

In: Optimization in Polymer Processing

ISBN # 978-1-61122-818-2

Editor: A.Gaspar-Cunha, J. A.Covas, pp.1-9 ©2011 Nova Science Publishers, Inc.

Chapter 1

INTRODUCTION

José António Covas, António Gaspar-Cunha

IPC/I3N, Institute of Polymers and Composites, University of Minho,
Guimarães, Portugal

The World's consumption of Plastics has increased steadily for several decades, thus mirroring the technological and societal advances within the same period. The forecast for 2010 reaches 259 million tons, up from 190 in 2004 and from 86 in 1990 (source: Plastics Europe Deutschland, WG Statistics and Market Research). In fact, the plastics consumption per capita is nowadays a well know economical indicator, given its good correlation with the Gross National Income of a specific economy. This widespread use of plastics in packaging, electrical and electronics, building, medical, automotive, aeronautics, sports and leisure, fishing, agriculture, textile and toys applications results from a number of inherent favorable characteristics, such as low density, thermal, electrical and acoustical insulation, low permeability to liquids and gases, good mechanical performance (tensile, impact), good aesthetical characteristics (namely in terms of color, gloss and touch) and easy conversion into useful products, even if with complex shapes. For a given polymer, these properties can be easily tuned via additivation (for example, plasticizers, impact modifiers, reinforcements), but the polymer itself can be modified in terms of its molecular weight and/or molecular weight distribution, or grafting of specific chemical species, in order to make it more adequate to a particular application of processing technology (known as *grade* in the industrial jargon). However, the full range of properties - e.g., from

elastomeric to quite rigid, from transparent to opaque, from low to high service temperature - can be explored via the selection of a material from hundreds of possibilities (including polyolefins, polyamides, vinyls, polyesters, polyurethanes, or their blends).

A number of processing technologies has been made progressively available to convert the above polymeric systems into industrial successful products, with adequate dimensional tolerances, required aesthetics and sufficient performance under service conditions. In the case of thermoplastics, the most important are injection molding, extrusion, blow molding and thermoforming. Most of these techniques rely on the same working principle: the raw material, generally in the form of solid pellets, is heated until full melting; this melt is then forced to take the shape of the product (e.g., flow through a die in the case of extrusion, filling of the mold cavity in injection molding); the melt is cooled down until solidification (in practice, until it becomes sufficiently rigid to be handled). The spectacular developments in sensing, informatics and electronics have been applied to these technologies, yielding significant increases in precision, accuracy, reproducibility, control, automation and energy savings. Thus, processing equipments show increasing output capacity, flexibility and control capability.

Nevertheless, the chief contribution to equipment enhancement is associated to the progress of the knowledge of the physical phenomena involved in a production cycle. Polymers have low thermal conductivity (this is usually a very useful property in terms of final application, but a drawback whilst heating or cooling for processing purposes), may degrade upon exposure to the processing temperatures, may crystallize upon cooling (this affecting the optical characteristics) and their melts are generally highly viscous and exhibit some elasticity. In practice, the development of flow, temperature, material morphology and homogeneity inside/along a processing unit is quite complex.

Scientific and technical studies of polymer processing began by identifying and then analyzing the major individual steps of each process, their related physical, thermal, rheological and chemical phenomena and their influencing parameters. Correlations between these phenomena and operating conditions and equipment geometry, as well as between the latter and final product properties were soon established. For example, thermoforming denotes a group of techniques that typically consist in heating a plastic sheet, pushing it against the contours of a mould and cooling the part before extraction from the mold. Applications range from food packaging to large parts for electric appliances. From a process analysis point of view, the

production cycle can be divided in three stages, heating, mechanically deforming the sheet and cooling the part. Thin sheets are generally heated by radiation, hence the first stage can be assumed as equivalent to heating a plastic sheet by radiation during a certain time, with possibly convective surface losses. The corresponding process parameters include the heater and initial sheet temperatures, sheet thickness and heating time (operating conditions), the distance between heater and sheet, the type of heater and oven layout (equipment characteristics), the sheet emissivity and thermal conductivity (material's properties). During heating, a complex temperature profile develops and the sheet may sag - thus affecting its thickness and distance to the heater - and its surface quality may be affected. In parallel, a vast amount of empirical knowledge has also been accumulated, namely on the processability and operating window of different materials and on the efficiency and working life of different types of heaters.

Only when the role of each parameter on the process response is known, it becomes possible to ameliorate the process performance in an efficient way. Practical information can be exclusively used for this purpose, although it is usually associated to expensive (and often time and material consuming) trial-and-error experiments. Also, it is difficult to extrapolate existing experience to new concepts or solutions. Despite of these limitations, many new technological solutions continue to pop up based on ideas from experienced practitioners, which are then validated and empirically developed. Alternatively, process modeling seems an elegant, powerful and efficient tool to improve the knowledge of a given processing sequence and, thus, enable its progress. There is an abundant, ever increasing literature on modeling of polymer processing. From early attempts assuming 1D isothermal flow and heat transfer, purely Newtonian viscous melts or elastic solids and simplified geometries of product or equipment, the field has developed significantly in the last two decades, producing sophisticated numerical codes with very good prediction capability (as ascertained from direct comparison of computational predictions with experimental measurements), not only of the flow kinematics, but also of morphology development and even of the final product dimensions and (some) properties. Depending on the processing technique, and on whether the computational model focus on a number of process stages or on the entire processing sequence, this may mean a 3D non-isothermal flow and heat transfer analysis, the consideration of the solid or of the melt viscoelastic behavior (through complex constitutive equations) and of the effect of normal stresses, the full description of the product and/or equipment geometry and the insertion of morphology development analyses and/or of multi-scale

approaches capable of predicting macroscopic properties. Some commercial software's are available on the market.

Generally, the greater the sophistication of a software, the greater the expertise required from the user and the greater the costs involved. Thus, the utilization of software for design and engineering purposes must be very efficient. Unfortunately, this is often not the case. Taking as an example single screw extrusion, the process engineer might want to use process modeling software to set up the operating conditions to be adopted for the manufacture of a new product. After entering into the program the geometrical characteristics of the extruder and die, the relevant polymer properties and a specific operating condition (screw speed and barrel temperature profile), the program runs and she or he will be confronted with a more or less complete description of flow and heat transfer along the screw. Usually, the data is presented as axial evolution of pressure, temperature, shear rate, viscosity and degree of mixing along the screw, mass output, power consumption, velocity profiles at specific channel cross-sections, et cetera. It is up to the user to "digest" this information and judge whether the predicted thermomechanical environment and global process response are adequate or not (for instance, is the output large enough? Is the final degree of mixing sufficient? Is the maximum melt temperature acceptable? Are local residence times excessive?). The user may decide to investigate the effect of screw speed on the machine performance, thus repeating a number of times the modeling and analysis process. At the end of the study, adequate set operating conditions may have been defined, but there is no evidence if it would have been possible to find a better solution.

From a mathematical point of view, process modeling consists in solving the relevant governing equations (in the case of melt flow they comprise mass, momentum and energy conservation equations), coupled to material constitutive equations (e.g., viscosity, density) and considering the relevant geometrical/operational boundary/initial conditions, in order to the process characteristics (velocity, stress, pressure and temperature). This is known as the *direct problem*. In the above example of single screw extrusion, it is the solution to the direct problem that provides the data for analysis (see Figure 1). However, the process engineer would probably be much more interested in defining the appropriate process responses and obtain from the program the corresponding set of operating conditions. Mathematically, this would correspond to solving the same set of governing equations, with the same set of constitutive equations, but now in order to some of the previous boundary conditions. Most of the previous process responses would now become

boundary conditions. This corresponds to solving the *inverse problem* (Figure 2). Unfortunately, the latter is mathematically ill-posed, namely because there is not a unique relationship between cause and effect (in other words, various operating conditions might fulfill the new variables).

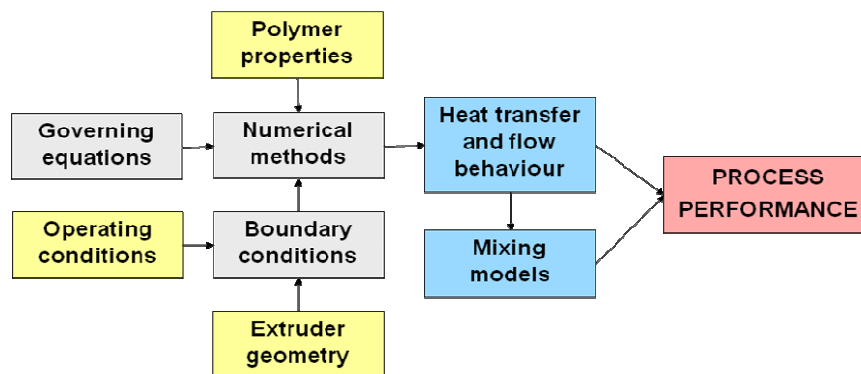


Figure 1. Numerical modeling of single screw extrusion.

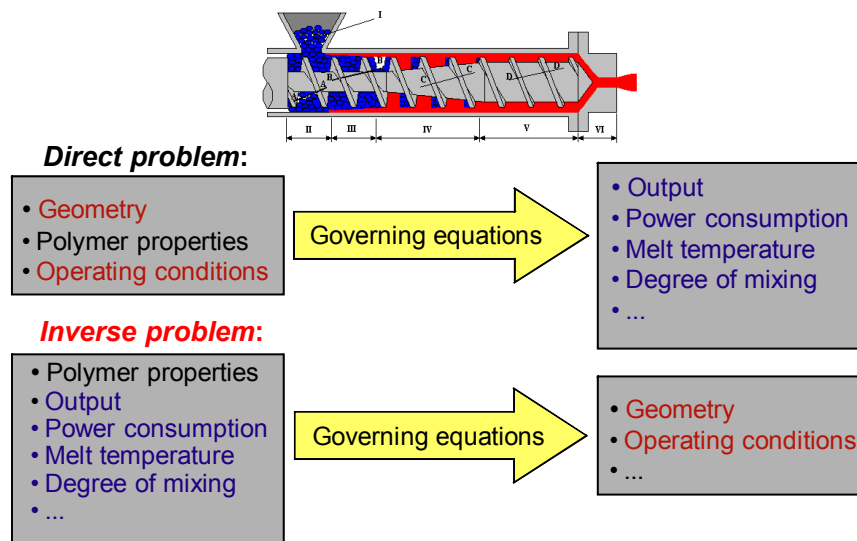


Figure 2. Direct and inverse problem in single screw extrusion.

An interesting alternative consists in considering the above tasks as optimization problems. For example, setting the operating conditions of a single screw extruder corresponds to defining the screw speed and barrel temperature that will maximize (optimize) process performance. As illustrated in Figure 3, this approach could typically use three inter-related modules: 1) a modeling package, that yields the process response to a given output, 2) an objective function, that quantifies the process performance (this function can combine several process parameters) and 3) an optimization algorithm. Thus, each possible solution is characterized by a value of the objective function that is determined via the use of the modeling package. The optimization algorithm provides progressively better solutions. An adequate user interface could provide automatically the results to the user.

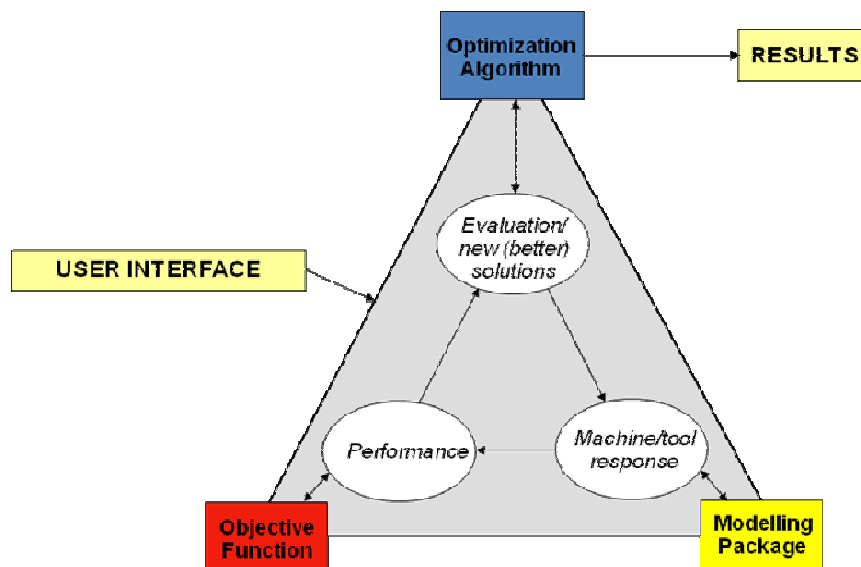


Figure 3. Process optimization approach.

The potential and advantages of this methodology are multiple:

- it is able to automatically provide the practical answers sought after by process engineers;

-
- it can use available process modeling packages (conventional direct problem solvers), thus benefiting from the sophistication reached in this field;
 - different optimization algorithms are available, depending on the specific characteristics of the processing problem to solve;
 - it can incorporate important practical knowledge (in the selection of the process parameters, in the definition of their range of variation, in the final decision of a solution to the problem);
 - the increase in computational power provided by computer manufacturers keeps the computation times required by the method within reasonable values.

The authors have successively applied this methodology to polymer extrusion, for screw design, process optimization and scale-up purposes. A number of commercial software's have added optimization routines to their menus. The amount of publications in this field is also growing. All these are indicators of the prospective more widespread practical adoption of the optimization approach.

This is why this book is about optimization in polymer processing. The work is a joint effort of a number of experts in polymer processing and/or optimization and is divided in two parts. The first presents and discusses optimization concepts (Chapters 2 to 4), the second reports applications in polymer processing (Chapters 5 to 9).

Chapter 2 is committed to the introduction of optimization concepts. It starts with the mathematical formulation of an optimization problem and with the distinction between continuous and discrete optimization. Then, the definitions of convexity, global and local optimization and optimality conditions are given. Some simple examples are presented to illustrate the different type of problems (e.g., constrained and unconstrained) and how the definitions introduced can be used to solve them. This is followed by the justification for the need of other types of optimization algorithms (namely metaheuristics). The chapter ends with a short introduction to Evolutionary Algorithms, a very efficient class of metaheuristics that are adopted in some chapters of this book.

Another important characteristic of real optimization problems is their multi-objective nature. This is the subject of Chapter 3. Multi-objective problems and optimality conditions for these types of problems are defined and traditional methods to deal with their multi-objective nature are presented.

The chapter concludes with the study of various evolutionary algorithms capable of dealing with multi-objective problems and the discussion of their advantages.

In Chapter 4, multi-objective evolutionary algorithms are extended to solve some specific and complex issues arising when solving real optimization problems, namely decision making, robustness of the solutions and required computation times. Since the result of a multi-objective optimization problem is not a single point, but a set of Pareto solutions, it is necessary to use a decision making strategy able to take into account the relative importance of all individual objectives. Also, the solutions obtained must be robust against variations of the decision variables, i.e., the performance should not deteriorate when the value of the decision variables changes slightly. Finally, due to the high number of solutions evaluations required by MOEAs and the corresponding high computation times, it is interesting to develop strategies to minimize these difficulties, which usually involves hybridization with local search methods. The methods proposed to deal with these three issues are illustrated towards the end of the chapter for a few benchmark test problems.

The methodologies presented in Chapters 3 and 4 are used in Chapter 5 to set the operating conditions and to define the screw geometry/configuration for plasticating single screw and co-rotating twin-screw extrusion, two major polymer processing and compounding technologies. The Chapter starts by presenting in some detail the process modeling routines that are used to evaluate the solutions proposed by the optimization algorithms during the search stage. Then, the most important characteristics capable of influencing the optimization procedure are presented for both extrusion processes. Finally, a few results obtained with the proposed optimization strategy are presented and discussed.

Chapter 6 is devoted to the optimization of two representative reactive extrusion processes making use of co-rotating twin-screw extruders, i.e., ϵ -caprolactone polymerization and starch cationization, using the methodology described in previous chapters. The chemical reactions are presented and modeled. Results concerning the optimization of operating conditions and screw configuration of the two chemical processes are then presented.

The design of extrusion dies and downstream calibration/cooling systems is the subject of Chapter 7. The state-of-the-art on the design of these tools is presented. The optimization methodology adopted is a metaheuristic where the improvement of the performance of the solutions generated in each iteration is obtained by changing iteratively the design controllable parameters - this is known as the Simplex method. An application example is discussed.

Sequential quadratic programming is used to optimize the injection molding process in Chapter 8. As in other process application chapters, the authors start by describing the numerical modeling routine developed, which in this case is based on the dual reciprocity boundary element method. Then, the modeling and optimization methods are used to solve an example dealing with the optimization of mold cooling.

The last Chapter is divided in two main parts. The first deals with the development of methods for the estimation and control of sheet temperature in thermoforming, while the second is dedicated to the resolution of the inverse heating problem using the conjugate gradient method. In both cases, the methodologies presented are illustrated with some typical examples.