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YE. V. TRACHUK

Postgraduate Student at the Department of Machines and Apparatus  
of Chemical and Oil Refining Industries  
National Technical University of Ukraine  
“Igor Sikorsky Kyiv Polytechnic Institute”  
ORCID: 0009-0006-1802-2058

M. P. SHVED

Ph.D., Associate Professor at the Department of Machines and Apparatus  
of Chemical and Oil Refining Industries  
National Technical University of Ukraine  
“Igor Sikorsky Kyiv Polytechnic Institute”  
ORCID: 0000-0001-7725-1447

## ANALYSIS OF THE INFLUENCE OF POLYMER MELT VISCOELASTIC PROPERTIES ON THE MIXING QUALITY IN A DISK EXTRUDER CALCULATION

The amount of virgin plastic produced is increasing every year. At the same time, to meet modern requirements, polymers are modified with various additives forming composite polymer materials. The production of this type of materials requires the use of equipment capable of ensuring high-quality mixing of components within a wide range of properties. One way to meet these requirements is to use cascade extrusion systems, in which a screw-disk extruder is used as a melter and homogenizer [1–2].

The article discusses the influence of the viscoelastic properties of polymer melt in modeling the mixing process in disc extruders, which is key to achieving homogeneous and isotropic composite materials. A Newtonian fluid model, which ignores the viscoelastic properties of the material, can be used to determine velocity fields and productivity during extrusion. However, its limitations lead to inaccurate predictions in cases where the material exhibits viscoelastic properties.

To overcome these shortcomings, a second-order rheological model can be used, which describes both the viscous and elastic properties of the material. Using numerical modeling, a comparison was made between the results obtained using the Newtonian fluid model and the modified second-order rheological equation in the Rivlin-Ericksen formulation. The results showed that when viscoelastic effects are taken into account, the radial flow velocity increases, and the value of the shear strain caused by this component decreases. The values of the shear strain caused by the tangential velocity do not depend on the magnitude of the radial velocity. The total shear strain when using different fluid models remained virtually unchanged: 1719,2 units for the Newtonian fluid model and 1695 units for the second-order model. Thus, the difference between the calculation results is 1,38 %, which is not significant for this indicator.

**Key words:** extrusion, disk extruder, clearance between disks, shear rate, shear strain, melt quality.

Є. В. ТРАЧУК

аспірант кафедри машин та апаратів хімічних  
і нафтопереробних виробництв  
Національний технічний університет України  
«Київський політехнічний інститут імені Ігоря Сікорського»  
ORCID: 0009-0006-1802-2058

M. P. ШВЕД

кандидат технічних наук,  
доцент кафедри машин та апаратів хімічних і нафтопереробних виробництв  
Національний технічний університет України  
«Київський політехнічний інститут імені Ігоря Сікорського»  
ORCID: 0000-0001-7725-1447

## АНАЛІЗ ВПЛИВУ В'ЯЗКОПРУЖНИХ ВЛАСТИВОСТЕЙ РОЗПЛАВУ ПОЛІМЕРУ ПРИ РОЗРАХУНКУ ЯКОСТІ ЗМІШУВАННЯ У ДИСКОВОМУ ЕКСТРУДЕРІ

Кількість первинного пластику, що виготовляється, збільшується з кожним роком. При цьому для забезпечення сучасних вимог полімери модифікують різними добавками, таким чином утворюючи композиційні полімерні матеріали. Виготовлення даного типу сировини потребує використання обладнання здатного

забезпечувати високу якість змішування компонентів у широких межах властивостей. Одним зі шляхів виконання таких вимог є використання каскадних екструзійних систем, в яких, у якості розплавлювача-гомогенізатора, використовується черв'ячно-дисковий екструдер [1–2].

У статті розглянуто вплив в'язкопружиних властивостей розплаву полімеру при моделюванні процесу змішування в дискових екструдерах, який є ключовим для досягнення однорідних та ізотропних композитних матеріалів. Модель ньютонівської рідини, що ігнорує в'язкопружні властивості матеріалу, може використовуватись для визначення полів швидкостей та продуктивності при екструзії. Проте її обмеження призводять до неточних прогнозів у випадках, коли матеріал проявляє в'язкопружні властивості.

Для подолання цих недоліків може використовуватись реологічна модель другого порядку, яка описує як в'язкісні, так і еластичні властивості матеріалу. За допомогою чисельного моделювання виконано порівняння результатів отриманих за моделлю ньютонівської рідини та модифікованим реологічним рівнянням другого порядку у формулуванні Рівліна-Еріксена. Результати показали, що при врахуванні в'язкопружиних ефектів радіальна швидкість потоку швидкості зростає, а значення накопиченої деформації, спричиненої цією компонентою, зменшується. Значення накопиченої деформації, спричиненої тангенціальною швидкістю, не залежать від величини радіальної швидкості. Загальна накопичена деформація зсуву при застосуванні різних моделей рідини залишилася практично незмінною: 1719,2 одиниць для моделі ньютонівської рідини і 1695 одиниць для моделі другого порядку. Таким чином, різниця між результатами розрахунків складає 1,38 %, що не є значущим для цього показника.

**Ключові слова:** екструзія, дисковий екструдер, зазор між дисками, швидкість деформації зсуву, деформація зсуву, якість розплаву.

### Problem statement

Due to their special operational characteristics, the availability of effective processing methods, and the existence of significant reserves of raw materials, polymers are used in almost every sector of the economy [3]. As a result, there has been a gradual increase in the mass of primary polymers worldwide, and there are currently no signs that this trend will stop in the near future [3–5].

To meet modern requirements for polymer products, polymers are modified using various fillers, additives, and dyes, creating composite materials with unique combinations of characteristics. The mixing process plays a special role in the manufacture of composite materials. The uniformity of the distribution of components in the melt and, accordingly, the repeatability and isotropy of the characteristics of the resulting material depend on the quality of the mixing of the polymer with additives.

Although single- and twin-screw extruders are quite versatile, they are physically incapable of processing different materials equally well, especially those with different fillers. In this regard, cascade extrusion units are becoming more and more popular. They are more flexible because in such units, different operations are performed not by a single working body (screw) with a fixed geometry, but by different machines with the possibility of autonomous control.

In cascade schemes for the production of filled compositions and polymer granulation, screw-disk extruder is particularly effective as melter and homogenizer (Fig. 1). These extruders are simple to manufacture, compact, and versatile [1]. Of particular interest is the ability to regulate and predict the degree of homogeneity of the melt at the outlet of the screw-disk extruder [6], since in cascade installations it is mainly used as a melter and homogenizer.

Despite the fact that disk extruders have been studied since the 1950s, there is currently no methodology that would allow quantitative assessment and prediction of melt homogenization quality depending on the technological parameters of the extrusion process. This significantly complicates both the optimization of equipment designs and the selection of rational technological modes for its operation.

### Analysis of the latest research and publications

One of the most convenient methods for assessing the quality of melt homogenization is to determine the average thickness of the material strips. Since polymer melts are characterized by high viscosity, their movement occurs in laminar mode [7], and mixing is caused by shear strain. In simple shear, the thickness of the strip is related to shear strain as follows [7]:

$$\frac{r}{r_0} = \frac{1}{\sqrt{1+\gamma^2}} = \frac{1}{\sqrt{1+\left(\frac{dV}{dS}t\right)^2}}, \quad (1)$$

where  $dV/dS$  – the coordinate-derivative of velocity,  $t$  – shear strain duration.

Thus, knowledge of the material flow velocity fields is a prerequisite for determining the mixing effect in the clearance of a disk extruder. Two velocity components are usually considered: radial and tangential, Fig. 2. The radial component determines the productivity of the extruder, while the tangential component is decisive in calculating the mixing capacity of the disk extruder.

Since the description of the disk extruder, many authors have attempted to theoretically justify the material flow processes that occur in the working clearance. Tomita and Kato [8] were among the first, who obtained the following

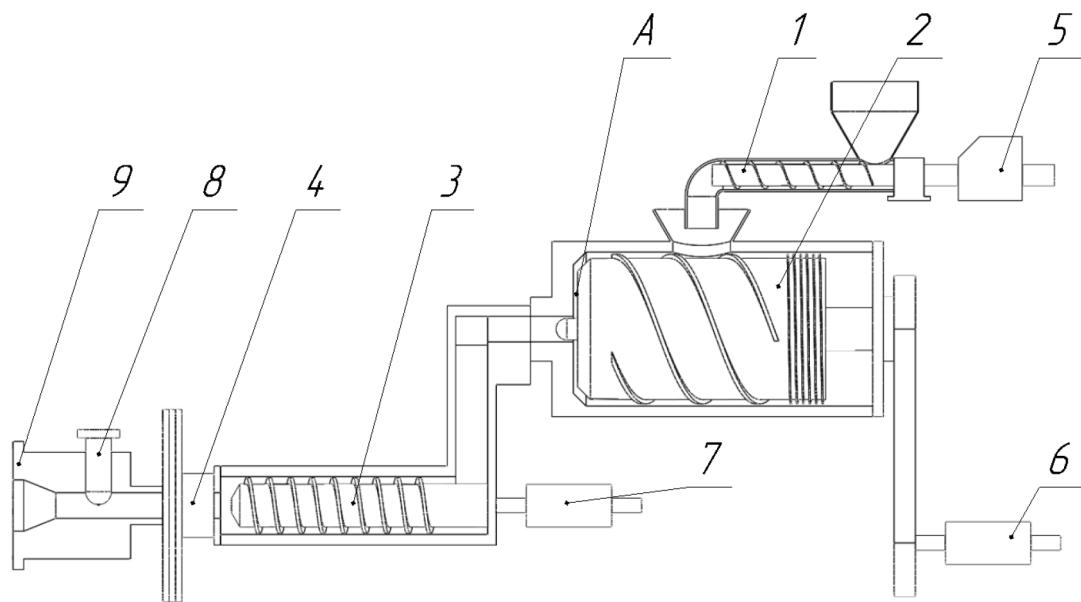


Fig. 1. Diagram of a cascade screw-disk extruder

(1 – screw feeder; 2 – screw-disk extruder; 3 – screw extruder; 4 – filter; 5, 6, 7 – drives of the rotating parts of the cascade extruder; 8 – throttling device; 9 – forming tool)

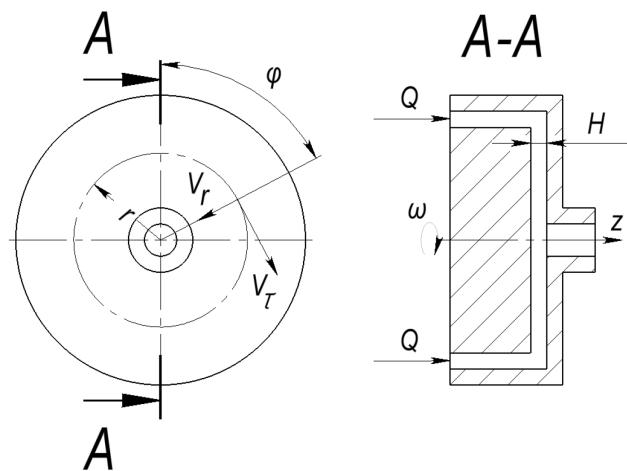


Fig. 2. Diagram of the clearance between the disks

equation for the radial component, using the assumption of a linear dependence of the tangential velocity on the coordinate across the width of the clearance:

$$V_r = \frac{3Q}{\pi r H^3} (z^2 - Hz), \quad (2)$$

where  $H$  – clearance between the disks,  $r$ ,  $z$  – coordinates on the corresponding axes,  $Q$  – extruder volumetric productivity.

Equation 2 does not take into account the influence of the viscoelastic properties of the polymer melt. This result is rather questionable, since it is known that normal stress effects occur during the processing of polymers in disk extruders [9]. This causes the radial velocity and, accordingly, the productivity of the apparatus to depend on the rotation frequency of the moving disk. Nevertheless, many researchers use this dependence when developing mathematical models and simulating disk extruders [1, 10–12].

The obtained results allow us to describe the general trends in melt flow, but their accuracy remains limited due to the neglect of the viscoelastic properties of polymer materials. Considering the key role of these properties in the formation of velocity fields, further development of disk extruder models is impossible without taking into account the rheological characteristics of polymer melts.

### The study aims

The purpose of this work is to compare the velocity fields of polymer melt in a clearance between the disks of a screw-disk extruder and the amount of shear strain using a Newtonian fluid model and a viscoelastic fluid model, which is described by a modified second-order rheological equation in the Rivlin-Ericksen formulation.

### Main research material

In a disk extruder, two mutually perpendicular velocity components are at work: tangential and radial. Taking this into account, for a disk extruder, it is necessary to modify formula 1 for the case of a two-axis simple shear:

$$\frac{r}{r_0} = \frac{1}{\theta_\kappa \cdot (1 + \sqrt{1 + \gamma_r^2} + \sqrt{1 + \gamma_\tau^2})}. \quad (3)$$

It is known that during extrusion, shear deformations are much greater than unity. Then equation 3 can be simplified to the form

$$\frac{r}{r_0} = \frac{1}{\theta_\kappa \cdot (\gamma_r + \gamma_\tau)} = \frac{1}{\theta_\kappa \cdot (\dot{\gamma}_r t + \dot{\gamma}_\tau t)}. \quad (4)$$

In a disk extruder, the most significant change of the parameters is in the channel width direction. Therefore, the derivatives of the greatest importance are  $\dot{\gamma}_r = dV_r/dz$  and  $\dot{\gamma}_\tau = dV_\tau/dz$ .

In works [13–15], the movement of polymer in the clearance between disks of a disk extruder was analyzed using a modified second-order rheological equation in the Rivlin-Ericksen formulation. For the case of the combined action of disc rotation and screw thread pressure, the following equations were obtained to determine the pressure distribution along the disk radius, as well as the tangential and radial velocity components:

$$V_r = \frac{1}{r} \left[ \frac{K_2}{K_1} \cdot r \cdot g1 + \frac{r^{(2-n)} \cdot g1^{(1-n)}}{K_1} \cdot \frac{dP}{dr} \right] \cdot \frac{H^2}{8} \cdot \left[ \left( \frac{2 \cdot z}{H} \right)^2 - 1 \right] + \left| \frac{1}{K_1} \cdot \frac{dP}{dr} \right|^{\frac{1}{n}} \cdot \frac{n}{n+1} \cdot \left( \frac{H}{2} \right)^{(1+n)/n} \cdot \left[ \left| \frac{2 \cdot z}{H} \right|^2 - 1 \right]; \quad (5)$$

$$V_\tau = \frac{2 \cdot \pi \cdot \omega}{H} \cdot z. \quad (6)$$

A linear dependence was used to describe the tangential component, as it was determined that this simplifies the mathematical model and does not lead to significant deviations in the performance calculation results [15].

The pressure gradient  $dP/dr$  is determined from the equation

$$2 \cdot \pi \cdot \int_{\frac{H}{2}}^{\frac{H}{2}} \left[ \left( \frac{K_2}{K_1} \cdot r \cdot g1 + \frac{r^{(2-n)} \cdot g1^{(1-n)}}{K_1} \cdot \frac{dP}{dr} \right) \cdot \frac{H^2}{8} \cdot \left[ \left( \frac{2 \cdot z}{H} \right)^2 - 1 \right] + r \cdot \left| \frac{1}{K_1} \cdot \frac{dP}{dr} \right|^{\frac{1}{n}} \cdot \frac{n}{n+1} \cdot \left( \frac{H}{2} \right)^{(1+n)/n} \cdot \left[ \left| \frac{2 \cdot z}{H} \right|^2 - 1 \right] \right] zd + + Q - 2 \cdot \pi \cdot \int_{\frac{H}{2}}^{\frac{H}{2}} \frac{K_2 \cdot g1 \cdot H^2 \cdot r}{8 \cdot K_1} \cdot \left[ \left| \frac{2 \cdot z}{H} \right|^2 - 1 \right] dz = 0. \quad (7)$$

When modeling extrusion processes, a stepwise approximation method is often a pretty effective approach. Its essence lies in the fact that the extrusion process is presented as a set of sequentially arranged small volumetric elements, within which certain parameters are considered constant, while their change occurs abruptly at the boundaries between these elements [12].

The flow process in a clearance between disks is an axisymmetric process. With this in mind, it is advisable to divide the working volume into strips of thickness  $dr$ , which in turn are divided into elements of thickness  $dr$  and width  $dz$ , Fig. 3.

In the case of the accepted calculation scheme, the productivity of each strip with a thickness of  $dr$  is the same and equals  $Q$ . Then the productivity of each element with a thickness of  $dr$  and a width of  $dz$  is determined by the equation

$$\Delta Q_i = 2 \cdot \pi \cdot R_i \cdot dz \cdot V_{ri}. \quad (8)$$

The time the material spends under the conditions prevailing inside the element is calculated using the following equation:

$$t_i = \frac{dr}{V_{ri}}. \quad (9)$$

According to the no-slip boundary condition, the velocity of the material on the walls is assumed to be zero. Thus, in virtually any continuous mixer, the material at the walls undergoes significantly greater deformation than the material in the central areas of the flow, Fig. 5 [7].

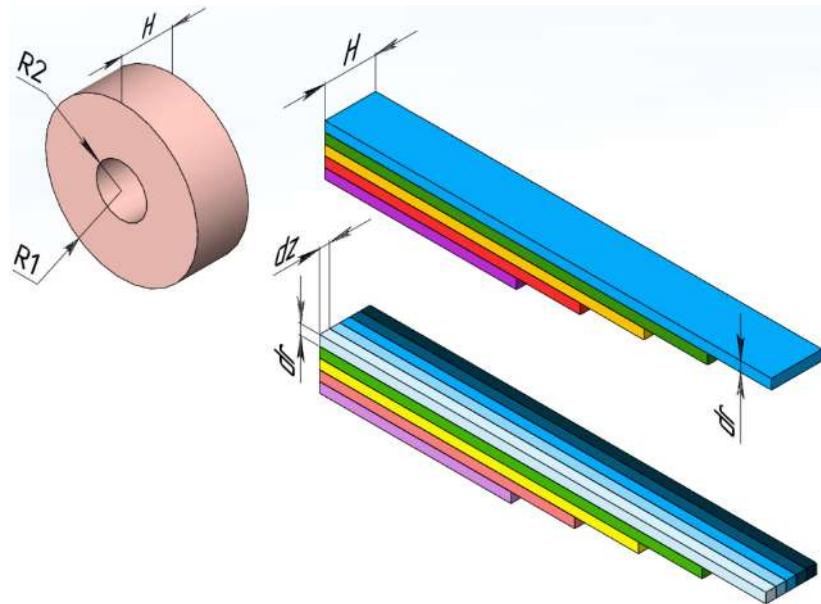


Fig. 3. Diagram of the division of a clearance between disks into calculation elements

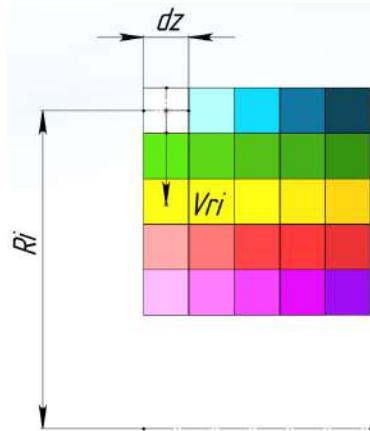


Fig. 4. Diagram for determining parameters inside a calculation element

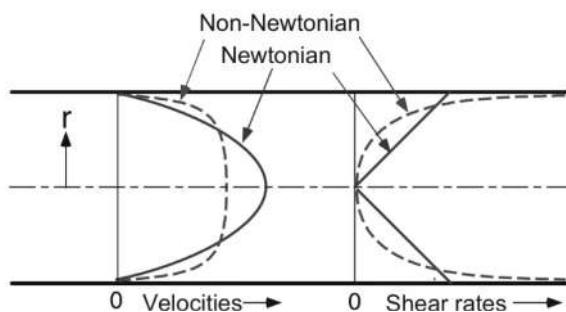


Fig. 5. Velocity and shear rate profiles in a pressurized flow through a straight channel [7]

However, due to their low speed, the layers near the walls are characterized by low productivity and therefore have a negligible effect on the overall mixing quality in the extruder. Therefore, the average shear deformation of the material should be calculated not as an arithmetic mean, but using the equation

$$\gamma_{cp} = \sum_i \frac{\Delta Q_i \cdot \gamma_i}{Q}. \quad (10)$$

Based on the described dependencies, the program was developed using Python. It is capable of calculating the amount of shear strain which the material gets when passing through the clearance between the disks of the disk extruder.

This allows predicting the quality of material mixing at the outlet of the disk extruder, taking into account the viscoelastic properties of the material, the geometric characteristics of the clearance, the productivity of the screw thread, and the disk rotation frequency. By substituting different equations to determine the velocity components, it is possible to compare the velocity fields when using both the Newtonian fluid model and the viscoelastic fluid model, which is described by a modified second-order rheological equation in the Rivlin-Ericksen formulation.

The parameters were determined using the following initial data: clearance width  $H = 0,006$  m, outer radius  $R_1 = 0,15$  m, inner radius  $R_2 = 0,09$  m, rotation frequency  $\omega = 3$  s<sup>-1</sup>, number of calculation points along the  $R$  axis – 50, number of calculation points along the  $z$  axis – 50, productivity  $Q = 6,184 \cdot 10^{-5} \frac{\text{m}^3}{\text{s}}$ . Polystyrene with the following characteristics was taken as the test material:  $n = 0,31$ ;  $K_1 = 1,73 \cdot 10^4 \text{ Pa} \cdot \text{s}^n$ ;  $K_2 = 1,77 \cdot 10^4 \text{ Pa} \cdot \text{s}^n$ ;  $K_3 = 1,64 \cdot 10^4 \text{ Pa} \cdot \text{s}^n$ .

Calculations showed that the flow velocity in the radial direction, taking into account viscoelastic properties, is greater than in the Newtonian fluid model, Fig. 6. This is explained by the consideration of the normal stress effect, which additionally directs the material towards the axis of rotation.

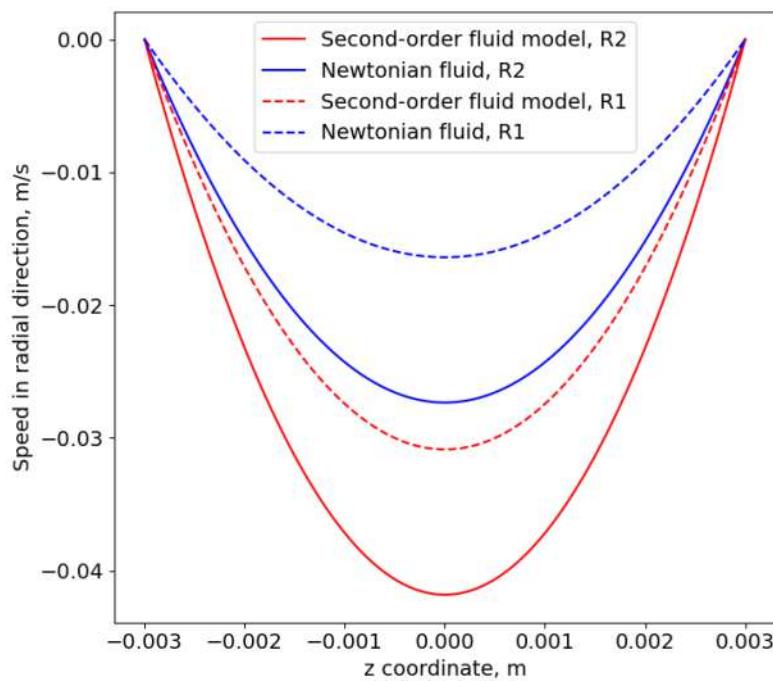


Fig. 6. Velocity profiles in the radial direction

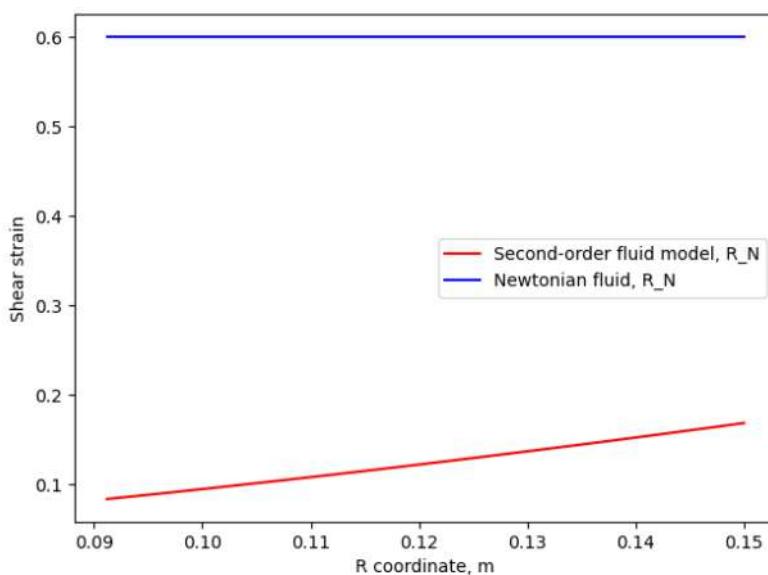
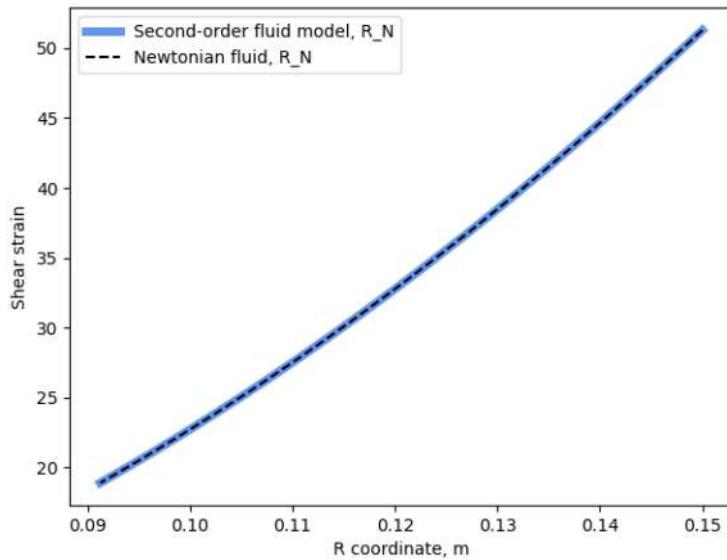


Fig. 7. Dependence of the magnitude of the radial velocity component shear deformation on the radius



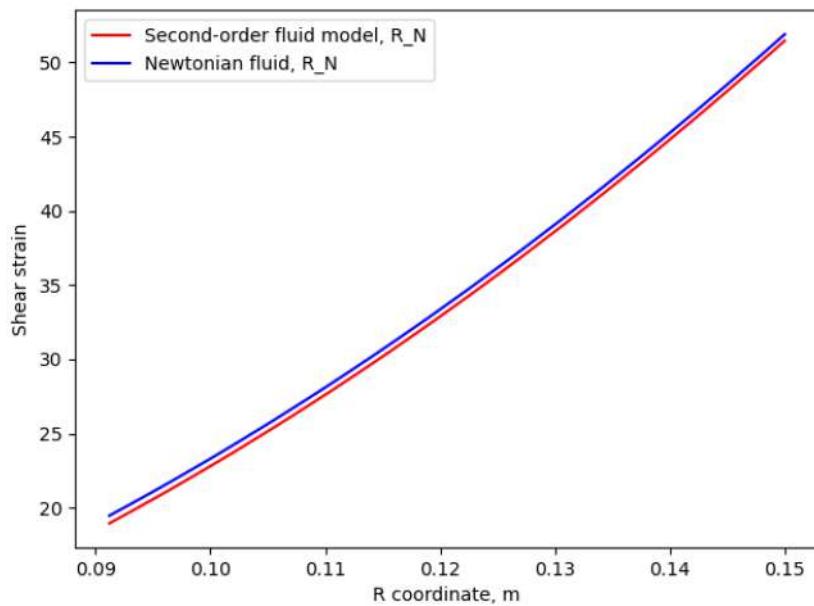
**Fig. 8. Dependence of the magnitude of shear deformation of the tangential velocity component on the radius**

The nature of the dependence of the shear deformation of the radial velocity component on the radius when using both models differs greatly. As can be seen in Figure 7, when using the Newtonian fluid model, the shear deformation does not depend on the radius value and is equal to a certain constant. It has been determined that this value depends on the step size  $\Delta R$  and is described by the equation

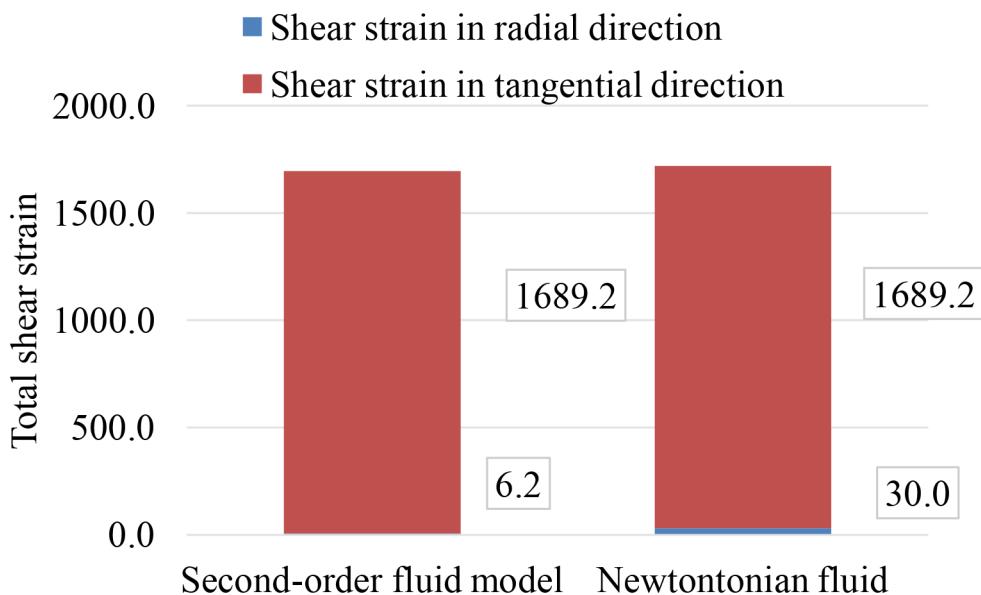
$$\gamma_r = \sum_i \frac{\Delta Q_i \cdot \gamma_{ri}}{Q} = \sum_i \sum_j \frac{6 \cdot (H - 2 \cdot z) \cdot \Delta R_i}{H^3} \Delta z_j. \quad (11)$$

Since both models use the same equations for the tangential velocity component, the values of shear deformation caused by this component are identical (Fig. 8). At first glance, this result seems counterintuitive, since the radial velocities are not equal, which means that the time during which the material perceives shear rate also differs. However, the independence of the shear strain in the radial direction from the value of the radial velocity component becomes obvious upon detailed consideration of the equation for determining the shear strain in the tangential direction.

$$\gamma_t = \sum_i \frac{\Delta Q_i \cdot \gamma_{ti}}{Q} = \sum_i \frac{\Delta Q_i \cdot \dot{\gamma}_k \cdot t}{Q} = \sum_i \sum_j \frac{(2 \cdot \pi \cdot R_i \cdot \Delta z_j \cdot V_{ri}) \cdot \dot{\gamma}_k \cdot \left( \frac{\Delta R}{V_{ri}} \right)}{Q} = \sum_i \sum_j \frac{2 \cdot \pi \cdot R_i \cdot \Delta z_j \cdot \dot{\gamma}_k \cdot \Delta R}{Q}. \quad (12)$$



**Fig. 9. Dependence of the magnitude of the radial velocity component shear strain on the radius**



**Fig. 10. Comparative diagram of the total shear strain obtained using the Newtonian fluid model and the modified second-order rheological equation**

Summing up the corresponding results, we obtain graphs of the distribution of the total shear strain when using one and the other fluid model (Fig. 9). The graphs are very similar, which is reflected in the final results. Thus, when using the Newtonian fluid model, the value of the shear strain was 1719,2 units, and when using the second-order rheological equation, it was 1695 units (Fig. 10). The difference in the results is 1,38 %, which is not a significant difference when calculating the quality of melt homogenization.

#### Conclusions

As a result of analyzing the movement of polymer melt in the clearance between the disks of the screw-disk extruder, it was determined that the material undergoes shear strain in two mutually perpendicular directions: radial and tangential. Thus, to determine the quality of melt homogenization using the amount of shear strain, it is necessary to perform calculations for the case of biaxial shear strain, taking into account the productivity of each calculation element. Since the process is axisymmetric, the working volume was divided into calculation elements with a thickness of  $dr$  and a width of  $dz$ .

A Python program has been created that can calculate the amount of shear strain accumulated by the material as it passes through the clearance between the disks of a disk extruder. To determine the velocity fields, both the rheological model of Newtonian fluid and the modified second-order rheological equation in the Rivlin-Ericksen formulation can be used.

It has been determined that when viscoelastic properties are taken into account, the values of the radial component of velocity increase, and the time the material remains in the clearance decreases accordingly, which is explained by the effect of normal stresses. This is reflected in the amount of deformation accumulated by the material in the radial direction. When applying the Newtonian fluid model, this value is 30 units, and when taking into account viscoelastic properties, it is 6 units. It has been determined that when applying the Newtonian fluid model, the value of shear deformation does not depend on the value of the calculated radius.

The calculation of the shear deformation in the tangential direction showed identical values when applying both models, which is an obvious result when analyzing the dependencies used.

It has been determined that the values of the total accumulated deformation, taking into account viscoelastic properties and without taking them into account, are 1695,4 and 1719,2 units, respectively. Thus, the deviation of the obtained values is 1,38 %, which is not a significant difference when calculating the quality of melt homogenization.

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