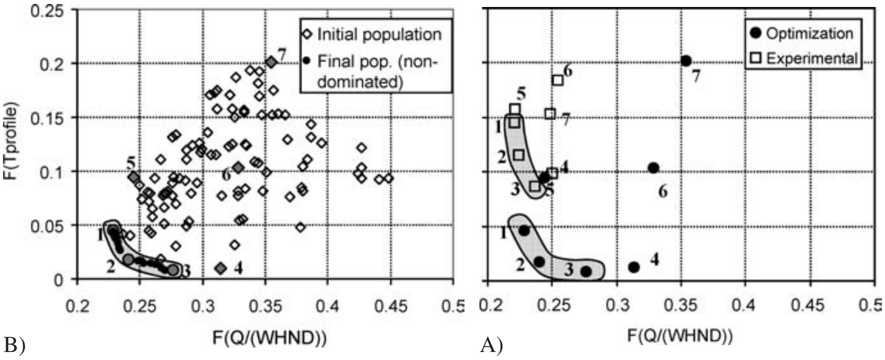

Fig. 17. Pareto plot of a practical scale-up problem. A) Initial and final populations, using the optimization procedure; points 1–3 are non-dominated and are part of the optimal front, whereas points 4–7 are non-dominated. B) Coordinates of points 1–7, as obtained computationally (solid points) and experimentally (open points); the respective optimal fronts are also indicated

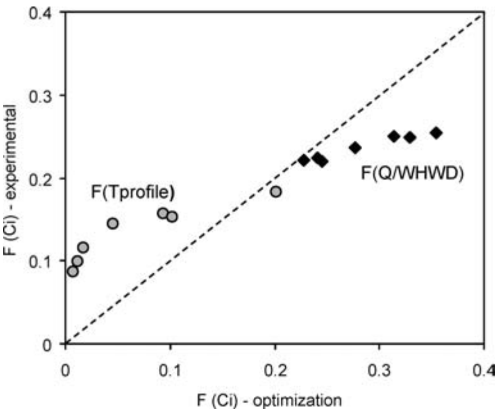

Fig. 18. Experimental versus calculated values of the objective functions

4. The computational solutions extend more along the x-axis than those based on experimental data (again, the difference can attain 0.1 in terms of F values).

Comments 1 and 2 are positive in terms of the practical validation of the methodology proposed in this work. Fig. 18 correlates the values of the individual objective functions determined from optimization and from experimental data. In the case of the Q/(WHND) ratio, the relationship is similar to that shown in Fig. 16, i. e., the computational values are generally higher and extend through broader range than the experimental ones, thus explaining also the differences in the X-axis of Fig. 17. In other words, the differences between experiments and predictions seem to be mainly accountable to the modelling routine. In the case of the temperature profile, the experimental F values are higher than the predicted ones, especially in the lower F range. This explains the vertical shift in Fig. 17, particularly for the points that incorporate the optimal front (by definition, these are the solutions with lower $F(T_{profile})$). Observation 4 was predictable, as it had already been observed that the experimental extruder response is less sensitive to variations in screw speed than the modelling routine.

6 Conclusions

This work proposed an optimization approach for extrusion scale-up, taking single screw extrusion as an example. The methodology is able to consider simultaneously various criteria and can take into account their relative importance. It can be applied to the scale-up of either operating parameters and/or geometry. The efficiency of the scaling-up can be easily assessed, not only due to the quantitative nature of the objective function associated to each criterion, but also by monitoring the implication of the exercise on the satisfaction of other process measures.

It was demonstrated that multicriteria scale-up is more efficient than scaling-up on the basis of a single process response, as the optimization algorithm searches for and generally finds solutions yielding good compromises in terms of the simultaneous satisfaction of various criteria. Also, the more process parameters are included in scale-up exercise, the more efficient scale-up can be, as more degrees of freedom for optimization are provided.

The experiments performed to validate the method provided encouraging results, although further efforts are required.

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

Although this work aimed at proposing a new methodology to tackle extrusion scale-up, it is evident that its practical usefulness depends strongly on the sophistication of the modelling routine. Therefore, since the thermomechanical environment the polymer system is subjected to inside the extruder determines its morphology and consequently its properties, future work should concentrate on coupling models accounting for morphology evolution to improved mathematical descriptions of extrusion.

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