MATERIALS AND MANUFACTURING PROCESSES
Vol. 18, No. 3, pp. 523–532, 2003

Applications of Genetic Algorithm in Polymer Science and Engineering

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ABSTRACT

In the last several years, genetic algorithm (GA) has gained wide acceptance as a robust optimization algorithm in almost all areas of science and engineering. Polymer science and engineering is no exception. Researchers in this field have devoted considerable attention to the optimization of polymer *production* using objective functions and constraints that lead to products having desired material properties. Multiple-objective functions have been optimized simultaneously. An example is the minimization of the reaction time in a reactor (lower costs) while simultaneously minimizing the concentration of side products (that affect the properties of the product adversely). Several end-point constraints (equality or inequality) may also be present, as, e.g., obtaining polymer of a desired molecular weight. Again, this requirement stems from producing polymer having desired strength. Solving such problems usually result in Pareto sets. A variety of adaptations of GA have been developed to obtain optimal solutions for such complex problems. These adaptations can be used to advantage in other fields too. The applications of GA in areas of polymer science and engineering other than polymerization systems are few and far between, but this field is now maturing, and it is hoped that the future will see several newer applications.

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DOI: 10.1081/AMP-120022026
1042-6914 (Print); 1532-2475 (Online)

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Key Words: Genetic algorithm; Multi-objective optimization; Pareto sets; Optimization; Optimization in polymer reaction engineering; Optimization in polymer science and engineering; Scheduling in polymers; Optimization in polymer processing; Optimization in polymer molecular design; Nondominated sorting GA.

1. INTRODUCTION

Even though all animals and plants are comprised of long-chain molecules, synthetic macromolecules were developed only in the 19th century. Their unusual properties helped replace natural polymers in almost all fields. Indeed, polymers are one of the most important materials today. Polymer science and engineering has matured considerably over the past several decades, and the knowledge in this area has grown immensely in diverse areas. Many paradigm shifts have taken place in each of its various substreams over the years.[1] In recent years, a robust optimization technique, namely, genetic algorithm (GA),[2–4] has been applied to solve several interesting and often complex problems in different fields of polymer science and engineering. These parallel similar developments in other fields of materials science and engineering. Most of these developments have taken place in the realm of polymer *production*. A common thread passes through these studies—the aim is to produce product having desired material properties, while minimizing their cost of production. Several adaptations have been developed in the original algorithm, and real-life problems involving single-[2–6] as well as multiple[7–10]-objective functions have been formulated and solved for the manufacture of polymers. Relatively few optimization problems have been solved by using GA in other areas of polymer science and engineering. These studies are reviewed here in the hope that it will spur further optimization activity in these and other hitherto unexplored areas of polymer science.

2. APPLICATIONS OF GA IN POLYMER SCIENCE AND ENGINEERING

A short summary of the applications of GA in polymer science and engineering is now presented. There are different stages in the production of polymers, starting from the molecular design of molecules, running through their manufacture in reactors, and finally ending with their processing. In each stage, GA can be and has been used. The maximum and most advanced applications are in the realm of polymerization reactors, with only a few applications in the other spheres. We review these applications here, with special emphasis on the several algorithmic adaptations developed to obtain the optimal solutions.

2.1. Polymer Production

Chakravarthy et al.[5] and Ho et al.[6] were the first to adapt simple GA (SGA)[2–4] and use it to optimize polymer production using decision variables that

are *continuous functions* of time. Chakravarthy et al.[5] studied the optimization of the bulk polymerization of methyl methacrylate (MMA). This is an interesting and complex system, because it exhibits the Trommsdorff effect, which is associated with an extremely sharp increase in the monomer conversion with time, at some stage of polymerization. They used the temperature history, T(t), to minimize the reaction time, t_f, in a batch reactor, while simultaneously requiring the attainment of the design values, x_{md} and μ_{nd}, of both the *final* (at $t = t_f$) monomer conversion, $x_m(t_f)$, and the number average chain length, $\mu_n(t_f)$, of the polymer product. The latter constraint ensures the production of polymer having the desired material properties (strength, etc.). Thus, they solved the following problem

$$\begin{aligned} &\text{Min } I[T(t)] = t_f \\ &\text{subject to:} \\ &x_m(t_f) = x_{md} \\ &\mu_n(t_f) = \mu_{nd} \\ &\text{bounds on } T(t) \\ &\text{model equations} \end{aligned} \tag{1}$$

The following equivalent mathematical problem involving penalty functions was used to take care of the end-point constraints on x_m and μ_n:

$$\begin{aligned} &\text{Min } I[T(t)] = t_f + w_1[1 - \{x_m(t_f)/x_{md}\}]^2 + w_2[1 - \{\mu_n(t_f)/\mu_{nd}\}]^2 \\ &\text{subject to:} \\ &\text{bounds on } T(t) \\ &\text{model equations} \end{aligned} \tag{2}$$

The values of the two penalty parameters, w_1 and w_2, are taken to be *very* large so that the second and third terms on the right-hand side of the expression for I in Eq. (2) dominate over t_f when $x_m(t_f)$ and $\mu_n(t_f)$ deviate from their design values. These terms, thus, act as penalties and force the constraints to be satisfied.

Ho et al.[6] carried out a similar time-optimal control of a continuous-flow stirred tank reactor (CSTR) in which random copolymerization of MMA and vinyl alcohol (VA) was taking place, during start-up or grade-change. Clearly, the use of two comonomers leads to desirable material properties. They used an adaptation of SGA. This system does not show the Trommsdorff effect but is quite complex because of the simultaneous polymerization of two monomers. They obtained the optimal jacket temperature *history* and the *history* of the flow rate of VA to minimize the transition time (during start-up or grade-change). At the same time, they used two end-point constraints: the polymer product was forced to be of a desired molecular weight (strength, etc., of the material), and the average mole fraction of VA in the polymer product was to have a desired value. Penalty functions were used.

More recently, *guided* SGA was used by Mankar et al.[11] to carry out an *experimental* on-line optimization study on MMA polymerization in a specially made viscometer-reactor assembly. An off-line computed optimal temperature history was

implemented on this system. A planned disturbance (heater failure) was introduced after the start of polymerization. The temperature history was reoptimized *on-line* after the introduction of this disturbance, to *save the batch*, i.e., to produce a polymer product having the originally planned value of μ_n, in the minimum possible (remaining) reaction time, and implemented experimentally. The results were quite satisfactory and demonstrated the power of (guided) SGA for on-line experimental work.

The first use of multiple-objective functions in polymer reaction engineering was for an industrial nylon-6 semibatch reactor.[9] The two objective functions used were to minimize (i) the total reaction time, t_f, and (ii) the concentration, $[C_2]_f$, of the cyclic dimer, an undesired by-product, in the product. The second objective function is related to the material properties of the final polymeric product. Cyclics in the product lead to processing problems as well as give an unacceptable finished fabric and so are minimized. End-point constraints were imposed on the monomer conversion, x_m, in the product stream, as well as on the number average chain length, μ_n, of the product, so that design values, $x_{m,d}$ and $\mu_{n,d}$, are attained. The decision variables used in this study were (i) the rate of release, $V_T(t)$, of the vapor from the semibatch reactor (a function of time, t) that influenced the pressure in the reactor and (ii) the jacket fluid temperature, T_J, a scalar. Non-dominated sorting genetic algorithm, NSGA-I,[7–9] first developed by Srinivas and Deb[8] for decision variables that were *scalars*, was adapted to apply to decision variables that were continuous *functions* of time. Pareto sets of optimal solutions were obtained for a specified value of the feed water concentration (see Fig. 1). For a two-objective function problem, e.g., the Pareto set is the locus of (equally good) optimal points so that if one moves from any

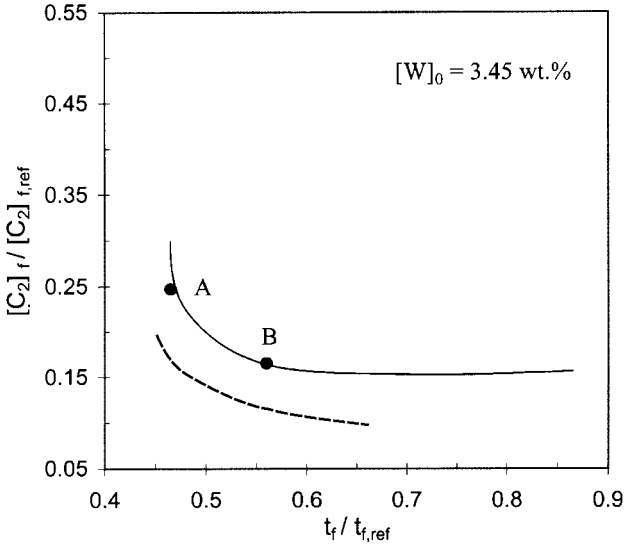

Figure 1. Comparison of the Pareto solutions for an industrial semibatch nylon-6 reactor for two different choices of decision variables [solid lines:[12]; broken lines:[9]]. Subscript, ref., indicates values being used in industry before changeover to near-optimal conditions.

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one point (say, point A in Fig. 1) to any other (say, point B), one objective function improves while the other worsens. The choice of the *preferred* solution from among these optimal sets of points depends on additional information, which often takes a non-quantifiable form.

It is interesting that considerable improvement in the operation of the industrial reactor was indicated by this study, and we understand that these results have been implemented on the industrial reactor.

Gupta and Gupta[12] extended this work on the industrial nylon-6 reactor system to consider the multiobjective optimization of the reactor-cum-control valve assembly. They considered the fractional opening of the control valve as one of the decision variables (again, a function of time), instead of the rate of release of vapor from the reactor. The second decision variable was the temperature of the jacket fluid, a scalar. The Pareto optimal solutions obtained for this *system* were found to be worse when compared to the solutions obtained by Mitra et al., who had studied the reactor *alone* (see Fig. 1). This was because the operation of the control valve that released the vapor excluded certain sets of values of $V_T(t)$, which were permitted in the study of Mitra et al.[9]. It is clear that for industrial systems, the optimization of the entire *system* should be carried out.

Garg and Gupta[13] applied NSGA to the multiobjective optimization of free radical bulk polymerization reactors for PMMA, in which diffusional effects (the Trommsdorff, cage, and glass effects) are manifested. The two-objective functions used were the minimization of (i) the total reaction time, t_f, and (ii) the polydispersity index, Q_f, of the product. It is well known that the polymer properties are not only related to the average molecular weight but to the breadth of the molecular weight distribution, reflected through Q. End-point constraints were used on μ_n and x_m, similar to that for nylon-6. Optimal temperature histories, T(t), were generated. It is interesting that a unique optimal solution, instead of a Pareto set of several optimal points, was obtained. This result was of considerable importance because a controversy had existed on this point for several years, based on earlier optimization studies that used a scalar objective function composed of a weighted sum of the two objectives.

Polyethylene terephthalate (PET) is another commercially important commodity polymer, mostly used in the manufacture of synthetic fibers. Bhaskar et al.[14] formulated a multi-objective optimization problem for an industrial, third-stage, continuous wiped-film finishing reactor used to produce this polymer. The objective functions used in this problem were to minimize the concentrations of two undesirable side products, namely, that of the (i) acid end groups (these lead to breakage of filaments during the high-humidity spinning operation) and (ii) the vinyl end-groups (this leads to a coloration of the fiber) in the output stream. An equality constraint was imposed on the degree of polymerization, DP_{out}, of the product, to produce PET having a desired value, DP_d (i.e., $DP_{out} = DP_d$), of about 82. The acid end-group concentration in the product was further restricted to lie below a certain value (an inequality constraint), whereas the concentration of the diethylene glycol end group—which affects the crystallinity and, therefore, the melting point of the PET-adversely, but helps improve the dyeability of the fiber—in the product was restricted to lie in a specified *range* (two inequality constraints). The three inequality constraints were taken care of by ''penalty-killing'' of the chromosomes that violated

these constraints. The solution of the problem was found to be a unique point, and no Pareto set of optimal solutions was obtained when temperature was included among the decision variables. The unique optimal solution was found to be superior to the current operating conditions in the industrial reactor studied. It is interesting that a *single* application of NSGA-I could not provide the correct optimal point (or Pareto, whenever that existed), and multiple applications of the algorithm (with different seeds for the random-number generator) were necessary. Clearly, the algorithm fails in this case. Thus, this problem, is an unusual one and can be used as a test problem for improved optimization codes.

Another application of considerable industrial importance is the optimization of the continuous casting of polymethyl methacrylate (PMMA) films in a furnace. The two objective functions[15] are (i) the maximization of the cross section-average value of the monomer conversion at the end of the furnace, $x_{m,av,f}$, and (ii) the minimization of the length, z_f, of the furnace. The end-point constraint used was that the section-average value of the number average chain length in the product, $\mu_{n,av,f}$, should be equal to a desired value, $\mu_{n,d}$., again because of strength considerations. In addition, a ''local'' constraint is to be satisfied in this problem. This takes the form that the temperature at *any* point in the film must be below an upper safe value, to prevent degradation (discoloration) of the polymer film. The decision variables used were the temperature of the isothermal plug-flow tubular reactor (PFTR), used as a pre-polymerizer, concentration of the initiator in the feed to this PFTR, monomer conversion at the end of this PFTR, film thickness in the furnace (all *scalars*), and the temperature programming, $T_w(z)$, in the furnace (a continuous *function*). The local constraint was taken care of by using the penalty killing procedure.

Recently, Kasat et al.[16] studied the multiobjective optimization of a polystyrene reactor using GA. The algorithm used here is an algorithm based on elitism, viz., NSGA-II,[10] an improved version of NSGA-I. The two-objective functions used here are i) minimization of the residence time in the reactor and ii) maximization of the monomer conversion. The decision variables used are the temperature *history* and the initiator concentration (scalar) in the feed. An end-point constraint is imposed on the μ_n of the product. NSGA-II has been adapted to apply to decision variables that are continuous functions of time. Pareto optimal solutions are obtained (see Fig. 2).

2.2. Scheduling

Although most of the applications of GA in polymer science and engineering have been in the area of polymerization engineering, as described above, SGA has been applied in *a few* other areas as well. Again, the important aspect in *all* these studies is the emphasis on achieving desired material properties. Wang et al.[17] used GA for on-line scheduling of an industrial unit manufacturing several grain-size fractions of two types of expandable polystyrene. This plant involves several batch reactors, followed by mixers and then continuous finishing units. The task was to determine the sequence and timing of the several units in the plant, as well as to choose the feed rates for the two finishing lines following the mixers. The objective was to produce the required grain-size fractions before the due dates without

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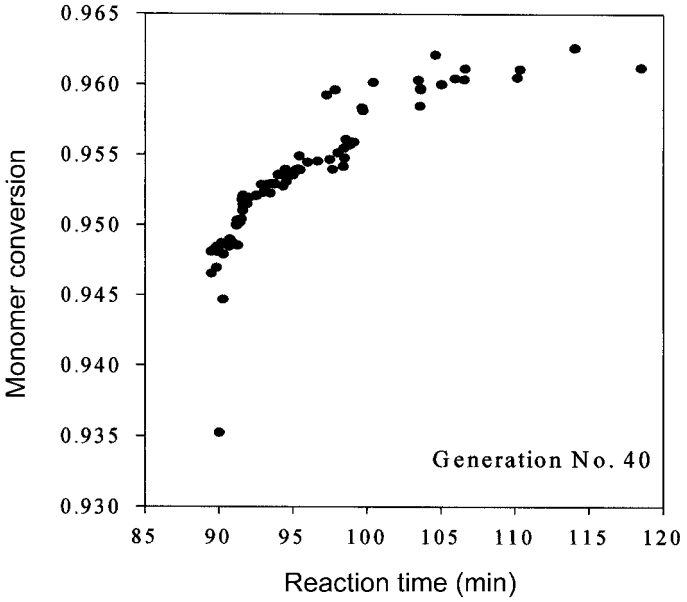

Figure 2. Pareto solutions for a polystyrene reactor[16] $\mu_{n,d} = 700$.

unnecessary production of unwanted fractions. In the algorithm, overproduction and underproduction were penalized with different weights. They found that the quality of solutions obtained by GA was comparable with those obtained by mixed-integer non-linear programming while the computing times were moderate.

2.3. Polymer Science

Nagasaka and Yada[18] carried out the reverse design of polymers using GA. This is achieved by generating several chromosomes representing the structure of the polymer and then predicting the corresponding fitness functions (properties). Quantitative structure-property relationship (QSPR) methods have been used. These workers have constructed a code, EXPOD, for the reverse design of polymers. A similar study on the computer-aided molecular design of polymers has been reported by Venkatasubramanian et al.[19]. This uses GA to design new molecules having desired properties. They illustrate this with some case studies in polymer design. Anantha and Venkatasubramanian[20] studied the influence of the computational parameters of GA on its performance for large-scale molecular design of polymers. They showed that the performance of GA could be enhanced by using diversified sampling schemes, adaptive parameter tuning, and interactive inclusion of additional design knowledge.

Patel et al.[21] developed quantitative structure-property relationships using GA for a training set of 16 polymers for which the gaseous diffusion constants of CO_2, N_2, and O_2 were measured. They found that the bulk modulus of the polymer is

the dominant physicochemical polymer property that influences the diffusion of these gases. They constructed QSPR diffusion models for these three gases. This information could be used for the selection of processing and packaging materials.

Hanagandi et al.[22] modeled polymer adsorption on a solid surface using a self-consistent field approach. The governing equations were cast in terms of an optimization problem, and GA was used to solve it. The objective function was to minimize the sum of square errors between the guess values of the several volume fractions, ϕ_i, of the polymer in the ith layer (lattice theory) and the predicted values. It is interesting that it was observed that use of GA cascaded with a gradient search technique was superior to GA alone. A similar cascaded approach was also found to be superior by Chakravarthy et al.[5] for MMA polymerization.

It is clear that multiobjective function optimization has not yet been used in these other areas of polymer materials science, and there is considerable potential available.

2.4. Polymer Processing

The manufacture of polymer composites using liquid composite molding involves the injection of a reactive resin into a closed mold with preplaced fibrous reinforcements. Simulation codes that provide results on mold filling for a specified location of the gates are available. Young[23] developed an optimization scheme using GA to search for the optimal locations of the gates that minimize the mold-filling pressure, uneven filling pattern, and the temperature difference during the mold-filling process.

McKay et al.[24] compared two data-based extruder modeling paradigms. A locally recurrent neural network and GA were used to develop inferential models of the polymer viscosity using measurements from an industrial plasticating extruder. They demonstrated that both of these two techniques produced adequate non-linear dynamic inferential models. However, GA produced models that performed better than those obtained with use of the locally recurrent neural network. Covas et al.[25] obtained Pareto optimal operating conditions of plasticating single screw extruders using GA.

Resin transfer molding (RTM) is one of the most promising fabrication methods for midvolume, high-performance polymer composite structures. Liang et al.[26] and Luo et al.[27] introduced a systematic approach for the optimal design of RTM tooling. The approach was built on a three-dimensional RTM simulation model coupled with a neural network-GA optimization procedure. The simulation model was used to predict resin flow patterns (potential quality problems) and processing efficiency (mold-filling time). The GA is applied to this rapid RTM process model to search for the optimum solution. This tooling design scheme enables an engineer to determine the optimum locations of injection gates and vents for the best processing performance [i.e., short filling times and high levels of quality (minimum defects)]. It is evident that optimal processing conditions would lead to the production of final products having desired mechanical properties. These studies in the optimization of polymer processing operations can easily be applied to other *non-polymer* processing applications.

3. CONCLUSIONS

It can be seen that several workers have started using GA in polymer science and engineering in the last decade. The more advanced applications involve multi-objective optimizations. These have been reported primarily in the area of polymer reaction engineering. Several improvements and "tricks" have been used to obtain optimal solutions. These could be used to advantage in other areas as well, even beyond the realm of polymer science and engineering. Some effort involving single-objective functions also has been reported in other areas of polymer science and engineering such as polymer processing, polymer science, and scheduling of manufacturing processes. With the increase in awareness about GA, we hope to see an increase in its applications in the next few years.

ACKNOWLEDGMENT

Partial financial support from the Department of Science and Technology, Government of India, New Delhi [through grant III-5(13)/2001-ET] is gratefully acknowledged.

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