

Discovered functions for Shear Stress and Pressure Drop of Linear Low Density Polyethylene Using Genetic programming

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Abstract: The estimation of the functions that describe the shear stress and the pressure drop across the short orifice die as a function of shear rate at different mean pressures for linear-low-density polyethylene copolymer (LLDPE) at 190oC is obtained using Genetic Programming (GP) . The GP has been running based on experimental data in two cases; shear stress and pressure drop at different mean pressures to produce shear stress and pressure drop for each target mean pressure. The shear rate and mean pressure of linear-low-density polyethylene copolymer have been used as input variables to find the discovered functions. The experimental, calculated and predicted shear stress and pressure drop are compared. The discovered function shows a good match to the experimental data. We find that the GP technique is a good new mechanism of determination of the shear stress and the pressure drop linear-low-density polyethylene copolymer.

Keywords: Genetic Programming, pressure drop , shear stress , shear rate, linear-low- density polyethylene copolymer

1. Introduction

Numerous experimental studies (Maxwell and Jung[1] [1957](#); Hatzikiriakos and Dealy [2][1992](#); Binding et al. [3][1998](#); Couch and Binding [4][2000](#); Goubert et al. [5][2001](#); Laun,[6,7] [2003](#), [2004](#); Sedlacek [8][2004](#)) have been carried out to quantify coefficients and values which describe a number of polymer grades. Papers on the subject by Binding et al. [3]([1998](#)) and Goubert et al.[5] ([2001](#)) have already presented very good reviews of the historical background and the reader is encouraged to consult them for further insight. The different experimental techniques commonly used have also been reviewed in the work of Goubert et al. [5]([2001](#)). Within experimental errors, Couch and Binding[4] ([2000](#)) find these values of the LDPE polymer grades [low-density polyethylene].

Flow instabilities are an important aspect which seems to have been overlooked in several studies concerning the effects of pressure on viscosity (Hatzikiriakos and Dealy[2] [1992](#); Binding et al.[3] [1998](#); Couch and Binding[4] [2000](#); Laun [6,7][2003](#), [2004](#); Sedlacek [8][2004](#)). Experiments may take place at apparent shear rates ten times greater than the critical shear rate at which upstream instabilities (also named melt fracture) appear under atmospheric pressure. In the presence of the upstream instability, the flow field in the die and near its entrance is highly viscoelastic and

unsteady, rendering any numerical simulation extremely difficult. Couette-Bagley corrections used here may be several times larger (Laun[6] [2003](#)) than typical viscous Couette-Bagley corrections.

Flow stability during extrusion has already been the subject of several reviews which are too numerous to list (Denn,[9] [2001](#); Piau et al.[10] [1995](#)). It is clear that flow curves show a change in slope when upstream instabilities appear. The sharpness of this slope change depends on the nature of the polymer and on the length of the die used. In general, the shorter the die is, the more distinct the change in slope will be in the flow curve.

To our knowledge, no work except Carreras et. al [11] has focused on the effects of pressure on flow instabilities (oscillatory flow, upstream instability) prone to occur during polymer processing operations, which brings us to the following questions: do these instabilities still take place in flows under high pressures? And if so, how does pressure affect them in terms of stability criteria and in terms of pressure drop?

As an example to illustrate the relevance of accounting for flow instabilities, the work by Hatzikiriakos and Dealy[2] ([1992](#)) can be considered. They calculated apparent slow slip laws by means of a sliding plate rheometer and capillary rheometry experiments. From their capillary rheometry measurements, they concluded that the effects of pressure on pressure drop were negligible and that any deviations in the flow curve were due to slip at the wall. It is true that the deviations observed in their study were not due to pressure effects, but only because the pressure drops were too small. The apparent slip calculated in their work seems to correspond to flow regimes presenting the upstream instability.

A few years later, the same group successfully determined a pressure coefficient of $14 \times 10^{-9} \text{ Pa}^{-1}$ for a linear-low-density polyethylene copolymer (LLDPE) (Koran and Dealy[12] [1999](#)) using a new version of their high-pressure sliding plate rheometer. Since then, it has been well established that pressure affects viscosity.

In their work, Binding and his co-workers [3,4]([1998](#), [2000](#)) do not mention flow instabilities either, though they attain apparent shear rates as high as $2,500 \text{ s}^{-1}$. For LDPE, and most noticeably for the short orifice curves, one observes sharp slope changes characteristic of the onset of upstream instabilities. Moreover, regardless of extrusion temperature, the slope change appears at the same critical shear stress level reported by Laun [6,7]([2003](#), [2004](#)) for the same LDPE.

The results of Carreras et. al [11] is subdivided into two parts: the first one examines the existence of pressure effects on flow stability. To see the effects of pressure, we chose shear rates that lay on both sides of the stable/unstable flow transition under atmospheric pressure. Moreover, pressure drops were kept small to ensure that viscous heating was negligible. Finally, the effect of pressure on flow stability is shown as upstream instabilities and/or oscillating flow conditions at the wall are observed. The second part is devoted to the influence of ramifications on the effects of pressure under stable flow regime conditions. For stable flow regimes, these effects of pressure are measured and quantified in both shear and entrance flows. In contrast, and to complement work by Binding and his co-workers [3,4]([1998](#), [2000](#)) the backbones of

the molecules are quite similar but the number and length of these ramifications are changed.

In the present work, the effects of pressure on the viscosity and flow stability of one of the commercial grade polyethylenes (PEs) which is linear-low-density polyethylene copolymer have been studied using Genetic Programming (GP). The range of shear rates considered covers both stable and unstable flow regimes. “Enhanced exit-pressure” experiments have been performed attaining pressures of the order of 500×10^5 Pa at the die exit. The necessary experimental conditions have been clearly defined so that dissipative heating can be neglected.

Very high pressures can be exerted on polymers during processing. At these pressure levels, polymer melt properties, and flow stability, evolve according to laws that are different from those used at moderate pressures. Following work by Couch and Binding [4], temperature and pressure dependence of shear stress can be modeled. Carreras et. al [11] studied these effects experimentally using different rheometers. The data obtained by Carreras et. al [11] is chosen to be carried out using the Genetic Programming

The information about the mechanical properties of solutions and melts is very important for the processing of these materials in almost all branches of industries. The theoretical and experimental studies concerning the flow viscous or viscoelastic fluids through different bodies are established [13-17].

Making use of the capability of the GP, we have estimated the function that describes the shear stress and the other function that describes the pressure drop using genetic programming. Genetic programming technique has been also one of researcher’s interests in modeling of different branches of physics [18-20].

Recently, Mostafa.Y.El-Bakry et .al. studied genetic programming technique for the flow of viscoelastic fluid between two eccentric spheres [21]

The shear stress and the pressure drop are highly polarizable targets. Therefore, reliable estimates of the effect of shear rate at certain value of mean pressure is rather essential to predict at other mean pressures. GP is fed with shear rates and the mean pressure, so that the outputs imitate the experimental data. Also, we predict the pressure drop at different values of the mean pressures using the reliable estimation of the effect of pressure drop at certain value of mean pressure. GP is fed pressure drop and the mean pressure, so that the outputs imitate the experimental data. The next section deals with the introduction and the input parameters of GP. Finally, in Section 3, we present our results and conclusion.

2. The representation for the Shear Stress and Pressure Drop of Linear Low Density Polyethylene using Genetic Programming

2.1. Introduction to Genetic Programming

Genetic programming is one of a number of machine learning techniques in which a computer program is given the elements of possible solutions to the problem (in our case shear rate and mean pressure). This technique, through a feedback mechanism, attempts to discover the best solution (in our case it will be a function) to the problem at hand, based on the programmers definition of success. The Genetic programming framework creates a program which consists of a series of linked nodes. Each node takes a number of arguments and supplies a single return value. There are two general types of nodes: functions (or operators) and terminals (variables and constants) [22]. The series of linked nodes can be represented as a tree where the leaves of the tree represent terminals and operators reside at the forks of the tree. In other words, in GP the programs are written as function which is represented in expression trees. The tree elements are called nodes. The functions (F) have one or more inputs and produce a single output value. These provide the internal nodes in expression trees. The terminals (T) represent external inputs, constants and zero argument functions. For example, Fig.(1) shows the representation of the function $(A*(A+B))$ i.e. $*(A,+(A,B))$. To read trees in this fashion, one resolves the sub-trees in a bottom-up fashion, where $F = \{*,+\}$ and $T = \{A,B\}$. The genetic programming model seeks to imitate the biological processes of evolution, treating each of these trees or programs as an “organism”. Through natural selection and reproduction over a number of generations, the fitness (i.e., how well the program solves the specific problem) of a population of organisms is improved.

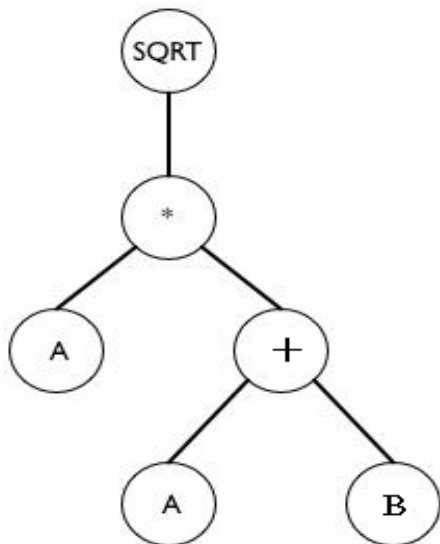


Fig. (1): Tree representation of the equation square root $*(A,+(A,B))$ i.e. $(A*(A+B))$.

A typical implementation of GP (i.e., the process of determining the best (or nearly best) solution to a problem in GP) involves the following steps:

- 1) GP begins with a randomly generated initial population of solutions.
- 2) A fitness value is assigned to each solution of the populations
- 3) A genetic operator is selected probabilistically.

Case i) If it is the reproduction operator, then an individual is selected (we use

fitness proportion-based selection) from the current population and it is copied into the new population. Reproduction replicates the principle of natural selection and survival of the fittest.

Case ii) If it is the crossover operator, then two individuals are selected. We use tournament selection where number of individuals is taken randomly from the current population, and out of these, the best two individuals (in terms of fitness value) are chosen for the crossover operation. Then, we randomly select a sub tree from each of the selected individuals and interchange these two sub-trees. These two offspring are included in the new population. Crossover plays a vital role in the evolutionary process.

Case iii) if the selected operator is mutation, then a solution is (randomly) selected. Now; a sub-tree of the selected individual is randomly selected and replaced by a new randomly generated sub-tree. This mutated solution is allowed to survive in the new population. Mutation maintains diversity.

4) Continue step 3 for any case of the above three cases, until the new population gets solutions. This completes one generation.

5) GP will not converge. Then, step 2)-4) are repeated till a desired solution is achieved. Other-wise, terminate the GP operation after a predefined number of generations.

2.2. Genetic Programming Approach

We use the experimental data of the shear stress at certain values of the shear rates and the mean pressures to produce the shear stress (calculated) for each case. Also, the experimental data of the pressure drop at certain values of the shear rates and the mean pressures are used to produce the pressure drop (calculated) for each case. The shear rates and the mean pressures are used as input variables to find the suitable function that describes the experimental data.

Our representation, the fitness function is calculated as a negative value of the total absolute performance error of the discovered function on the experimental data set, i.e. a lower error must correspond to a higher fitness. The total performance error can be defined for all the experimental data ($j = 1 \dots, n$) set as:

$$E = \sum_{j=1}^n |X_j - Y_j|^2 \quad (1)$$

Where X_j represents the experimental data for element j and Y_j represents the calculated data for element j . The running process stops when the error E is reduced to an acceptable level (0.00001). The training data set which is used based on the experimental data for shear rates at different mean pressures [11].

GP was run for 1000 generations with a maximum population size of 800. The operators were: crossover with probability 0.9 and mutation with probability 0.01. The function set is $\{+, -, *, \backslash\}$, and the terminal set is $\{\text{random constant from 0 to 10, the shear stress and the pressure drop}\}$. The "half" initialization method was used with an initial maximum depth of 17, and tournament selection with a tournament size of 9. The GP was run until

the fitness function is reduced to an acceptable level (0.00001). The discovered function has been tested to associate the input patterns to the target output patterns using the error function. The final discovered function for describing the shear stress, τ is given by

$$\tau = X_2 - 3.1618 X_1 + 131.894335 + 229.67553 + (229.67553 X_1) / (1 - X_1) + 100 / (1/b + 0.25908) \quad (2)$$

Where X_1 is the mean pressure and X_2 is the shear rate

$$a = ((19.681552 - 2 X_1) - 0.30997)^{-1}$$

$$b = (19.681552 - X_1)^{-1}$$

The final discovered function for describing the pressure drop, Δp , is given by

$$\Delta p = 0.85470 X_2 + 2.96235 X_1 + 138.12535 (X_2 - 0.03450 X_1) / [(15.82558 X_2 + 96137) (0.69132 + 0.197333 X_2)] \quad (3)$$

3. Results and conclusion

Our discovered shear stress function, τ , Eq.(2) and pressure drop function, Δp , (3) were tested using the experimental data of the shear stress and pressure drop for linear-low-density polyethylene copolymer (LLDPE) at 190°C. The training data is based on experimental observations at shear rate ranging from 1 (1/s) to 600 (1/s) [11]. The values of mean pressure are taken as 1, 200, 400 and 600 multiplied by $(10)^5$ pa for the shear stress and for the pressure drop the mean pressures are, 1, 100, 300 and 500 multiplied by $(10)^5$ pa.

Fig.(2) displays a good match between the experimental data of the shear stress function and the calculated ones by employing our discovered function Eq.(2). After convergence, the discovered function has been used to predict shear stress with two values of mean pressure 100 and 300 multiplied by $(10)^5$ pa, at shear rate ranging from 1 (1/s) to 600 (1/s) which corresponds to the available experimental data [11] and Fig.(3) illustrates the predicted shear stress compared with experimental data.

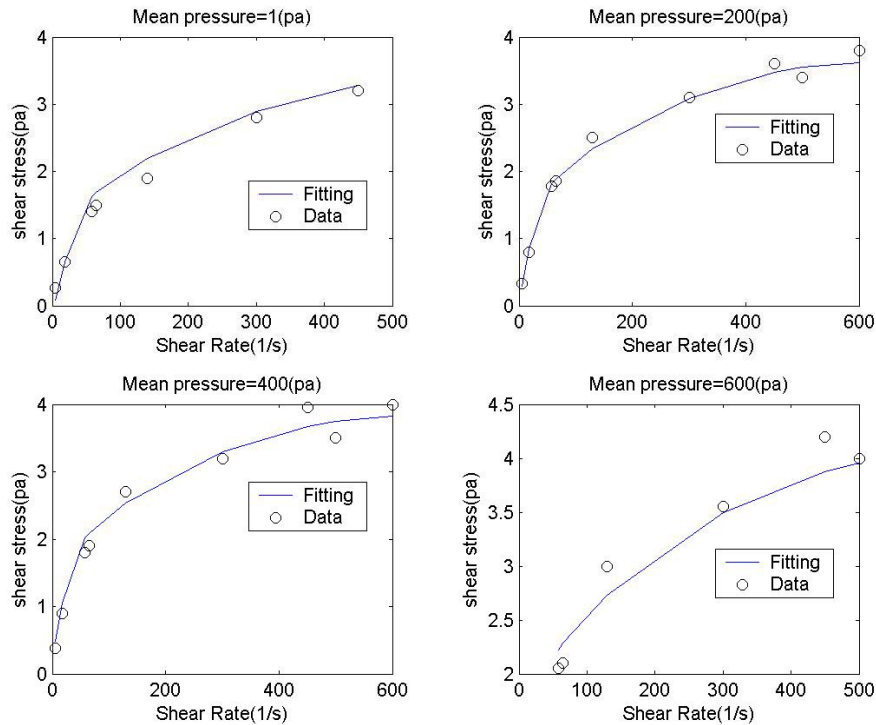


Fig.(2):Comparison between the shear stress calculated by employing our discovered function given in Eq.(2) and the corresponding experimental points of mean pressures 1, 200, 400 and 600 multiplied by $(10)^5$ pa .

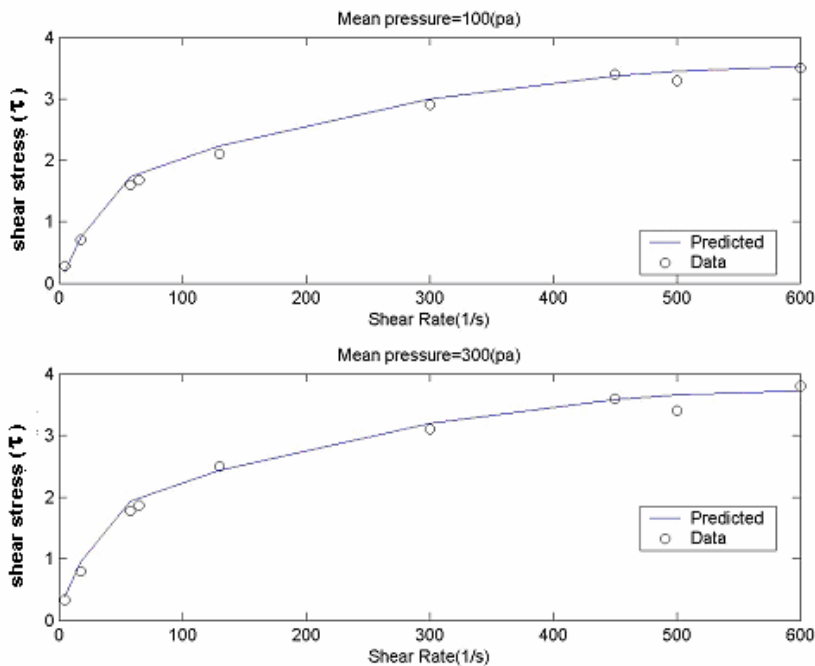


Fig.(3):Comparison between the experimental and predicted shear stress of mean pressures 100 and 300 multiplied by $(10)^5$ pa .

Fig.(4) displays also a good match between the experimental data of the pressure drop for (LLDPE) and the calculated ones by employing our discovered

function (3). After convergence, the discovered function has been used to predict pressure drop at values of mean pressures 200, 400 and 600 multiplied by $(10)^5$ pa, at shear rate ranging from 100 (1/s) to 600 (1/s) which corresponds to the available experimental data [11] and Fig.(5) illustrates the predicted pressure drop compared with experimental data.

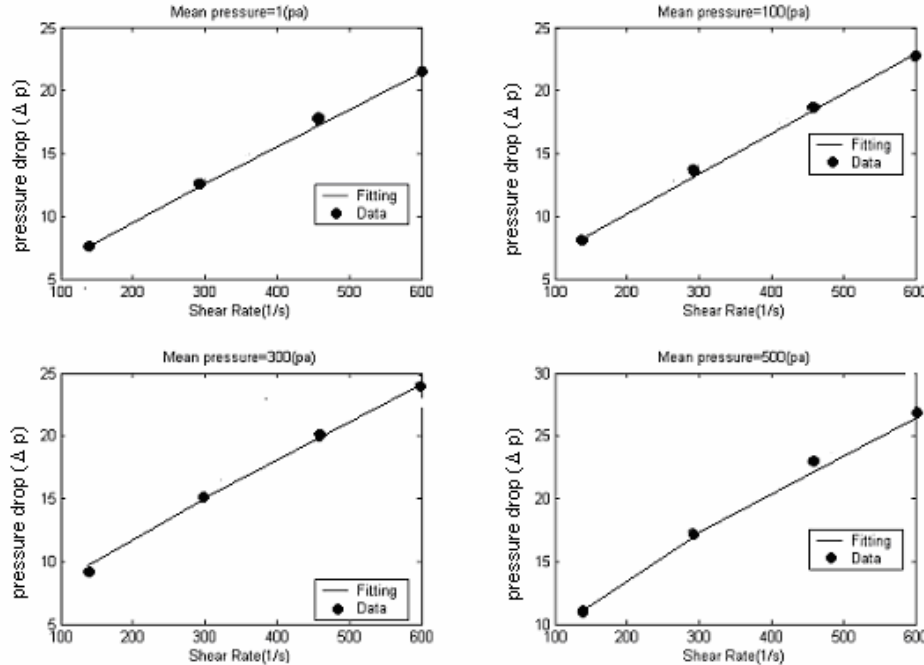


Fig.(4): Comparison between the pressure drop calculated by employing our discovered function given in (3) and the corresponding experimental points of mean pressures 1, 200, 400 and 600 multiplied by $(10)^5$ pa .

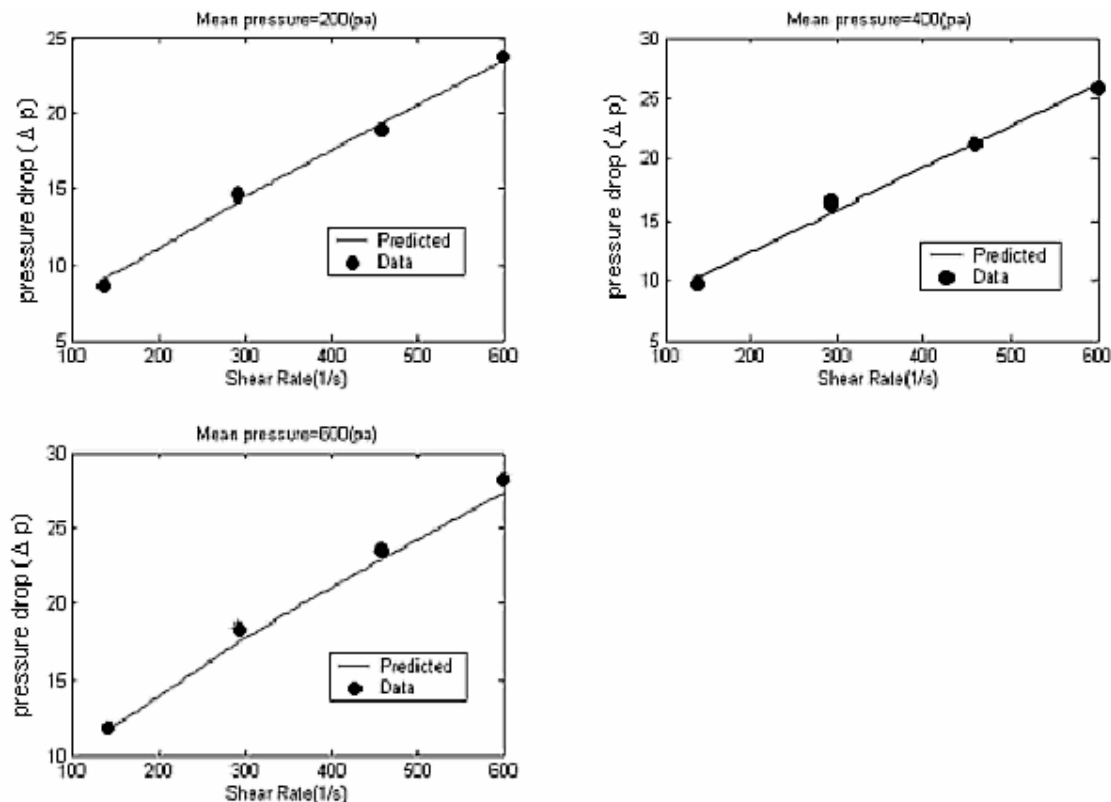


Fig.(5):Comparison between the experimental and predicted pressure drop at values of mean pressures 200, 400 and 600 multiplied by $(10)^5$ pa .

Finally, we conclude that GP has become a relevant research area in the field of fluid mechanics. The present work presents a new technique for modeling the shear stress and pressure drop for linear-low-density polyethylene copolymer (LLDPE) based on GP technique. The discovered function shows a good match to the experimental data for both the shear stress and the pressure drop. We find also that the GP technique is able to improve upon more traditional methods in different branches of physics, see e.g. Refs. [23,24,25].

References

- [1] Maxwell B and Jung A ; Hydrostatic pressure effects on polymer melt viscosity. *Mod Plastics* 35 (1957) 74–180
- [2] Hatzikiriakos SG, Dealy JM ; Wall slip of molten high density polyethylenes. II. Capillary rheometer studies. *J . Rheol* 36 (1992)703–741
- [3] Binding DM, Couch MA, Walters K ; The pressure dependence of the shear and elongational properties of polymer melts. *J Non-Newtonian Fluid Mech* 79 (1998) 137–155
- [4] Couch MA, Binding DM ; High-pressure capillary rheometry of polymeric fluids. *Polymer* 41 (2000) 6323–6334
- [5] Goubert A., Vermant J., Moldenaers P., Göttfert A., Ernst B. ; Comparison of measurement techniques for evaluating the pressure dependence of viscosity. *Appl Rheol* 11 (2001) 26–37
- [6] Laun HM ; Pressure dependent viscosity and dissipative heating in capillary Rheometry of polymer melts. *Rheol Acta* 42(2003) 295–308
- [7] Laun HM; Capillary Rheometry for polymer melts revisited. *Rheol Acta* 43 (2004) 509–528
- [8] Sedlacek T, Zatloukl M, Filip P, Boldizar A, Saha P ; On the effect of pressure on the shear and elongational viscosities of polymer melts, *Polym. Eng. Sci.* 44 (2004) 1328–1337
- [9] Denn MM ; Extrusion instabilities and wall slip. *Annu Rev Fluid Mech* 33 (2001)

265–297

- [10] Piau JM, El Kissi N., Toussaint F., Mezghani A. ; Distortions of polymer melt extrudates and their elimination using slippery surfaces. *Rheol Acta* 34 (1995)40–57
- [11] Carreras, E.S., Elkissi, N., Piau, J.M., Toussaint, F. and Nigen, S.; pressure effects on viscosity and flow stability of polyethylene melts during extrusion", *Rheologica Acta*, vol.45, No.3(2006)209-222
- [12] Koran F, Dealy JM ; A high pressure sliding plate Rheometer for polymer melts. *J Rheol* 43 (1999)1279–1290
- [13] Peysson, Y., Aubry, T. and Moan, M.; Phenomenological Approach of the Effective Viscosity of Hard Sphere Suspensions in Shear-Thinning Media , *Appl. Rheol.* 16:3 (2006) 145-151.
- [14] Koenigsberg, W. and Selverian, J.H.; Zone Method for Representing Relaxation Characteristics of Viscoelastic Materials , *Appl. Rheol.* 15:3 (2005) 160-171.
- [15] Anderson, P.D., Dooly, J. and Meijer, H.E.H.; Viscoelastic Effects In Multilayer Polymer Extrusion, *Appl. Rheol.* 16:4 (2006) 198-205 .
- [16] Edwin, C.C. and Montgomery, T.S.; Creeping Sphere-plane Squeeze Flow To Determine The Zero Shear Rate Viscosity Of HDPE Melts, *Appl. Rheol.* 14:1 (2004) 33-39 .
- [17] Abu-El Hasan, A., Abdel Wahab, M., El-Bakry, M. and Zidan, M.; flow of fluids of grade two between two eccentric rotating spheres, *ZAMP*, 47 (1996) 313 .
- [18] Banzhaf, W., Nordin, P., Keller, R. and Francone, F.; Genetic Programming An Introduction: On the Automatic Evolution of Computer Programs and Its Applications, Morgan Kaufmann Publishers, Inc. San Francisco, California, (1998).
- [19] Riolo, R.; Genetic Programming Theory and Practice, Bill worzel– Computers (2003).
- [20] El-Bakry, M.Y. and Radi, A.; Genetic Programming for hadronic interactions at high energies, *Int. J. Mod. Phys.C*.18 (2007) 1-6.
- [21] El-Bakry, Mostafa. Y. and Radi, A.; Genetic Programming Approach For Flow of Steady State Fluid Between Two Eccentric Spheres, To be published in *Appl. Rheol.* 17:6 (2007) 68210
- [22] Poli, R.; Genetic Programming for Feature Detection and Image Segmentation, "Dec" School of Computer Science, University of Birmingham. (1995).
- [23] Kwan, C.K., Kauppila, W.E., Lukaszew, R.A., Parikh, S.P., Stein, T.S., Wan, Y.J. and Dababneh, M.S.; *Phys. Rev. A* 44 (1991) 1620.
- [24] Parikh, S.P., Kauppila, W.E., Kwan, C.K., Lukaszew, R.A., Przybyla, D., Stein, T.S. and Zhou, S.; *Phys. Rev. A* 47 (1993) 1535.
- [25] El-Bakry, S.Y. and Radi, A.; Discovered function for positron collisions with alkali-metal atoms using genetic programming, *Int. Journal of Mod Phys.C*, Vol.18 No.3 (2007) 351-358 .