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SSEM-AG COMPUTER MODEL FOR OPTIMIZATION OF POLYMER EXTRUSION

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ABSTRACT

The optimization of an extrusion process is a conflicting, multi-objective problem. It is complicated by the number of variables (screw/die geometry, operating conditions, material data) and their non-linear relations, as well as by the opposing criteria, for example extrusion throughput and power consumption. It is difficult to find the global optimum for the process avoiding local optima. There are two approaches to solve the problem, experimental and using a mathematical model of extrusion. Optimization techniques based on an experimentation are time-consuming and very expensive.

In this paper we present an optimization methodology based on the Genetic Algorithms (AG), where response surface is given by the extrusion model. A mathematical Single-Screw Extrusion Model SSEM developed at the Warsaw University of Technology is used to predict the extruder behavior, and AG approach is used for optimization. An integrated SSEM-AG system was developed to study optimization of the single-screw extrusion process. Three design criteria (output variables) are selected for optimization: maximum extrusion throughput, minimum power consumption and low melt temperature. As input variables, screw speed, barrel temperature and screw channel depth are chosen.

INTRODUCTION

There are two approaches to solve the problem of extrusion optimization, experimental and using a mathematical model of the process. Optimization techniques started with experiments using various screws and different operating conditions. The optimum data were simply the best one tried. This method is time-consuming and expensive, and nothing warrants that optimum screw design and operating conditions are found.

Statistical methods, regression analysis and response surface analysis may be used both for optimization by computer simulation and by analyzing data from experiment. Underwood [1] was the first to use factorial design of experiments to optimize extrusion. The optimum data were found by locating the extremum on the response surfaces relating the input variables, e.g. screw geometry, and the output variables that are the design criteria, e.g. low power consumption or high output. The main drawback of this method is the number of required experiments.

In this aspect, using the mathematical model of the process is much more efficient. First approaches to optimization of the extrusion process by computer simulation were limited to the conventional screws [2-4]. Recently, much more sophisticated global extrusion models have been developed, and simulations conventional and non-conventional screws, as well as dies of various geometries are available. Potente [5] developed a strategy for screw optimization by means of DOE (Design of Experiments) and multiple regression introducing a global extrusion model REX. Lafleur [6] used the STATISTICA software to locate the optimum on a response surface given by the model developed at the Ecole Polytechnique de Montreal.

Another approach proposed Covas [7,8] who developed an optimization methodology based on Genetic Algorithms, where response surface is also given by the extrusion model. Unlike other approaches, Genetic Algorithms do not require any derivative data and do not impose any restrictions for the convexity of the search space.

OPTIMIZATION STRATEGY

Extrusion models are able to predict the response of the system in terms of important process parameters such as throughput, power consumption, solid bed profile SBP, pressure and temperature profiles, mixing degree and material properties. An input data are material properties, screw and die geometry, as well as operating conditions (screw speed, barrel temperature). To predict the response of the system is the direct problem. The inverse problem, i.e. the selection of the input data to obtain a good extrusion performance, involves important difficulties; it is an optimization problem (Fig.1).

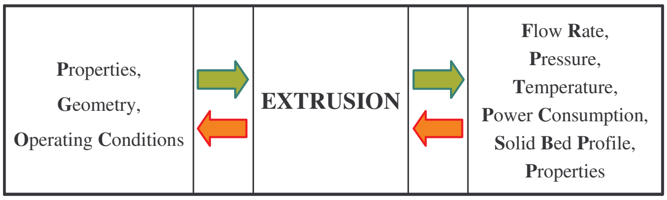

Fig.1. Direct and inverse problem for polymer extrusion: ⇒ - direct problem, ⇐ - inverse problem

The aim of optimization is to find the global optimum on a search space, by maximizing or minimizing an objective function. Polymer extrusion must satisfy simultaneously several objectives, e.g. power consumption, throughput, melt temperature, mixing degree etc.

In this paper, a global objective function is defined as

$$F_i = \sqrt[k]{f_{i(1)} * f_{i(2)} * \ldots * f_{i(k)}} \qquad (1)$$

where F_i is the global objective function for i-set of input data, k is the number of optimization criteria (individual objectives, output variables), and $f_{i(k)}$ is the objective function of criterion k which can take two forms:

- for the criterion to be maximized

$$f_i = \frac{y_i - y_{\min}}{y_{\max} - y_{\min}} \qquad (2)$$

- for the criterion to be minimized

$$f_i = \frac{y_{\max} - y_i}{y_{\max} - y_{\min}} \qquad (3)$$

where y is the output variable (optimization criterion, e.g. throughput); $y_{\max}$, $y_{\min}$ are the maximum and minimum values that this output variable y can reach, respectively.

SINGLE SCREW EXTRUSION MODEL

The Single Screw Extrusion Model SSEM [9] is used to predict the extruder behavior and to provide the response surface. This model simulates an operation of the extruder-die system, and describes solids conveying in the hopper, solids conveying in the screw, delay zone, melting zone, melt conveying in the screw and polymer melt flow through the die (Fig.2). Given the material and rheological properties of the polymer; the screw, hopper and die geometry; and the extrusion operating conditions (screw speed and barrel/die temperature profile), the model predicts: flow rate of the polymer, pressure and temperature profiles along the extruder screw channel and in the die, solid bed profile, and power consumption.

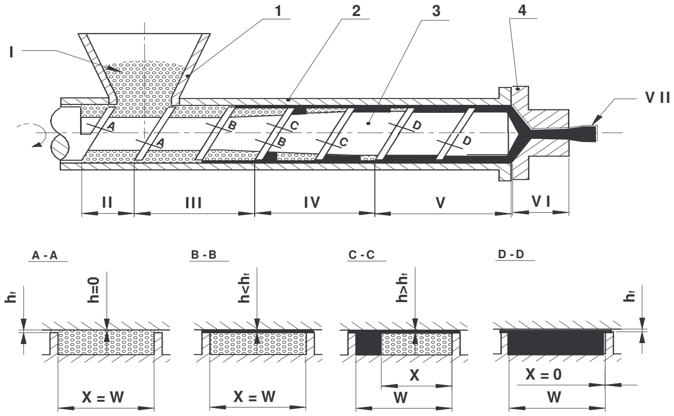

Fig.2. Extrusion process: 1 – hopper, 2 – barrel, 3 – screw, 4 – die; I – solid particles in the hopper, II – solid conveying, III – delay section, IV – melting, V – melt conveying, VI – melt flow in the die, VII – extrudate; X – solid bed, W – screw channel width, h_f – flight clearance, h – melt film thickness

Main assumptions of the model are the following:

- The solid bed behaviour is described by the plug flow, the velocity of the solid bed is constant.
- The melting behaviour is described by the 3-zones Tadmor model.
- The molten polymer is considered to be a shear-thinning fluid, obeying the following expression:

$$\ln\eta = A_0 + A_1\ln\gamma^* + A_{11}\ln^2\gamma^* + A_{12}T\ln\gamma^* + A_2T + A_{22}T^2 \qquad (4)$$

where: η - viscosity, T - temperature, γ^* - shear rate, $A_0 \dots A_{22}$ - coefficients of the polynomial,

- The flow in the melt conveying zone is considered to be one-dimensional, newtonian and locally isothermal in a flat channel. The non-linear superposition factor theory of (drag and pressure) unidirectional flow of the power law fluid as well as an approximative solution of two-directional flow of the power law fluid are also considered.
- The effects of flights, channel curvature, flight clearance and varying channel height are expressed in terms of correction factors for the drag and pressure flow.
- The flow through the die is considered to be one-dimensional and locally isothermal flow of a power law fluid.

A new version of the program based on the presented model has been developed. The program is written in Delphi 5 of Borland. A general structure of the program is shown in Fig.3.

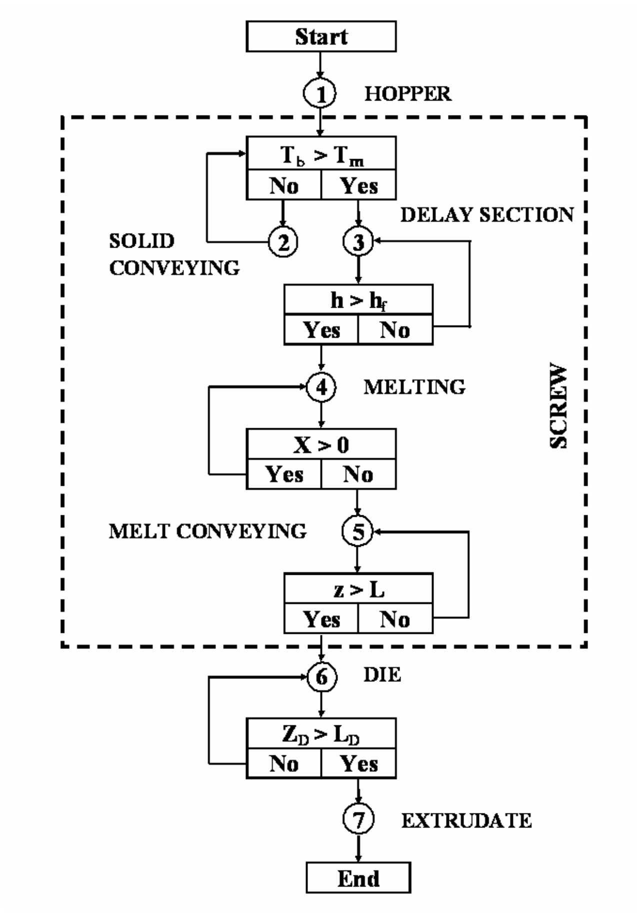

Fig.3. Overall computation structure for SSEM program

The developed computer program is general-purpose, and makes it possible to simulate the extrusion process for conventional and non-conventional screws, and various dies. A screw profile can be visualized as a connected series of sections, each with some specific geometry: conventional section, torpedo section, mixing fluted section and mixing ring section. Specifying the screw geometry involves declaring the type of geometrical sections and their dimensions. The same procedure is valid for a die visualization. Various cross-sections are available: circle, circular slit, rectangular slit, rectangle, square, ellipse, semicircle, etc.

Examples of simulation for a typical three-sectional conventional screw presented in Fig.4 are shown in Fig.5. Pressure and temperature profiles, power consumption, and solid bed profile SBP were computed.

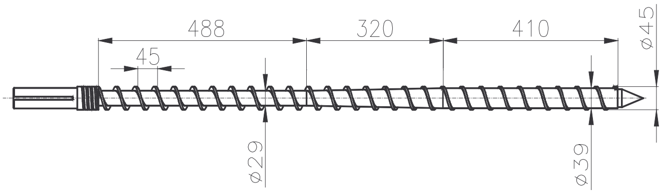

Fig.4. Three-sectional conventional screw

Symbol of Dataset : 1G3PE80 date: 2003-07-03 17:16:53

Chart for : Extruder

Chart
☑ Pressure
☑ Temperature
☑ SBP
☑ Power
☐ ------------

☐ Logarithmic

Range
1
0 1545
0
☑ Automatic

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Fig.5. Simulation for conventional screw

Examples of simulation for a rod cylindrical die shown in Fig.6 are presented in Fig. 7. Pressure and temperature profiles, as well as a mean velocity and residence time were calculated.

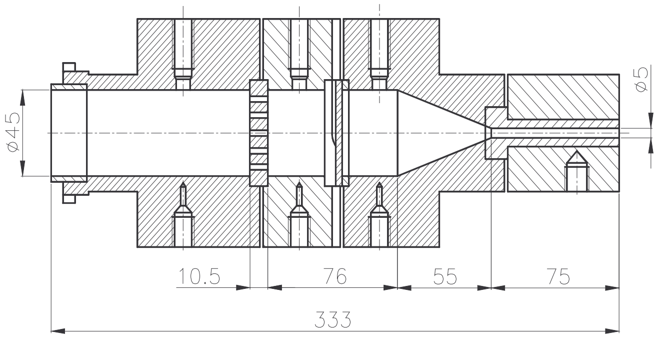

Fig.6. Rod cylindrical die

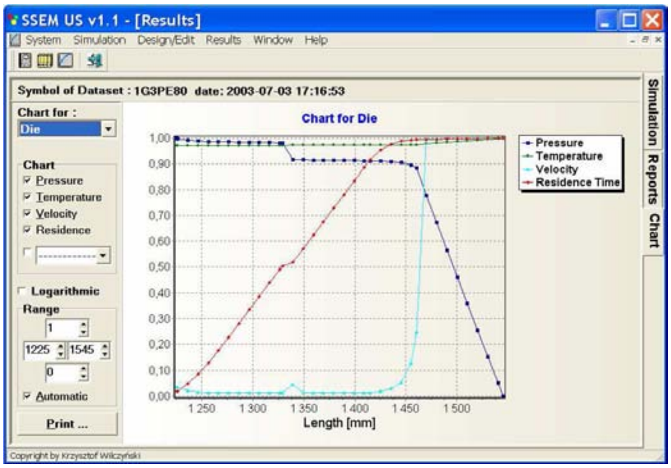

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Fig.7. Simulation for rod cylindrical die

GENETIC ALGORITHMS

Genetic Algorithms GA are search and optimization methods that imitate the natural evolution process [10]. They start from a set of randomly generated points and apply genetic operators like crossover and mutation to confine the region where the optimum is located (Fig.8). It prevents the algorithm from being trapped in a local minimum.

The Genetic Algorithm procedure requires [10]:

- encoding of input variables, which are represented as strings of bits, referred to as chromosomes,
- definition of an objective function, that evaluates a value of each genotype, i.e. set of chromosomes,
- generation of initial population, randomly selected,
- definition of genetic operators, i.e. reproduction, crossover and mutation, which search the response space using probabilistic rules.

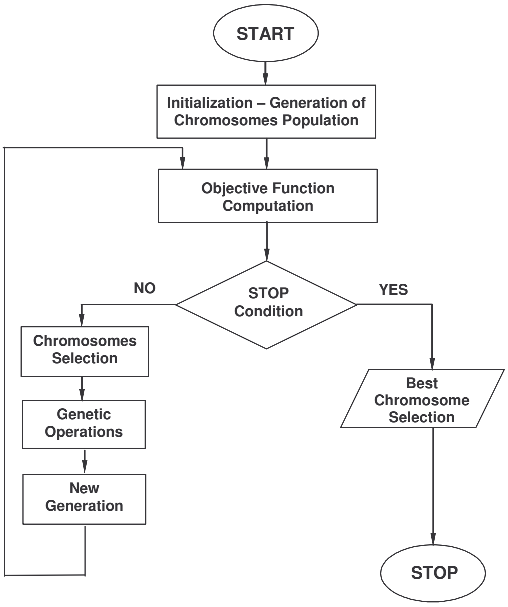


Fig.8. An overall Genetic Algorithm scheme

AN INTEGRATED SSEM-AG OPTIMIZATION SYSTEM

An optimization SSEM-AG system was developed by integration of the SSEM mathematical model of the single-screw extrusion process with the especially built AG program (Fig.9).

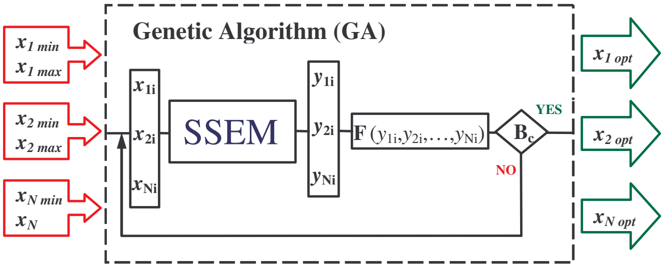


Fig.9. An integrated SSEM-AG system

The AG program is written in Delphi 5 of Borland. This program makes it possible, working with SSEM program, to optimize extrusion process with unlimited input variables. The accuracy of the search of response space is defined by the number of partitions of input variables scope. A roulette wheel method is used for selection of best solution. An overall SSEM-AG algorithm scheme is shown in Fig.10.

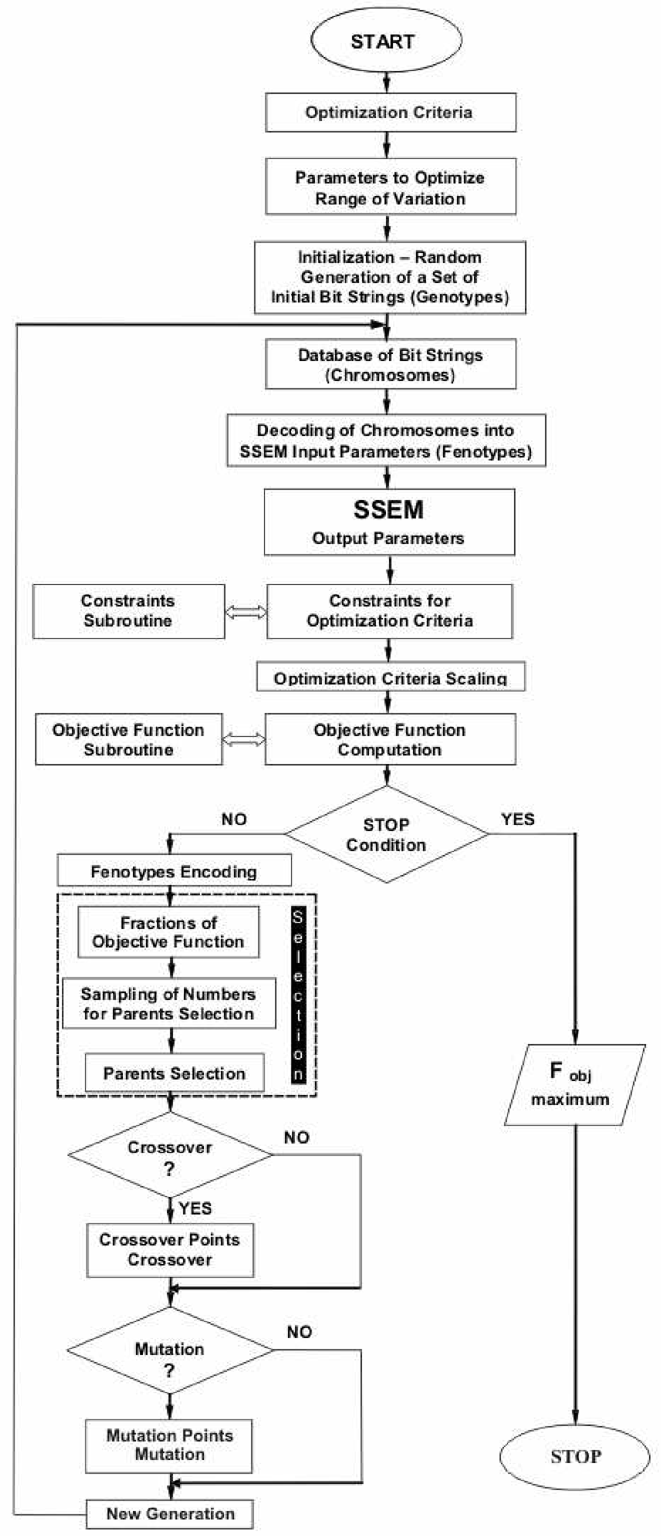
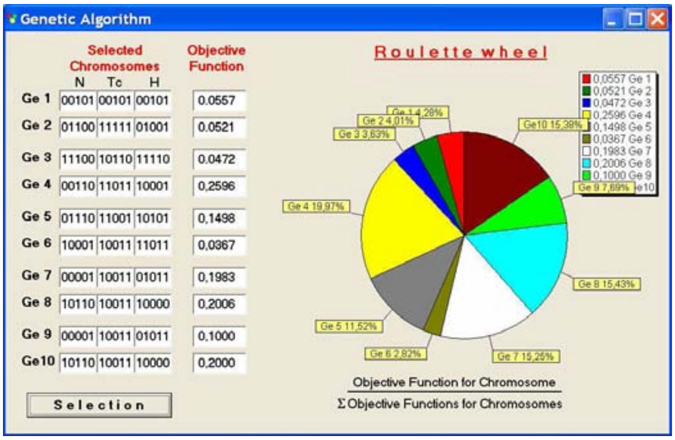


Fig.10. An overall SSEM-AG algorithm scheme

In this paper, three input variables are considered, screw speed N, barrel temperature T_b and depth of the screw channel in the metering section H. A binary representation of length 5 is applied to encode these variables, and produce a chromosomes of length 15. A roulette wheel selection is used as a reproduction operator which is shown in Fig.11.

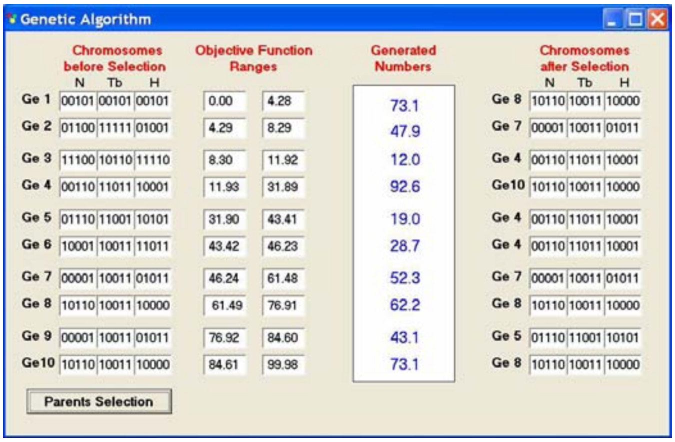


	Selected Chromosomes N	Tc	H	Objective Function
Ge 1	00101	00101	00101	0.0557
Ge 2	01100	11111	01001	0.0521
Ge 3	11100	10110	11110	0.0472
Ge 4	00110	11011	10001	0,2596
Ge 5	01110	11001	10101	0,1498
Ge 6	10001	10011	11011	0,0367
Ge 7	00001	10011	01011	0,1983
Ge 8	10110	10011	10000	0,2006
Ge 9	00001	10011	01011	0,1000
Ge10	10110	10011	10000	0,2000

$$\frac{\text{Objective Function for Chromosome}}{\Sigma\,\text{Objective Functions for Chromosomes}}$$

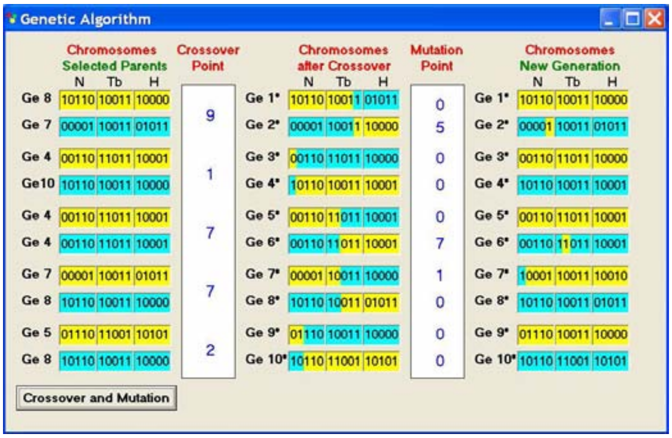
Fig.11. A roulette wheel selection of genotypes

Genetic operations, reproduction, crossover and mutation, are shown in Figs.12 and 13.



	Chromosomes before Selection N	Tb	H	Objective Function Ranges		Generated Numbers		Chromosomes after Selection N	Tb	H
Ge 1	00101	00101	00101	0.00	4.28	73.1	Ge 8	10110	10011	10000
Ge 2	01100	11111	01001	4.29	8.29	47.9	Ge 7	00001	10011	01011
Ge 3	11100	10110	11110	8.30	11.92	12.0	Ge 4	00110	11011	10001
Ge 4	00110	11011	10001	11.93	31.89	92.6	Ge10	10110	10011	10000
Ge 5	01110	11001	10101	31.90	43.41	19.0	Ge 4	00110	11011	10001
Ge 6	10001	10011	11011	43.42	46.23	28.7	Ge 4	00110	11011	10001
Ge 7	00001	10011	01011	46.24	61.48	52.3	Ge 7	00001	10011	01011
Ge 8	10110	10011	10000	61.49	76.91	62.2	Ge 8	10110	10011	10000
Ge 9	00001	10011	01011	76.92	84.60	43.1	Ge 5	01110	11001	10101
Ge10	10110	10011	10000	84.61	99.98	73.1	Ge 8	10110	10011	10000

Fig.12. Reproduction procedure (parents selection)



	Chromosomes Selected Parents N	Tb	H	Crossover Point		Chromosomes after Crossover N	Tb	H	Mutation Point		Chromosomes New Generation N	Tb	H
Ge 8	10110	10011	10000	9	Ge 1*	10110	10011	01011	0	Ge 1*	10110	10011	10000
Ge 7	00001	10011	01011		Ge 2*	00001	10011	10000	5	Ge 2*	00001	10011	01011
Ge 4	00110	11011	10001	1	Ge 3*	00110	11011	10000	0	Ge 3*	00110	11011	10000
Ge10	10110	10011	10000		Ge 4*	10110	10011	10001	0	Ge 4*	10110	10011	10001
Ge 4	00110	11011	10001	7	Ge 5*	00110	11011	10001	0	Ge 5*	00110	11011	10001
Ge 4	00110	11011	10001		Ge 6*	00110	11011	10001	7	Ge 6*	00110	11011	10001
Ge 7	00001	10011	01011	7	Ge 7*	00001	10011	10000	1	Ge 7*	10001	10011	10010
Ge 8	10110	10011	10000		Ge 8*	10110	10011	01011	0	Ge 8*	10110	10011	01011
Ge 5	01110	11001	10101	2	Ge 9*	01110	10011	10000	0	Ge 9*	01110	10011	10000
Ge 8	10110	10011	10000		Ge 10*	10110	11001	10101	0	Ge 10*	10110	11001	10101

Fig.13. Crossover and mutation

EXTRUSION OPTIMIZATION

Three design criteria are selected for optimization: maximum extrusion throughput Q, minimum power consumption P and minimum melt temperature T. As input variables: screw speed N, barrel temperature T_b and channel depth H are chosen.

Then, the individual objective functions are defined as

$$Q_i = \frac{Q_i - Q_{\min}}{Q_{\max} - Q_{\min}} \tag{5}$$

$$P_i = \frac{P_{\max} - P_i}{P_{\max} - P_{\min}} \tag{6}$$

$$T_{ti} = \frac{T_{t\max} - T_{ti}}{T_{t\max} - T_{t\min}} \tag{7}$$

and the global objective function is represented by

$$F_i = \sqrt[3]{Q_i * P_i * T_{ti}} \tag{8}$$

where F_i is the value of the global objective function for i-set of variables; $f_{i(Q)}$, $f_{i(P)}$, $f_{i(T)}$ are the individual optimization criteria of max. throughput, min. power consumption and min. melt temperature.

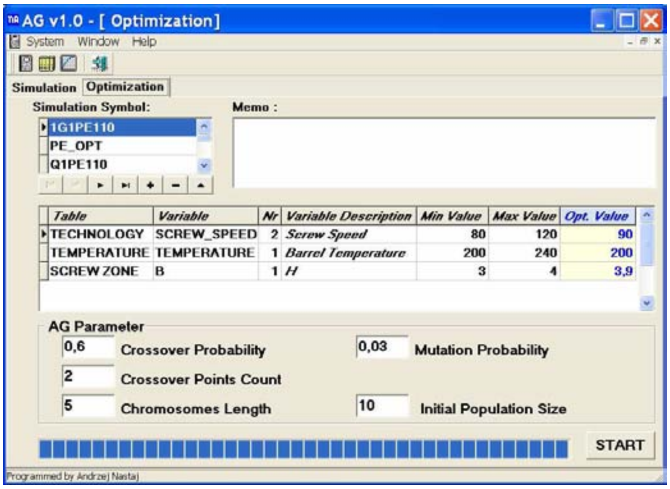
The objective of optimization is to define the screw speed N, the barrel temperature T_b and the depth of the screw channel in the metering zone H, for the conventional, 3-sectional screw, of 45 mm in diameter, length/diameter ratio L/D=27, depth of the screw channel in the feeding zone H_f =8 mm, feeding and metering lengths L_f =11D and L_m=9D, within the following range of input data variation:

N = 80 - 120 rpm,
T_b = 200 - 240 °C,
H = 3.0 - 4.0 mm

The following AG parameters were assumed:

- length of chromosomes: n = 5,
- initial population: k = 10,
- probability of crossover: $p_c = 0.6$,
- number of points of crossover: $n_c = 2$.
- probability of mutation: $p_m = 0.03$,

The input data for extrusion optimization, as well as results of optimization, that is optimal values of the extrusion parameters: N, T_b, H are shown in Fig.14.



Simulation Symbol:
1G1PE110
PE_OPT
Q1PE110

Memo :

Table	Variable	Nr	Variable Description	Min Value	Max Value	Opt. Value
TECHNOLOGY	SCREW_SPEED	2	*Screw Speed*	80	120	90
TEMPERATURE	TEMPERATURE	1	*Barrel Temperature*	200	240	200
SCREW ZONE	B	1	*H*	3	4	3,9

AG Parameter
0,6 Crossover Probability
0,03 Mutation Probability
2 Crossover Points Count
5 Chromosomes Length
10 Initial Population Size

Programmed by Andrzej Nastaj

Fig.14. The input data for optimization,
and results: optimal parameters N, T_b, H for extrusion

The following set of input variables was obtained as an optimum of the discussed extrusion process:

N_{opt} = 90 rpm, $T_{b\ opt}$ = 200 °C, H_{opt} = 3.9 mm

Output variables related to these values are equal to:

Q_{opt} = 0.0123 kg/s, P_{opt} = 5911 W, T_{opt} = 220 °C

CONCLUSIONS

An integrated SSEM-AG system was developed to study optimization of the single-screw extrusion process. SSEM program is a computer model of extrusion based on the mathematical description of the process. AG program is an optimization module for the system.

An example of optimization has been presented. Three design criteria (output variables) were selected for optimization: maximum extrusion throughput, minimum power consumption and low melt temperature. As input variables, screw speed, barrel temperature and screw channel depth were chosen. Convergence of the optimization procedure was rather fast obtained.

Genetic Algorithms seem to be powerful tool for optimization in polymer processing. AG starts from a set of randomly generated points, which prevents the algorithm from being trapped in a local optimum. It does not require any derivatives and do not impose any restrictions in terms of convexity of the search space.

Neural Networks can be used for modeling of the optimized process based on experimental or simulation data. A hybrid Neural Network and Genetic Algorithm approach might be a new approach for modeling and optimization of the plasticating single-screw extrusion.

NOMENCLATURE

$A_0 \ldots A_{22}$ – coefficients of the polynomial,
B_c – break condition,
F_i – global objective function for i-set of input data,
G_e – genotype (set of chromosomes),
H – channel depth,
L – screw channel length,
L_D – die length,
N – screw speed,
P – power consumption,
Q – throughput,
T – temperature,
T_b – barrel temperature,
T_m – melting point,
W – screw channel width,
X – solid bed width,
$f_{i(k)}$ – objective function of criterion k,
$f_{i(P)}$ – individual optimization criterion of min. power,
$f_{i(Q)}$ – individual optimization criterion of max. throughput,
$f_{i(T)}$ – individual optimization criterion of min. melt temperature,
h – melt film thickness,
h_f – flight clearance,
k – number of optimization criteria,
$x_{1,2\ldots N}$ – input variables,
y – output variable,
$y_{1,2\ldots N}$ – output variables,
$y_{1,2\ldots N\ opt}$ – optimal values of output variables,
y_{max}, y_{min} – max. and min. values of output variable y,
z – coordinate in the screw channel length direction,
z_D – coordinate in the die length direction,
η – viscosity,
γ^* – shear rate.

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