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# A finite-difference method for the prediction of velocity field in extrusion process

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#### Abstract

Extrusion defects and flow instabilities are an important limitation in most product processing operations. Investigation of the fluid kinematics to deduce the dynamical response of the fluid can be very useful to characterize these instabilities and understand the mechanisms involved in their triggering and enhancement. To do so, the flow of a Newtonian fluid through a screw press has been studied in order to predict the downstream velocity field in extrusion process. Flow in the screw press is modeled by adapting the classical theory of single screw extrusion. Some publications have addressed this subject matter, especially in the nineties. However, most of these publications develop models that are not so easy to apply. To complement those earlier works, an approximate model base on finite-difference method is developed. The models in this paper may be considered as of pedagogical value because of the ease of their application; none-theless, results are obtained basing on the real extruding conditions, such as a general screw geometry. In order to achieve this pedagogical purpose, three important properties pertaining to model building are considered in this article. These properties are applicability, simplicity, and level of technique applied. Moreover, the models introduced in this paper are straightforward application by both practitioners and students. The ease of the applicability is confirmed by the suitability to adopt a widely employed software, such as Microsoft Excel, to implement the model developed.

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Keywords: Extrusion; Finite-difference; Downstream velocity field

## 1. Introduction

At the beginning, single screw extruders have been widely used in the polymer industry, but in the last decades they have been extensively applied in the ceramic, food and pharmaceutical industries, due to the fact that they are cheap, robust and continuous.

Extruders geometry is an important parameter of the extrusion process, since it affects shear rate and residence time values, involving direct outcomes on the quality of the final product. Defects and flow instabilities are important limitations in processing operations of most extruded products. Investigating fluid kinematics to deduce the dynamical response of the fluid can be very useful to characterize those instabilities and understand the mechanisms involved in their triggering and enhancement. In addition, better control on the downstream velocity field in extrusion process can be a significant source of quality differentiation between food products. In other words, a more regular profile and lower values of the mean shear rate along the extruder determine a reduced gelatinization of the compound. Conversely, extruders characterized by high values of shear rate can involve several issues in controlling the final quality of the products, due to the complex behavior of the shear rate profile along the screw axis.

On the ground of these premises, models for predicting the extrusion process variables have been receiving ever increasing attention by the researchers. Until the 1970s, food extrusion was regarded as an art rather than a science; thus, only trained and experienced personnel could handle

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#### Nomenclature

$D_{b}$ $R_{s}$ $\omega$ $W$ $H$ $\theta$ $\theta_{b}$ $\mu$ $V_{s}$ $x$	internal barrel diameter screw root radius rotation sped of screw width of channel at the internal radius of barrel channel depth helix angle of screw helix angle of screw at internal barrel radius that is $R_s + H$ viscosity of the Newtonian fluid screw root velocity down channel coordinate	$Z = V_x, V_y, \frac{\partial P}{\partial x} = \frac{\partial P}{\partial y} = \frac{\partial P}{\partial z} = n_{i,j} = nW, nE = h_z, h_y$ $Q_{\text{leakage}}$	channel width coordinate $V_z$ velocity component of x, y and z directions pressure gradient in down channel direction pressure gradient in channel depth direction pressure gradient in channel width direction generic node $(i,j)$ in a $nW^*nH$ grid mesh <i>I</i> number of nodes along z and y direction distance between two adjacent nodes along z and y direction volumetric flow rate of leakage flow
x y	down channel coordinate channel depth coordinate	<i>Q</i> leakage	volumetric flow rate of leakage flow

such equipment. However, over the past 30 years and especially in the nineties, several models have been developed to predict process throughput, energy requirements, mixing patterns and residence time distribution of extruders. One of the earliest models for single screw extrusion was presented by Darnell and Mol (1956). The model developed by the authors described plug flow of a solid feed material along a screw of constant pitch and depth. The original approach proposed by Darnell and Mol (1956) has been subsequently developed by Burbidge and Bridgwater (1995), Englander, Burbidge, and Blackburn (2000), by adding the rheological parameters characterizing pasty feed materials. Following a similar approach, further authors focused on extrusion process for food materials. Among recent works, Vergnes, Le Roux, Chaurand, and Abécassis (1995), developed and experimentally validated a thermomechanical model for pasta extrusion. More specifically, the flow along the screw channel was computed using finite element simulation and described by means of an approximate model, which has been derived starting from wellknown analyses of plastic extrusion. Karwe, Chiruvella, and Jaluria (1996), studied the behavior of starch-based materials under high temperature environment, by a numerical simulation of flow inside a single screw extruder. Elsey, Riepenhausen, Mckay, Barton, and Willis (1997), developed a flexible dynamic model of the extrusion process in order to predict and control realistic quality variables, such as product gelatinization fraction. Along the same line, the earlier work of Blackburn, Bottena, and Burbidgea (2003), presented a general one-dimensional model for the prediction of the pressure field in single screw extrusion including corrections for non-constant channel depth in the screw.

As stated above, several models have been developed and presented on extrusion processes. Nevertheless, the analysis of the scientific literature has pointed out that the issue of accurate predicting the velocity distributions has been somehow neglected. In particular, issues such as how to predict the downstream velocity field in extrusion processes have not received the required attention in technical literature and only few authors faced this challenge. Both mathematical and experimental approaches have been employed to achieve the required accuracy in order to describe and solve more realistic generalized problems. Choo, Neelakantan, and Pittman (1980), developed a computer model for flow in a single-screw extruder, pumping a Newtonian liquid under isothermal and developed flow conditions. Flow rate, screw speed, and pressure gradient characteristics were measured, and a tracer particle technique was employed to determine channel velocity profiles. The data were required for the testing the model which takes into consideration channel curvature. Using the resulting experimental data, Li and Hsieh (1996), developed and tested an analytical solution of an isothermal, Newtonian fluid in a single screw extruder with finite channel. Following this analytical approach, Yu and Gunasekaran (2003), proposed and tested a numerical approach to analyze flow field and heat transfer developed inside a single-screw channel. Finite-difference and finite element methods were used to obtain numerical solutions for flow and energy equations also in the case of non-Newtonian fluids. Along the same line, but more focused on experimental approaches, Bakalis, Cox, Russell, Parker, and Fryer (2006), analyzed velocity distributions in single-screw extruder a specially designed and manufactured, by using positron emitting particle tracking. In particular, velocity profiles in the extruder, that could be predicted by computational fluid dynamics were generated, measured and compared to the experimental data by setting process parameters, flow rate and rotational speed in the range used in commercial processes.

On the ground of literature analysis, it can be right stated that most of the papers examined present approaches that are able to accurately predict the downstream velocity field in extrusion process. However, it is also self-evident that the way approaches were developed has can significantly affect both their practical applicability and their degree of current adoption. Generally speaking, the higher the accuracy of the approach proposed, the higher the resulting complexity of the model; consequently, higher difficulties may be involved in practical implementation of the model itself. As a result, a necessary trade-offs between model complexity and practical applicability rise. Moreover, in some cases a detailed explanation on how to apply well-know techniques, such as finite-difference methods, exploiting widely employed software (e.g. MS Excel) should be considered as essential for the applicability of the models developed. The analysis of scientific literature related to the extrusion process, and in particular to the downstream velocity field, has pointed out that the issue of how readers could apply the proposed models has been somehow neglected.

Based on these premises, the aim of this paper is twofold. First, we propose a finite-difference approach for predicting the downstream velocity field in extrusion process. Fluid flow in the screw press is modeled by adopting the classical theory of single screw extrusion for Newtonian fluids in a general screw geometry. In addition, we present a detailed numerical case study, in order to provide the required knowledge for a quickly propagation of the model without expensive and obscure software. Usually, these tools act as black boxes where only few people know how they work and consequently only few people have a full control on them. To overcome this problem the numerical case study is developed step by step by user-friendly and widely employed software as MS Excel.

The model proposed in this paper may be considered as of pedagogical value because of its applicability, simplicity, and good performance in predicting the velocity field values. Moreover, the model introduced in this paper is of straightforward application by both practitioners and students. The ease of the applicability is confirmed by the suitability to adopt a widely employed software, such as Microsoft Excel, to implement the model developed. The good performance of the model is confirmed by the comparison between numerical results and experimental data from published literature.

This study is part of a wider project aiming to control microbiological parameters of extruded products. The whole project is founded by Regione Emilia-Romagna inside the PRRITT (Programma Regionale per la Ricerca Industriale, l'Innovazione e il Trasferimento Tecnologico).

## 2. Safety emphasis

This study is part of a wider project whose aim is to define process operative leverages in order to control microbiological polluters in food extruded products. In particular, a mathematical model, and subsequently a simulation software, will be developed in order to predict physical properties affecting the proliferation of microbiological polluters in products during the whole process. Thanks to the software developed, proper conditions could be designed to optimize the safety of the extrusion process.

#### 3. Mathematical formulation

The material fed to the screw extruder passes through a relatively long, shallow helical channel formed by the flight of the screw.

The channel bounded by the inner surface of the barrel, the root of the screw and the flight. In order to simplify the problem many approaches hypothesize stationary screws and rotating barrels (in opposite direction). This does not alter the analysis when the internal barrel diameter is much larger then the channel depth. Nevertheless, Li and Hsieh (1996), underlined the source of error and they proposed a new analytical solution for flow in extruder with a rotating screw and stationary barrel. In accordance with Li and Hsieh (1996), and in order to provide better and more realistic results, the model developed exploits a rotating screw and stationary barrel approach. The channel and the screw geometry studied is qualitatively shown in Fig. 1; in the scheme, x, y and z represent channel down stream, channel height and channel width directions, respectively.

Since in many practical extruders the height of the screw channel is much less than the barrel diameter, the screw curvature is assumed to be very small. As a consequence, the barrel surface and the screw channels can be mathematically modelled as unwrapped. In other words, from a geometrical point of view, the higher the ratio of the barrel diameter to the height of screw channel, the lower screw curvature should be and the screw channel tends to become flat plate. This does not alter the analysis, since centrifugal force are negligible. In order to further simplify the problem, the following assumptions are commonly used without losses in accuracy:

- fluids flow is assumed as laminar, since the very high viscosity of the common extruded fluid (>10<sup>3</sup> Pa s) leads to Reynolds numbers much less than unity;
- the inertia terms in the Navier–Stokes equation can be neglected in comparison with viscous and pressure terms;
- gravitational force is negligible;
- the fluid is incompressible and Newtonian;
- the flow is fully developed;
- no slips at the walls occur.

Under these hypotheses, equations describing fluid motion for this problem in rectangular coordinates can be expressed as follows:

$$\frac{\partial P}{\partial x} = \mu \left( \frac{\partial^2 V_x}{\partial y^2} + \frac{\partial^2 V_x}{\partial z^2} \right) \quad x \text{ component}$$

$$\frac{\partial P}{\partial y} = \mu \left( \frac{\partial^2 V_y}{\partial y^2} + \frac{\partial^2 V_y}{\partial z^2} \right) \quad y \text{ component}$$

$$\frac{\partial P}{\partial z} = \mu \left( \frac{\partial^2 V_z}{\partial y^2} + \frac{\partial^2 V_z}{\partial z^2} \right) \quad z \text{ component}$$
(1)

Assuming that  $V_y \approx 0$ , which is a reasonable assumption for screws with a small channel depth to width ratio,



Fig. 1. Real and "unwrapped" geometry of a single screw extruder.

H/W, and using the continuity equation; then,  $\partial V_y/\partial z \approx 0$ ,  $\partial V_z/\partial x \approx 0$ , and  $\partial V_y/\partial y \approx 0$ . Thus Eq. (1) becomes:

$$\frac{\partial P}{\partial x} = \mu \left( \frac{\partial^2 V_x}{\partial y^2} + \frac{\partial^2 V_x}{\partial z^2} \right) \quad x \text{ component}$$

$$\frac{\partial P}{\partial y} \approx 0 \qquad \qquad y \text{ component}$$

$$\frac{\partial P}{\partial z} \approx \mu \frac{\partial^2 V_z}{\partial y^2} \qquad \qquad z \text{ component}$$
(2)

The above simplified equations of motion can be found in Li and Hsieh (1996). Since the proposed model utilizes a rotating screw and stationary barrel approach, boundary conditions should take into account the screw velocity. In particular, the screw flight velocities are not constant but variable as a function of the radius; from the mathematical point of view, in the case of the *x*-component the function is expressed in the following boundary conditions:

Barrel 
$$V_x(z, H) = 0$$
  
Screw root  $V_x(0, y) = \omega R_s \cos(\theta)$   
 $V_x(0, y) = \omega (R_s + y) \cos(\theta)$   
Screw flights  $V_x(W, y) = \omega (R_s + y) \cos(\theta)$ 
(3)

As can be seen from the above equations, the x-component of Eq. (2) is a non-homogeneous, second order partial differential equation with non-homogeneous boundary conditions. Li and Hsieh (1996), proposed an analytical solution of this problem for finite rectangular channel. In order to extend the solution to a general duct geometry, a finite-difference method is applied to solve the differential x-component equation. To this extent, the domain is discretized by imposing a grid defined for a set of nodes  $n_{i,j}$  (see Fig. 2).

On the ground of these premises, the x-component of the above equation can be written in discrete form as follows (the mesh is an  $nW^*nH$  grid along z and y direction, respectively):

$$\frac{\partial P}{\partial x} \approx \mu \left( \frac{V_x(i+1,j) - 2V_x(i,j) + V_x(i-1,j)}{h_y^2} + \frac{V_x(i,j+1) - 2V_x(i,j) + V_x(i,j-1)}{h_z^2} \right)$$
(4)

Hence, for an estimated pressure gradient in the down channel direction, the component of velocity  $V_x(i,j)$  for the (i,j) node in x direction becomes:



Fig. 2. Discretized domain.

$$V_{x}(i,j) \approx \frac{h_{y}^{2}h_{z}^{2}}{2(h_{y}^{2}+h_{z}^{2})} \left[ \frac{V_{x}(i+1,j)+V_{x}(i-1,j)}{h_{y}^{2}} + \frac{V_{x}(i,j+1)+V_{x}(i,j-1)}{h_{z}^{2}} - \frac{1}{\mu} \frac{\partial P}{\partial x} \right]$$
(5)

It is noteworthy that the velocity value in the generic node (i,j) is a function of the velocity values close to the node itself, and, in particular, these are the velocity value at the up node  $V_x(i+1,j)$ , the velocity value at the down node  $V_x(i-1,j)$ , the velocity value on the right side node  $V_x(i,j+1)$ , and the velocity value on the left side node  $V_x(i,j-1)$  as shown in Figs. 2 and 4. These velocity values have been derived in the previous iteration and are assumed as constants for the current iteration. Since boundary conditions are constant along the procedure, Eq. (5) can be adopted iteratively for each node in the mesh (except the boundary nodes) until a required level of accuracy is achieved.

Based on the same rationale, slanted walls of the channel can be taken into account by a suitable mesh as shown in Fig. 3.

As an oblique line can be shown in a PC monitor by pixels, slanted walls of the channel can be modeled by rectangular grid and, as can be seen in Fig. 3, the higher the number of nodes, the higher the quality of the model should be.

As shown in Li and Hsieh (1996), for the cross channel flow, z component of Eq. (2) can be integrated twice to yield:

$$V_z = \frac{R_{\rm s} \ \omega \ \sin \theta_{\rm b} (H-y)}{H} \left[ 3 \frac{y}{H} - 1 \right] + \frac{6Q_{\rm leakage} \ [Hy - y^2]}{H^3}$$

#### 4. Software implementation

Nowadays, commercial solutions are available to solve complex fluid dynamic problem, although these solutions are often expensive, unknown, and not user friendly if compared to spreadsheet programs which are available in widespread, cheap and user friendly software packages as MS Office, Star Office or Open Office. Besides, as stated above, the commercial solutions for solving complex fluid dynamic problem, in several cases, act as black boxes and only few people know how they exactly work; consequently, few people have a full control on them. This means that few people can utilize and fully understand the outcomes from the software. Conversely, when adopting user friendly and widely employed softwares, a general model can become a powerful tool for a large number of users. To this extent, and due to its wide employment, a MS Excel implementation of the presented approach has been developed.

Due to its framework, MS Excel is particularly suitable to solve the finite different approach. As well known, it is structured by cells can contain labels, numerical values and mathematical relationships between cells. Due to its similarity to the finite different approach, this structure is particularly appropriate to describe the mesh and the mathematical relationships between each node. In other words, each cell in MS Excel is approached as a node, where both numerical value and analytical formula represent the down stream velocity and the mathematical relationship to solve the problem, respectively. Moreover, thank to the large number of available cells, MS Excel is particularly suitable to be adopted to implement the iterative approach required to achieve a defined level of accuracy.

Once the number of nodes is defined, the cells in MS Excel to be implemented, can be identified. Clearly, the higher the number of nodes of the mesh, and consequently the number of cells involved, the higher the resulting accuracy of the model. Following the boundary conditions of Eqs. (3), the boundary cells have to be implemented with the respective formulation, whereas the others cells have to be initially set to 0. Fig. 4 shows the mesh (the boundary cells are in grey) at the iterative step 0, the related data and the screw flights velocity formulation in a boundary cell on the left side.



Fig. 3. Discretized domain with slanted walls.



Fig. 4. MS Excel application at the iterative step 0.

In order to develop the iterative procedure, a set of tables have to be computed. In other words, Eq. (5) has to be adopted for the inside cells where the velocity

values close to the specific cell (i.e.  $V_x(i,j+1)$ ,  $V_x(i,j-1)$ ,  $V_x(i+1,j)$  and  $V_x(i-1,j)$ ) are obtained in the previous table and are treated as constants values

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Fig. 5. Iterative MS Excel application.

for the current table (see Fig. 5). To this extent, to implementing the iterative procedure the user can quickly copy the second table as shown in Fig. 5. The higher the number of iterations, and consequently the number of tables computed, the higher the accuracy of the model.

It is noteworthy that the above implementation developed for a rectangular channel can be easily extended to applications for general channel geometry: different geometries can be built by simply adding and/or removing opportune cells in MS Excel.

## 5. Results

To assess validity and accuracy of the proposed approach, results provided by the finite-difference methodology are compared with those presented in published papers. Since experimental and/or analytical data are currently available only for rectangular channel, the application is developed with a rectangular dept. The

Table 1	
Pertinent	data

Н	10	mm
W	30	mm
$h_{y}$	1	mm
$h_z$	1	mm
nH	11	
nW	31	
R <sub>s</sub>	9	mm
μ	10,000	Pa s
$\phi_{ m b}$	0.7889	Rad
ω	3.125	1/s
$V_x$	19.818	mm/s
$\partial P/\partial x$	5000	Pa/mm

Table 2 Down channel velocity

x = 15  mm	V <sub>x</sub>				
<i>y</i> (mm)	Numerical (mm/s)	Analytical (mm/s)	Comparison (%)		
9.0	-0.06657	-0.0664	-0.265		
8.0	0.326844	0.326229	0.188		
7.0	1.194325	1.185439	0.744		
6.0	2.512203	2.498218	0.557		
5.0	4.272357	4.256302	0.376		
4.0	6.472487	6.456927	0.240		
3.0	9.116147	9.103026	0.144		
2.0	12.21223	12.20286	0.077		
1.0	15.77401	15.76917	0.031		

predicted down channel velocity is compared with the analytical solution proposed by Li and Hsieh (1996), whose approach was validated by experimental results measured by Choo et al. (1980). Table 1 shows the pertinent data, while Table 2 shows the down channel velocity computed and the comparison results in the middle of the channel.

As can be observed from Table 2, the difference is less than 1% even when only a  $10 \times 30$  mesh is used. These results are obtained after only 79 iterations. Clearly, the higher the number of iterations and the higher the number of nodes in the mesh, the higher the accuracy should be. It is noteworthy that the user can suitably set these two parameters in order to achieve a desired level of accuracy. In this case study, the maximum difference less than 1% from the analytical solution proposed by Li and Hsieh (1996), is the criteria utilized for deciding when the solution had converged.

In Fig. 6, the three dimensional down channel velocity representation is shown by MS Excel surface graph.



Fig. 6. A three dimensional down channel velocity representation.

## 6. Conclusions

The paper proposes a finite-difference approach for solving the down channel velocity in a single screw extruder of a Newtonian fluid. The approach completes those existing in today's literature by adding an efficient as well as easy to apply procedure to obtain the velocity field. Moreover, the model may be considered as of pedagogical value because of its applicability, simplicity, and level of technique applied. Moreover, the model introduced in this paper is of straightforward application by both practitioners and students. Since of a user friendly, widely employed, and cheap software as MS Excel is utilized for implementing the model, the proposed approach becomes an interesting and practical tool aiming at a quickly propagation. In other words, this study has presented a tool that can be adopted by every people for constructing the screw characteristics and the analyzing the extruder performance.

The predicted down channel velocity data are compared with the analytical data of Li and Hsieh (1996), that were validated with the experimental data of Choo et al. (1980). Testing the proposed approach for a small mash ( $10 \times 30$  nodes), has yielded less than 1% difference, providing good findings of the methodology developed.

The fully developed velocity profile reveals important information about the effect of the screw flight. Besides, it represents the starting point for the fluid dynamic and thermodynamic approach for the purposes of screw design and extrusion simulation.

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