THE DESIGN OF EXTRUSION SCREWS: AN OPTIMIZATION APPROACH

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Abstract

The design of a screw for plasticating polymer extrusion based on scientific principles is still a challenging task, which has received surprisingly little attention in the literature. In the present work the design of a screw is considered as an optimization problem. The corresponding design methodology is discussed. Two alternative approaches are considered. In the first case, the aim is to maximize the value of an objective function that describes quantitatively the process performance in terms of pre-selected important process criteria. A multiobjective optimization scheme resorting to the use of optimal or non-dominated Pareto frontiers is also implemented, where the set of feasible individual solutions in terms of the various criteria is correlated, thus evidencing the compromise between them. The relevance of the solutions and the sensitivity of the method to changes in the criteria considered are demonstrated with a case study.

1- INTRODUCTION

Computational modeling of plasticating extrusion for a particular extruder/polymer/die combination in order to predict the response of the system in terms of important process performance parameters such as output, power consumption, melt temperature and degree of mixing has reached a relative maturity [1-3], despite the need to further improve the theoretical models of specific process stages, such as solids conveying. The so-called direct formulation of the problem (see Figure 1) involves solving sequentially the governing equations relevant for each of the various process stages coupled to the corresponding constitutive equation and boundary conditions (geometry and operating conditions), in order to the velocity and stress components, pressure and temperature [1].

The use of the above equations to the definition of the screw geometry guaranteeing a good general process performance, i.e., the inverse formulation, involves important difficulties. The same governing equations – coupled to identical constitutive equations and to boundary conditions now prescribing flow conditions at specific locations and operating conditions - should be solved in order to the geometry of the channel and to velocity and stress components, pressure and temperature (see Figure 1). Since there is no unique relationship between cause and effect, the problem is mathematically ill-posed [4]. Also, different physical mechanisms may develop along the same screw sections. Therefore, in practice, screw design is accomplished on a trial-and-error basis and little scientific information on the subject has been provided in the open literature.

Nevertheless, some attempts do design a screw "scientifically" have been reported. Chung [5, 6] proposes that once the melting rate and melting capacity are predicted, the metering, compression and feeding sections are designed according to a series of steps with the aim of matching a prescribed output rate, followed by a final adjustment considering common practice and other relevant factors. Rauwendaal [3] considers various design criteria (mechanical

strength, output and power consumption) individually for each geometric zone. The analytical equations describing each extrusion stage are then solved in order to each criterion. For example, the simultaneous optimization of the channel depth and helix angle for melt conveying in order to maximize the output can be carried out. Other authors adopted a statistical analysis for screw design purposes. Potente *et. al* [7, 8] used a modeling package coupled to a multiple regression analysis to optimize the screw geometry. Graphic contour plots of quality functions determined from regression equations were used. Thibodeau and Lafleur [9, 10] adopted a 5 level central composite design method to define the helix angle and the depth and length of the feeding and metering zones that minimize both the extrusion temperature and abrasion in the feeding zone (in terms of slip velocity) and maximize the mixing capability. The optimum screw corresponds to the set of input values that produce the maximum of the global desirability function. Although the statistical methods referred to in these two studies are powerful and well proven, in the case of multimodal and complex response surfaces the number of points used for their description can be insufficient.

This work discusses a screw design methodology based on an optimization approach, where the equations available to solve the direct problem are used iteratively in order to optimize an objective function that evaluates the performance of a screw in terms of a number of relevant design criteria and of their relative importance. An alternative optimization scheme involving the use of optimal or non-dominated Pareto frontiers, which correlate the set of the best feasible individual solutions in terms of the various criteria, thus evidencing the compromise between them, is also implemented. Genetic Algorithms were adopted due to their capacity to deal with combinatorial-type problems and because they do not require derivative information nor additional knowledge on the process [11]. These techniques have been used previously with a considerable degree of success for setting the operating window for specific extrusion situations [12, 13].

2- OPTIMIZATION METHODOLOGY

In general, the aim of optimization is to find the global optimum (or to approach this optimum) on a given search space, by maximizing or minimizing an objective function that can be subjected to some constraints. For a maximization problem:

$$
\begin{aligned}
\text{maximise} \quad & f(x_i) & i &= 1, \ldots, N \\
\text{subject to} \quad & g_j(x_i) \geq 0 & j &= 1, \ldots, J \\
& h_k(x_i) \geq 0 & k &= 1, \ldots, K
\end{aligned}
\tag{1}
$$

where f is the objective function of the N parameters, x_i, g_j are the J ($J \geq 0$) inequality constraints and h_k are the K ($K \geq 0$) equality constraints. The knowledge of the type and number of the individual objectives, the characteristics of the input variables and of the constraints and the anticipated topography of the response surface determine the selection of the best suited optimization method to use in any specific problem.

As in most engineering problems, efficient polymer extrusion of a particular cross-section must satisfy simultaneously several objectives, such as mass output, melting rate, melt temperature, power consumption and degree of mixing. The relative importance of these parameters is subjective and can be considered in two ways.

A global objective function can take into account the individual objectives and weigh their relative importance:

$$
FO_i = \sum_{j=1}^{q} w_j \, F_j
\tag{2}
$$

where q is the number of criteria, w_j is the weight attributed to each criterion (which can vary between 0 and 1, with $\Sigma w_j = 1$) and F_j is the objective function of criterion j which can take two forms, depending on whether one wishes to maximize or minimize it:

$$F_j = \frac{X_j - X_{j_{min}}}{X_{j_{max}} - X_{j_{min}}}$$

(3)

$$F_j = 1 - \frac{X_j - X_{j_{min}}}{X_{j_{max}} - X_{j_{min}}}$$

(4)

In the above equations X_j results from the evaluation of criterion j, while X_{jmin} and X_{jmax} are the minimum and maximum values that this criterion can reach, respectively. All values are in the same non-dimensional linear scale, since by definition each F_j ranges between 0 and 1 and so does the global objective function. Not only the values of the individual and global objective functions provide a good estimation of the fulfillment of the corresponding target given the range of variation, but solutions that have a single criterion with a zero value can be easily eliminated. The aim of the optimization is to maximize the value of FO_i, which can be done using a search and optimization scheme, e.g., Genetic Algorithms [11], coupled to a mathematical model of extrusion. Since a single solution will be obtained, if the relative criteria weights are to be adjusted, the optimization procedure must be repeated. This limitation has been present in this type of studies [e.g., 7-10,13].

Genetic Algorithms, GAs, are stochastic search and optimization methods that mimic natural evolution through genetic operators like crossover and mutation. They work with a population of points, each representing a possible solution in the search space. Each individual has a value associated to it (fitness or objective function), which is a measure of its performance on the system. Individuals with greater performance have a bigger opportunity for reproduction, i.e. to pass their characteristics to future generations [11].

Figure 2 illustrates the above optimization concept, which makes use of an objective function, an optimization algorithm and a modeling package. First, the user defines which parameters should be optimized and their range of variation, and identifies which criteria should be considered and what is their relative importance. In the first generation (iteration) those parameters are defined randomly. Hence, for this set of input parameters, the modeling package predicts the extruder's

response in terms of the prescribed criteria, which is converted into specific relative performance by means of the objective function. The optimization algorithm assesses the quality of this performance and generates new (better) values for the parameters. The iterative process continues until the pre-established number of generations or a stable maximum is reached. The solution to the problem is now available. As discussed above, any modifications to the relative importance of the criteria require a new iterative procedure.

Alternatively, advantage can be taken from the fact that GAs work with a population of individuals to carry out a multiobjective optimization involving the simultaneous but independent optimization of the various criteria. The results are presented in terms of Pareto plots, where the set of feasible individual solutions in terms of the various criteria is represented showing the compromise between them [11]. This work applies for the first time this type of approach to the design of extrusion screws.

In a typical multiobjective optimization there is a set of solutions that is better than the remaining when all the objectives are considered simultaneously, although it can be worst than some solutions when only selected criteria are considered, i.e., since some criteria are conflicting, a solution corresponding to the optimum of all criteria does not exist. Figure 3 shows a Pareto plot of two individual criteria relevant to extrusion, melt temperature at die exit and mechanical power consumption. If both objectives are to be minimized, point 5 is dominated by point 2, since it represents a condition where both criteria have higher values. Points 5 and 6 are dominated, whereas points 1 to 4 are non-dominated and make-up the Pareto optimal or non-dominated frontier, which provides the solution to the problem [11, 14-16]. The exact location of the solution well depends on the relative importance of the criteria, i.e., the value of the weights. For example, point 2 corresponds to a solution where minimization of the mechanical power consumption is more important than reducing the melt temperature.

In practical terms, the optimization procedure is carried out as described above and represented in Figure 2, but considering each criterion separately. The option between both techniques is made when defining the type of optimization. In the case of a multiobjective optimization the results are presented as Pareto plots.

3- SCREW DESIGN METHODOLOGY

The optimization methodology discussed above is capable of dealing with a significant number of variables (criteria and geometrical parameters), computational capacity being the only practical limit. Conflicting criteria can be dealt with and different design strategies can be accommodated. Moreover, the optimization tool can provide a good physical understanding of the response of the extruder to changes in the most important process variables.

Figure 4 shows how the optimization is used for screw design purposes. Before defining the parameters to optimize and the relevant criteria to take into consideration, process economics, previous experience, or even equipment availability will dictate the type of screw to be designed. After establishing the geometrical parameters to be defined, the design criteria and their relative importance, the optimization algorithm will provide a solution to the problem, i.e., what is the most adequate screw to process a specific material under given operating conditions, in order to obey some well defined and precise criteria.

In practice, changes in polymer properties and/or operating conditions occur, either involuntarily (batch to batch differences), or because different material grades are processed in the same machine (and the operating set values are eventually adjusted). Also, although the designer identified a number of design criteria and established their relative importance, some flexibility is advisable, given the subjectivity of this matter. Consequently, a set of better screws (instead of the best one) should be selected, and each one tested in terms of its relative sensitivity to limit

changes in those variables. The best screw will exhibit on average a good and stable performance.

In principle, the design methodology can also define the need, location and geometry of mixing sections. Conventional and non-conventional screws could be directly compared (and the relevant geometrical variables optimized). This has not yet been implemented, because a cost function relating machining costs should also be developed.

4- EXTRUSION MODELLING

The modeling package must provide reliable predictions, be sensitive to changes in the input parameters and require moderate computational resources. Both univariate and multivariate statistical analyses have shown [17] that all main screw geometrical parameters and their combinations of second and third order are significant for the major screw design criteria.

The pioneering work of Maddock and Street [18, 19] on the phenomenological understanding of the mechanisms developing along the axis of a screw extruder provided a starting point for modeling attempts of plasticating extrusion. Currently, and after numerous and intensive efforts, it is possible to describe the process theoretically from hopper to die with a reasonable degree of accuracy, depending on the assumptions undertaken and on the numerical scheme adopted [1,2,20]. In the present case, models available in the literature describing each individual process stage were sequentially connected using the appropriate boundary conditions, in order to have a coherent link between adjacent zones. Six functional zones were considered (Figure 5):

    i) **Solids conveying in the hopper** - gravity conveying of granular materials;

    ii) **Solids conveying in the screw** - friction drag solids conveying;

    iii) **Delay zone** - conveying of solids (partially) surrounded by a melt film;

    iv) **Melting zone** with a specific melting mechanism;

    v) **Melt conveying**;

vi) **Melt flow** through the die.

The global program structure is presented in Figure 6 [12], while Figure 7 schematizes the assumptions for each zone along the screw. Calculations are carried out for small increments (Δz) along the hopper, screw channel and die. Convergence is obtained when the pressure at die exit is lower than a small predefined value (ε). This requires iterative computations assuming two initial values for output (Q_1 and Q_2) and the secant method is used to define new values for the following iteration.

Vertical pressure at the bottom of the hopper is taken as the initial condition for the calculations along the screw length. It is estimated from a force balance on an elemental horizontal slice of bulk solids material under static loading conditions [21]. Friction drag solids conveying in the initial turns of the screw considers the conveying of a solid plug under non-isothermal conditions with heat dissipation at all surfaces. Pressure generation was computed using the equations of Broyer and Tadmor [22] (isothermal solids conveying with non-isotropic pressure distribution) and the temperature profile was determined modifying the analysis of Tadmor and Broyer [23] (non-isothermal solids conveying with heat dissipation at the barrel surface due to friction) by considering heat dissipation at all metallic surfaces [12]. Delay in melting was modeled assuming the development of two sequential stages, and not by a single treatment. Since melting occurs due to the combined contribution of heat conduction (from the barrel/screw) and mechanical energy dissipation (proportional to local friction at the interface), it is anticipated that a melt film separating the solid bed from the inner barrel wall will be formed initially. Eventually, when the combined contribution of local mechanical and thermal energies is also sufficient to induce melting, the solid bed will be later surrounded by melt films separating it from the screw surfaces. The first step was described by a modification of the Kacir and Tadmor [24] analysis (which assumes a fully developed melt film in the down and cross channel directions) taking into account heat convection in the down-channel and radial directions and

heat conduction in the radial direction [12]. The second step was considered a particular case of melting [12, 25].

The five-zone melting model developed by Lindt *et al.* [25, 26] (solid bed surrounded by a melt pool and three melt films) was adopted. The temperature field in the melt films was assumed to be fully developed in the cross channel direction, heat conduction in the down channel direction being neglected and the solid bed velocity being taken as constant.

Finally, melt conveying was described assuming the two-dimensional non-isothermal flow of a non-Newtonian fluid in presence of convection [27, 28].

Bigg [29] developed a two-dimensional non-Newtonian isothermal model where the "degree of mixing" in an extruder is quantified in terms of WATS (Weighted Average Total Strain) [30]. This method is adopted, but considering that the velocity on the z direction varies with x and y and the flow is non-isothermal.

5- SCREW DESIGN

5.1- Case study

In the example pictured in Figure 8 the objective is to define the length of the feed and compression zones (L_1 and L_2), the internal screw diameter of the feed and metering zones (D_1 and D_3), the screw pitch (S) and the flight clearance (e) of a screw, a range of variation being prescribed for each variable. The diameter and total screw length must remain constant, in order to fit the available extruder. The screw should maximize the output (objective F_1) and the degree of mixing – WATS (F_2), and minimize the length of screw required for melting (F_3), the outlet melt temperature (F_4), the mechanical power consumption (F_5) and the viscous dissipation along the barrel. The latter will be assessed by two ratios: average melt temperature/barrel temperature (F_6) and maximum melt temperature/barrel temperature (F_7). The operating conditions used and the die geometry are also presented in Figure 8. A High Density Polyethylene blown film

extrusion grade (NCPE 0928, from BOREALIS), with the properties quantified in Table 1, was considered in the calculations. Although this is a relatively simple example that does not consider the effect of mixing sections, the validity of the computer predictions can be more easily assessed than if using a complex geometry, given the practical difficulty of planning an experimental validation scheme. Table 2 presents the criteria's range of variation (equations 3 and 4). Any solution outside the valid range for the criteria will be attributed a $FO_i=0$.

The two optimization strategies discussed above, i.e., using a global objective function and performing a multiobjective optimization based on Pareto curves, were studied. The GAs parameters used in the optimizations were [11]:

- Number of generations (i.e., number of iterations) – 50
- Genetic operators: crossover rate of 70%, mutation rate of 0.4% and no inversion rate
- Population size (i.e., number of individuals in each generation) – 500
- Chromosome length (i.e., length of the binary codification of each individual) – 48
- Multiobjective optimization parameters: sharing function [11] (σ_{share}) of 0.01, indifference limits [12] (*limit*) of 0.1% and 10 ranks for the reduction of Pareto set [12] (*N_Ranks*).

5.2- Optimization with objective function

As shown in Table 3, which presents the weights affecting each of the seven criteria for the twelve case studies considered, the optimization methodology was tested in two steps. First, the best screw geometry was defined for each individual criterion, since it is easier to assess the value of the predictions. Then, all the criteria were considered simultaneously.

Table 4 compares the geometrical parameters of the best screws obtained when the various criteria are considered individually (case studies 1 to 7). The solutions are clearly sensitive to the characteristic of the criterion under consideration. Figures 9 and 10 depict the actual screw profile for cases 1 and 2, respectively, i.e., when the geometry must maximize the output (F_1) and the degree of mixing (F_2). A screw with long transport section, high metering depth and

small compression ratio maximizes the output. The high metering depth follows the guidance provided by Rauwendaal [3] when his analytical method is applied to the simultaneous optimization of the channel depth and helix angle during melt conveying. Of course, in the present work the entire screw is optimized simultaneously. In the case of ensuring adequate mixing the metering section must be long and shallow to increase the average shear rate and maximize the residence time. These are obviously two conflicting criteria.

Even in such simple situations the objective function can be multimodal, i.e., various maxima with similar values might exist, as exemplified in Figure 11 where output is plotted against the screw length of feed (L_1) and compression (L_2) zones. In practice, when various identical optimizations using the same conditions are made, Genetic Algorithms converge for different results. The difficulties of the optimization process increase when the global objective function needs to take into consideration contradicting criteria simultaneously. Table 5 shows the geometry of the screws obtained for case studies 8 to 12 (see also Table 3). Again, the relative importance of the individual criteria within the global objective function influences the solution proposed. When output maximization is the major aim (case studies 9 to 11) the optimum screw is similar to that of case study 1, i.e., with a long transport section and small compression ratio, which is not surprising. In the remaining cases, the screw has a long shallow metering section.

As an example, Figure 12 represents the evolution of the individual and global objective functions for case study 8 (all criteria are assumed as equally important) as the optimization proceeds, leading to the results in the first row of Table 5. A stable optimum is found before the 50th generation, where the exercise is interrupted. Also, around the 20th generation most individual criteria have already reached a plateau, but GAs will attempt to find some place for improvement. For example, at the 40th generation the global objective function is slightly improved by an increase in output that more than counterbalances the decrease in the degree of mixing, and the increase in both the length of screw required for melting and in power

consumption. It is clear that this solution results from a compromise between the relative satisfaction of different conflicting individual criteria. The actual screw profile at the 50th generation is drawn in Figure 13 and appears to be a compromise between the geometry presented in Figures 9 and 10, which makes sense as those two criteria are included in the objective function. The sensitivity of this screw to changes in the operating conditions is estimated in Figure 14, which shows the predicted performance of the extruder working at three different screw speeds (N_1 = 45 rpm, N_2 = 50 rpm and N_3 = 55 rpm) with three distinct barrel temperature profiles (T_{b1} = 145-155-165 °C, T_{b2} =150-160-170 °C and T_{b3} = 155-165-175 °C). The best performance is obtained for the lowest screw speed and barrel temperature profile (N_1 and T_{b1}), which are different from the values prescribed initially (see Figure 8). Efficiency deteriorates with increasing barrel temperature and screw speed. This results from the fact that, as shown by an analysis of the behavior of the individual criteria, F_1 and F_2 increase with the screw speed and barrel temperature, contrarily to criteria F_3 to F_7, all criteria having the same importance.

Nothing prevents the operating conditions to be incorporated in the optimization as parameters to be optimized. Their range of variation must be defined a priori ($N \in [10;50]$ rpm and $T_b \in [150-160-170;190-200-210]$). The corresponding results for case study 8 (all seven criteria are equal) are synthesized in Figure 15 in terms of screw profile and set operating values. The screw is not very different from that obtained previously (Figure 16), but the recommended operating conditions are distinct, particularly the screw speed. This is a consequence of the fact that most criteria (outlet melt temperature, F_3, length of screw required for melting, F_4, mechanical power consumption, F_5 and viscous dissipation along the barrel, F_6 and F_7) are optimized for low screw speeds, the total sum of their weights being greater than that of the remaining criteria (output and degree of mixing).

5.3- Multiobjective optimization

In Multiobjective Optimization with GAs there is no need to define a priori the individual weights in a global objective function, since choosing any solution along the Pareto frontier corresponds to fixing those weights. Alternatively, the decision maker can apply equation 2 to the final/optimized population and obtain the best screws for a given set of weights. In parallel, a good physical description of the extruder's response to the relevant criteria can be obtained. The Pareto plots pictured in Figures 16 and 17 correspond to the optimization of the general case study presented in Figure 8. The figures show some of the correlations in the criteria and parameters to optimize domains, respectively, against output or length of transport section. In fact, a seven-dimensional response surface exists, given the number of criteria. For example, as one wishes to maximize the output while minimizing the power consumption and maximizing the degree of mixing, the Pareto optimal frontier lies along the abscissa axis, on top and on bottom of the clouds of points of the corresponding graphs, respectively (Figure 16). Some points that seem to be dominated in one particular Pareto plot are certainly non-dominated in another.

The results on the optimal criteria domain frontiers (Figure 16), i.e., the Pareto plots relating the optimization criteria for the 50th generation population, show that a high range of outputs can be obtained by changing the screw parameters. While melt temperature, mechanical power consumption and viscous dissipation seem to have little influence on output for the range of optimized geometries, the degree of mixing and the melting efficiency can vary considerably at constant output. Of course, different relations between the optimization criteria could have been plotted, e.g., all criteria against WATS. The corresponding correlation would then became evident. The analysis of the plots on the parameters to optimize domain (Figure 17) shows that most of the search space is feasible, i.e., many geometrically feasible combinations of the

configuration parameters can produce adequate screws, depending on the relative importance of the criteria.

The best solutions obtained with this technique are identified in Table 6, which can be compared directly with Table 3, when an objective function is adopted. The values of the global objective function are slightly lower in Table 6, which could be due to the fact that in multiobjective optimization the algorithm search solutions for all the combinations of criteria importance, whilst when using an objective function search is routed into one unique and specific direction. Nevertheless, the geometry of the screws proposed in both cases is very similar.

The last step in the design methodology consists in testing the solutions to limited changes in polymer properties, operating conditions and/or relative importance of the criteria (see Figure 4). For example, Table 7 lists the five best screws obtained when all the criteria have identical importance (case study 8). In order to study their performance under different processing conditions, simulations using three screw speeds ($N_1 = 45$ rpm, $N_2 = 50$ rpm and $N_3 = 55$ rpm) coupled to three barrel set temperature profiles ($T_{b1} = 145$-155-165 ºC, $T_{b2} = 150$-160-170 ºC and $T_{b3} = 155$-165-175 ºC) were carried out, and the corresponding response quantified in terms of the global objective function value. As illustrated in Figure 18, the behavior of the five screws for the various processing conditions is quite similar, solutions 1 and 2 being the preferred ones given their global (average) performance. The data compiled in Figure 19 refers to the response of the same five screws to changes in the rheological properties of the polymer. In this case, three power law indices ($n_1 = 0.31$, $n_2 = 0.345$ and $n_3 = 0.38$) and three consistencies ($k_1 = 27$ kPa.s, $k_2 = 29.94$ kPa.s and $k_3 = 33$ kPa.s) were selected. Screw 1 seems to have a slightly more consistent behavior, which makes it the adequate solution, given the previous result.

6- CONCLUSIONS

The optimization methodology adopted in this work for screw design purposes is sensitive to the type and relative importance of the design criteria and seems to provide meaningful results. The work needs experimental validation although this is not easy for obvious reasons. Also, the inclusion of distributive and dispersive mixing sections, or barrier compression zones in the basic screw profile will increase the practical interest of the analysis, despite the difficulties in assessing the value of the predictions.

Any scientific method for extrusion screw design will always depend on the ability of the theoretical model describing the process to predict the response of the extruder in terms of the most relevant parameters. Hence, the initial stages of solids conveying when loose pellets are present (and not a continuous elastic solid), the differences in behavior between semi-crystalline and amorphous polymers, or the dynamic stability of the process need to be taken into account more satisfactorily.

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Nomenclature

δ_C	thickness of melt film C
δ_{DE}	thickness of melt film D/E.
ρ_{share}	radius of a circumference that is the maximum distance between chromosomes
CR	compression ratio
D	internal barrel diameter
D_1, D_3	internal screw diameter of feed and metering zones, respectively
e	flight width
F_j	individual objective function
FO_i	global objective function
H	channel depth
k	constant of the power law viscosity equation
L	total screw length
L_1, L_2	length of feed and compression zones, respectively
$limit$	indifference limit above which the performance of the solutions is considered as similar
N	screw speed
N_Ranks	pre-defined number of ranks
n	constant of the power law viscosity equation
q	number of criteria
Q	volumetric flow rate
q_b	heat flux on the barrel
q_f	heat flux on the flights
q_s	heat flux on the root of the screw
S	screw pitch
T_b	barrel temperature
T_m	melting temperature
T_s	temperature at screw surface
T_{s0}	polymer temperature at extruder inlet
V_b	barrel velocity
V_{bx}	barrel velocity in cross-channel direction
V_{bz}	barrel velocity in down-channel direction
V_{sz}	velocity of the solid bed in the z direction
W_b	melt pool width
$\overline{W}$	average channel width
w_j	criteria weight
x	Cartesian coordinate
X_j	value of criterion j
X_{jmax}	maximum value of criterion j
X_{jmin}	minimum value of criterion j
y	Cartesian coordinate
z	Cartesian coordinate
Δz	differential element in the z direction

FIGURE CAPTIONS

Figure 1- Polymer extrusion direct and inverse problems.

Figure 2- Optimization methodology.

Figure 3- Example of a Pareto plot.

Figure 4- Screw design methodology.

Figure 5- Physical phenomena considered in plasticating screw extrusion.

Figure 6- Global program structure for extrusion modeling.

Figure 7- Physical assumptions for: a) solids conveying; b1) delay zone 1; b2) delay zone 2; c) melting; d) melt conveying (A- solid bed, B – melt pool, C, D, E – melt films).

Figure 8- Screw geometric parameters to optimize.

Figure 9- Optimum screw for output maximization – case study 1 (CR – screw compression ratio).

Figure 10- Optimum screw for mixing maximization – case study 2.

Figure 11- Output contour plot as a function of screw length of feed (L_1) and compression (L_2) sections.

Figure 12- Evolution of the individual and global objective functions during the optimization of case study 8.

Figure 13- Optimum screw for case study 8.

Figure 14- Sensitivity to changes in operating conditions – case study 8.

Figure 15- Screw and operating conditions (optimized simultaneously) for case study 8.

Figure 16- Pareto plots at the criteria domain.

Figure 17- Pareto plots at the parameters to optimize domain.

Figure 18 - Sensitivity of a set of screws to small changes in processing conditions – case study 8 (see text for details of N and T_b).

Figure 19 - Sensitivity of a set of screws to small changes in viscosity – case study 8 (see text for details of n and k).

Table 1- Polymer properties.

Property	Equation	Values
Solids density	$\rho = \rho_\infty + (\rho_0 - \rho_\infty)e^{FP}$ *with* $F = b_0 + b_1\,T + b_2\,T^2 + \dfrac{b_3}{T_g - T}$	ρ_∞ = 948 kg/m³ ρ_0= 560 kg/m³ Tg= -125 °C b_0= -1.276e-9 1/Pa b_1= 8.668e-9 1/°C Pa b_2= -5.351e-11 1/°C² Pa b_3 = -1.505e-4 °C/Pa
Melt density	$\rho_m = g_0 + g_1\,T + g_2\,P + g_3\,T\,P$	g_0 = 854.4 kg/m³ g_1 = -0.03236 kg/m³ °C g_2 = 2.182e-7 kg/m³ Pa g_3 = 3.937e-12 kg/m³ °C Pa
Friction coefficients		polymer-barrel = 0.45 polymer-screw = 0.25
Solids thermal conductivity		0.186 W/m °C
Melt thermal conductivity		0.097 W/m °C
Heat of fusion		196802 J/kg
Solids specific heat		1317 J/kg
Melt specific heat	$C_m = C_0 + C_1\,T + C_2\,T^2$	C_0 = -1289 J/kg C_1 = 86.01 J/kg °C C_2 = -0.3208 J/kg Pa
Melting temperature		119.6 °C
Viscosity	$\eta = k_0\,\dot{\gamma}^{n-1}e^{-a(T-T_0)}$	n = 0.345 k_0 = 29.94 kPa sⁿ a = 0.00681 1/°C T_0 = 190 °C

Table 2- Criteria limits of variation.

Criterion	$X_{i\ min}$	$X_{i\ max}$
F_1 (kg/hr)	1	20
F_2	0	1300
F_3 (m)	0.200	0.936
F_4 (°C)	150	210
F_5 (W)	0	10000
F_6	0	2
F_7	0	3

Table 3- Case studies and the corresponding individual weights.

Case studies		Weights						
		w_1	w_2	w_3	w_4	w_5	w_6	w_7
1	Individual criteria	**1.0**	0.0	0.0	0.0	0.0	0.0	0.0
2		0.0	**1.0**	0.0	0.0	0.0	0.0	0.0
3		0.0	0.0	**1.0**	0.0	0.0	0.0	0.0
4		0.0	0.0	0.0	**1.0**	0.0	0.0	0.0
5		0.0	0.0	0.0	0.0	**1.0**	0.0	0.0
6		0.0	0.0	0.0	0.0	0.0	**1.0**	0.0
7		0.0	0.0	0.0	0.0	0.0	0.0	**1.0**
8	Combined Criteria	1/7	1/7	1/7	1/7	1/7	1/7	1/7
9		0.4	0.1	0.1	0.1	0.1	0.1	0.1
10		0.6	0.1	0.05	0.05	0.05	0.1	0.05
11		0.6	0.3	0.1	0.0	0.0	0.0	0.0
12		0.1	0.3	0.4	0.1	0.0	0.1	0.0

Table 4- Optimum screw for various individual criteria (case studies 1 to 7).

Geometrical parameters	Case study (individual criteria)						
	1	2	3	4	5	6	7
L1 (mm)	390.0	100.0	100.0	100.1	390.0	110.0	110.0
L2 (mm)	200.1	240.0	170.0	200.1	381.6	290.0	215.5
D1 (mm)	23.1	25.3	25.6	25.7	20.0	25.8	24.7
D3 (mm)	26.1	31.9	30.7	31.9	28.2	30.0	31.9
P (mm)	41.9	30.0	41.6	41.1	30.5	41.7	41.7
E (mm)	3.0	3.6	3.0	3.9	3.0	3.2	3.6
H1 (mm)	6.5	5.4	5.2	5.2	8.0	5.1	5.7
H3 (mm)	5.0	2.1	2.7	2.1	3.9	3.0	2.1
CR	1.3	2.6	2.0	2.5	2.1	1.7	2.8

Table 5- Optimization with objective function: screw geometry for case studies 8 to 12.

Case Study	L_1 (mm)	L_2 (mm)	D_1 (mm)	D_3 (mm)	S (mm)	e (mm)	Global Objective Function
8	100.0	180.0	25.8	30.7	41.8	3.00	0.582
9	400.0	170.0	23.6	26.0	41.9	3.00	0.663
10	400.0	190.0	23.5	26.0	41.8	3.00	0.729
11	400.0	210.0	22.9	26.0	41.8	3.00	0.628
12	100.0	260.0	24.9	31.9	30.9	3.00	0.524

Table 6 – Multiobjective optimization: screw geometry for case studies 8 to 12.

Case Study	L_1 (mm)	L_2 (mm)	D_1 (mm)	D_3 (mm)	S (mm)	e (mm)	Global Objective Function
8	120.0	180.0	25.4	30.1	40.6	3.04	0.570
9	380.0	210.0	23.1	26.6	41.1	3.00	0.643
10	380.0	210.0	23.1	26.6	41.1	3.00	0.693
11	380.0	210.0	23.1	26.6	41.1	3.00	0.605
12	100.0	300.0	25.8	31.1	39.2	3.40	0.485

Table 7 – Multiobjective optimization: five best screws for case study 8.

L_1 (mm)	L_2 (mm)	D_1 (mm)	D_3 (mm)	S (mm)	e (mm)	Global Objective Function
120.0	180.0	25.4	30.1	40.6	3.04	0.570
100.0	180.0	21.8	29.3	41.8	3.10	0.569
120.0	180.0	25.6	29.5	40.4	3.00	0.568
120.0	180.0	25.4	30.7	40.4	3.12	0.568
120.0	180.0	25.0	30.3	40.6	3.16	0.568

Direct problem:

	Governing equations	
• Geometry • Polymer properties • Operating conditions	→	• Output • Power consumption • Melt temperature • Degree of mixing • ...
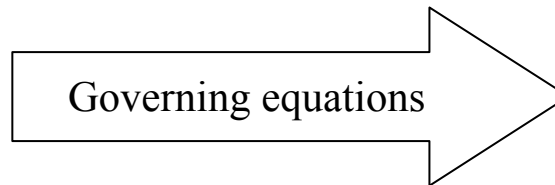
Inverse problem:

	Governing equations	
• Polymer properties • Output • Power consumption • Melt temperature • Degree of mixing • ...	→	• Geometry • Operating conditions • ...
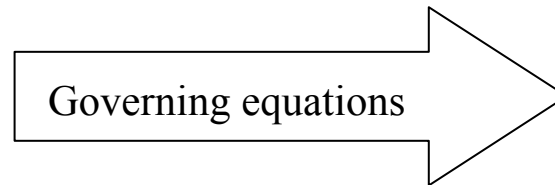
Optimization Algorithm

Objective function → Solution

Multiobjective optimization

USER

Definition of:
- Parameters to optimize
- Type of optimization

Definition of:
- Criteria
- Weights

Evaluation/ new (better) solutions

Pareto plot
Pareto plot
Pareto plot

Performance

Extruder response

Objective Function

Modeling Package

```
                    ┌─────────────────┐
                    │  Type of screw  │
                    └─────────────────┘
                             │
              ┌──────────────┴──────────────┐
              ▼                              ▼
     ┌─────────────────┐          ┌─────────────────────┐
     │    Relevant     │          │    Geometrical      │
     │    criteria     │          │     parameters      │
     └─────────────────┘          │   to be defined     │
              │                   └─────────────────────┘
              │                              │
              ▼                              ▼
     ┌────────────────────────────────────────────┐
     │           Optimization methodology          │
     └────────────────────────────────────────────┘
              │                              │
         Objective                      Multiobjective
         function                       optimization
              │                              │
              │                              ▼
              │                   ┌─────────────────────┐
              │                   │  Set of better      │
              │                   │      screws         │
              │                   └─────────────────────┘
              │                              │
              │                              ▼
              │                   ┌─────────────────────────┐
              │                   │ Sensitivity to limited  │
              │                   │ changes  in:            │
              │                   │  - polymer properties   │
              │                   │  - operating conditions │
              │                   │  - criteria             │
              │                   └─────────────────────────┘
              │                              │
              ▼                              ▼
              ╭──────────────────────────────────╮
              │                                  │
              │           BEST SCREW             │
              │                                  │
              ╰──────────────────────────────────╯
```

i) Hopper

Heater bands

ii)   **iii)**   **iv)**   **v)**   **vi)**

Die

Channel cross-sections

Solids Conveying   Delay   Melting   Melt Conveying

```
                    ┌─────────────┐
                    │    Start    │
                    └──────┬──────┘
                           │
                    ┌──────▼──────┐
                    │   Define:   │
                    │  Q₁ and Q₂  │
                    └──────┬──────┘
                           │
        ┌──────────┐       │
        │          │  ┌────▼─────────────────┐
        │   New    │  │ •Hopper              │
        │ Q₁and Q₂ │  │ •Solids Conveying    │   For each ΔZ
        │          │  │ •Delay               │
        └────▲─────┘  │ •Melting             │
             │        │ •Melt Conveying      │
             │        └────┬─────────────────┘
             │             │
             │        ┌────▼─────┐
             │        │   Die    │
             │        └────┬─────┘
             │             │
             No        ┌───▼────┐
             │         │ P_exit │
             └─────────┤ < ε    │
                       └───┬────┘
                          Yes
                       ┌───▼────┐
                       │  End   │
                       └────────┘
```

Start

Define:
Q_1 and Q_2

New
Q_1 and Q_2

- **Hopper**
- **Solids Conveying**
- **Delay**
- **Melting**
- **Melt Conveying**

For each ΔZ

Die

$P_{exit} < \varepsilon$

No

Yes

End

a)

b1)

b2)

c)

d)

D1 = [20,26] mm

D3 = [26,32] mm

Heater band

10.3D

7D

6D

20 mm

2 mm

D = 36 mm

2.7D

L1= [100,400] mm

L2 = [170,400] mm

235 mm

L = 936 mm

Operating conditions:
N = 50 rpm
Tb = 150 - 160 - 170 ºC

Pitch:
S = [30,42] mm

Flight thickness:
e = [3,4] mm

A)

B)

D=36 mm S=41.9 mm; e= 3 mm

$D1$= 23.1 mm

10.8D 5.6D 9.6D

$D3$= 26.1 mm

CR = 1.3

D=36 mm   *S*=30.0 mm; *e*= 3.6 mm

D1= 25.3 mm

2.8*D*   6.7*D*   16.5*D*

D3= 31.9 mm

CR = 2.6

D=36 mm S=41.8 mm; e= 3.0 mm

$D1$= 25.8 mm

2.8D 5.0D 18.2D

$D3$= 30.7 mm

CR = 1.92

D=36 mm S=37.8 mm; e= 3.1 mm

$D1$= 25.6 mm

2.8D 4.7D 18.5D

$D3$= 31.7 mm

CR = 2.42

Operating conditions:
  N = 12.2 rpm
  Tb = 160 - 165 - 170 ºC