Computer modeling for polymer processing co-rotating twin screw extrusion – nonconventional screw configurations

Komputerowe modelowanie procesów wytłaczania dwuślimakowego współbieżnego – układy niekonwencjonalne ślimaków

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Computer modeling of co-rotating twin screw extrusion with the use of nonconventional screw configurations has been presented. The polymer flow in the co-rotating twin screw extruder has been described. Some examples of three-dimensional, non-Newtonian modeling are shown. CFD generally oriented software ANSYS Polyflow has been used for modeling.

KEYWORDS: polymers, modelling of twin screw extrusion

Extrusion is the most basic and most technologically advanced plastics processing technology - about 2/3 of all plastics are processed using this method. Extrusion is widely used in the manufacture of plastic profile products (e.g. pipes, foils, plates), and is the basis for preparation processes, i.e. granulation, filling, strengthening, etc.).

One- and twin-screw extrusions, co-rotating and counter-rotating extrusions are distinguished. Extruders can be powered by gravity (without dosing) or with plastic dosing. Twin-screw extruders are most often powered by the other two methods. Extrusion with plastic dosing promotes faster plasticization and better mixing.

In case of supplying the extruder in a dosed manner, there are areas of incomplete filling of the screw in which no pressure is generated. Extrusion performance does not depend on the rotational speed of the screw, but on the performance of dispensing device.

Currently, extrusion design is aided by computer simulations based on global process models. They allow predicting the extrusion process based on technological parameters of the process, geometry parameters of the screw and the head and parameters of the material being processed [1, 2].

Single-screw extrusion models with conventional gravity feed are known [3, 4], and recently a single-screw extrusion model with dosing extrusion power has been developed [5, 6]. Twin-screw extrusion and counter-extrusion has also led to the construction of global models [4, 7, 8-13], which treat the extrusion process in a holistic way, taking into account solid state transport, plastics plasticization and plasticized flow. Such modeling requires comprehensive process calculations in multiple iterative loops until the convergence of the calculation follows a suitable convergence criterion.

Difficult and time-consuming numerical calculations of MES are not applicable to global modeling, but they can be a basis for the flow characteristics of the screws (dependence of the dimensional flow rate and dimensionless pressure gradient). After approximating these characteristics with regression models, they can then be implemented in the global process model. The authors presented this concept, among others, with respect to twin-screw extrusion [14].

Co-rotating twin screw extrusion

Twin-screw extrusion is used in the manufacture of profile products (counter-rotating extrusion) and in the preparatory processes of processing - for example in plastic filling, reinforcing and granulation (co-rotating extrusion). Twin-screw co-rotating and counter-rotating extrusions are extensively described in monographs [16, 17], where the basics of modeling these processes are also given. In twin-screw extruders, the flow is very complex and difficult to describe mathematically. On the other hand, the twin-screw extruders have good mixing and degassing properties, are characterized by good heat exchange and fast plasticization. The difficulty of describing such flow, however, implies that the twin-screw extrusion theory is less well developed than the one-screw extrusion theory.

It has been found that analytical flow analysis can be used with respect to conventional configurations of twin-screw systems. In industrial practice, twin-screw extruders are constructed of unconventional elements. Flow modeling in such components requires numerical MES calculations.

A scheme of the twin-screw co-rotation extrusion is shown in fig. 1. Material flows from one screw to the other and moves along the "twisted eighth" line. There is a counter-rotational movement in the crossover slot, which generates high shear stress (for this reason co-rotational extrusion is used in preparation processing).

The flow of material in co-rotational extruders is the result of relative movement of the screws and the cylinder as well as pressure gradient in the extruder. This is a pressure-drag flow, occurring in open channels between the screws (alternately) and the cylinder.

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In simplified terms, volume flow rate Q (extrusion yield) in the co-rotational extruder (in the area of the total screw filling) can be expressed as:

$$Q = Q_d + Q_a - Q_p - Q_l \quad (1)$$

where: Q_d - drag flow rate, Q_a - axial flow rate, Q_p - pressure flow rate, Q_l - leakage flow rate.

The drag flow rate, bypassing the mesh zone, can be defined as in the case of flow in a single screw extruder:

$$Q_d = \frac{V_{bz} WH}{2} F_d \quad (2)$$

where: V_{bz} = πDNcosφ - velocity component along the length of the screw channel (D - screw diameter, N - screw speed, φ - helical screw inclination angle, W – width of the screw channel, H – height of the screw channel, F_d = (1 – 0.571H/W) shape factor correcting the drag flow rate [1].

Pressure, axial and leakage flow rates can be expressed in the following formulas:

$$Q_p = \frac{WH^3}{12\eta} \frac{\partial p}{\partial z} F_p \quad (3)$$

$$Q_a = V_a A_a \quad (4)$$

$$Q_l = V_a (\pi - \beta) D h_f \quad (5)$$

where: p - pressure; z - coordinate along the length of the channel; η - viscosity; F_p = (1 - 0.625H/W) - pressure flow correction factor [1]; V_a = πDNtgφ - axial component (along axis of the screw system) of flow velocity; A_a - available flow area [1]; β - screw engagement angle; h_f - slot between the vortices of the screw windings and the cylinder.

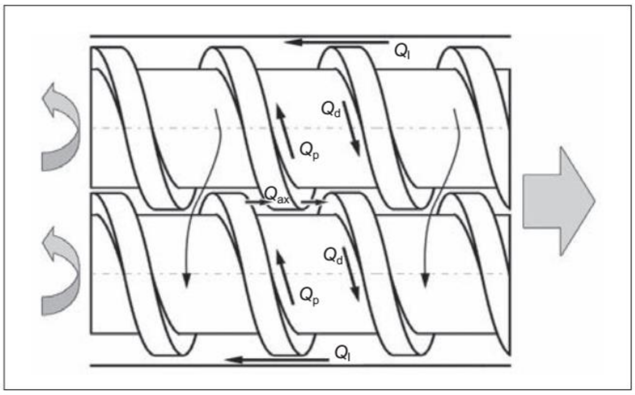

Fig. 1. Diagram of the flow in a co-rotational extruder: Q_d - drag flow, Q_p - pressure flow, Q_a - axial flow, Q_l - leakage flow

Flow in the screw extrusion systems is based on the motion of the material relative to the screw. The material flows in the extruder in the opposite direction than the screw rotates and the direction of flow depends on the direction of the screw windings and their rotation direction. Drag flow in extruder systems only occurs in case of viscous flows. This does not happen with ideal zero viscosity fluids.

Flow in the co-rotating extruder may be considered as a result of the relative traction of the drag flow (resulting from the relative motion of the screws and the cylinder) and the pressure flow (resulting from the pressure gradient). These relationships are defined by the magnitude a - ratio of the pressure flow rate to the drag flow rate. Following cases can be distinguished:

- when a<0, the pressure gradient is negative and the pressure flow is added to the drag flow,
- when a=0, the pressure gradient is zero and there is no pressure flow,
- when 0<a<1, the pressure gradient is positive and the pressure flow is subtracted from the drag flow.

Flow modeling

Modeling of twin-screw extruders using unconventional screw elements (i.e. three-dimensional, non-Newtonian modeling) requires the use of MES numerical methods. For this purpose, ANSYS Polyflow fluid analysis software package was used [15].

Three areas of analysis (fig. 2) were identified for the modeling of flow of material in a co-rotational extruder in a three-dimensional space: a fluid subdomain (a space between the cylinder wall and screw cores without screw windings) and two solids subdomains (first and second screws).

The discussed problem can be defined as a three-dimensional, isothermal, generalized Newtonian flow [18], for which the following boundary conditions can be formulated (fig. 2):

- at the inlet boundary of the flow space BS1: inflow condition, $Q = Q_0$;
- at the boundary of outlet from flow space BS2: outflow condition, normal forces and tangential velocities imposed (f_n & v_s): $f_n = 0$, $v_s = 0$;
- at the boundary of the inner surface of the flow space (core surface of the first screw) BS3: the Cartesian velocity condition (v_x, v_y, v_z): $\omega = N$;
- at the boundary of the inner surface of the flow space (core surface of the second screw) BS4: Cartesian velocity condition (v_x, v_y, v_z): $\omega = N$;
- at the boundary of the outer surface of the flow space (cylinder wall) BS5: normal condition and tangential velocities imposed (v_n & v_s): $v_n = 0$, $v_s = 0$.

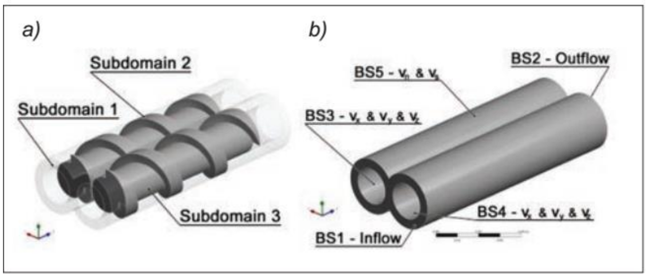

Fig. 2. Schematic flow conditions in a twin-screw system: *a)* flow geometry: subdomain 1, subdomain 2, subdomain 3; *b)* boundary conditions at the flow limits

The plastic flow modeling procedures differ slightly for the co-rotating and counter-rotating extruder [14]. The flow limits are determined identically, but the BS3 and BS4 conditions for the rotation direction of the screws are different. The BS3 and BS4 boundary conditions ($w = N$) defined here are described in [15, 18].

It was assumed that the rheological properties of the materials reflect the model of the power liquid [18]:

$$\underset{\sim}{\tau} = m\dot{\gamma}_{\mathrm{D}}^{\,n-1} 2\underset{\sim}{\boldsymbol{D}} \tag{6}$$

where: $\underset{\sim}{\tau}$ - extra-tension tensor; $\dot{\gamma}_{\mathrm{D}}$ - generalized shear rate; $\underset{\sim}{\boldsymbol{D}}$ - tensor of deformation speed; *m, n* - parameters of the power equation (m = 1.1 • 10^4 Pa • s^n - consistency coefficient, *n* = 0.4 - flow exponent, dimensionless).

Model studies were carried out with respect to a conventional element with a pitch of *t* = 30 mm and with a reduced pitch *t* = 25 mm and an increased pitch *t* = 35 mm, and then with respect to an element with an oppositely directed screw winding *t* = 30 mm. Schemes of the test screw systems are shown in fig. 3. The basic tests were carried out assuming the screw speed *N* = 80 rpm and the flow rate *G* = 8 kg/h.

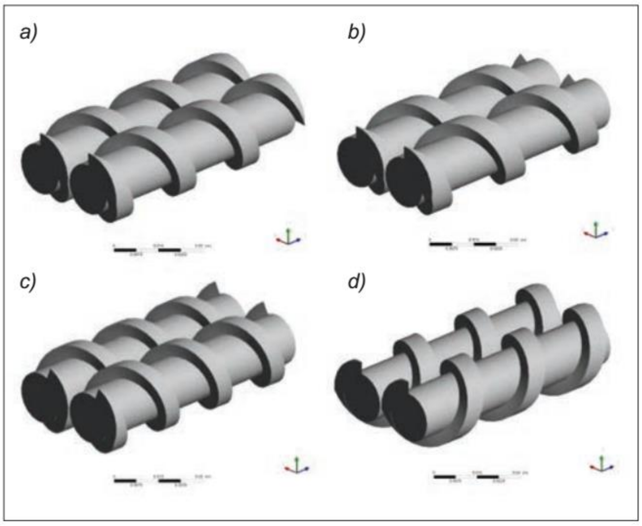

Fig. 3. Geometrical diagrams of the tested worm systems: *a)* conventional element, *t* = 30 mm; *b)* element with reduced pitch, *t* = 25 mm; *c)* element with increased pitch, *t* = 35 mm, *d)* element with opposite directed screw winding, *t* = 30 mm

The software ANSYS Polyflow v.17.0 [15] was used. The model was made of tetragonal (for rotating screw) and hexagonal (for liquid) elements. Calculations were made on HP/Supermicro Hydra supercomputer; eight 2.8 GHz processors and 204 800 MB RAM were used. Calculations were time consuming - for a model of several hundred thousand elements (including several tens of thousands of tetragonal elements) – they lasted several hours. Examples of flow simulation results are shown in figs. 4-10. Velocity distribution of the material and the pressure in conventional and unconventional system is shown - the opposite direction of the screw winding as well as in systems with different screw pitch.

In fig. 4, illustrating velocity components v_x, v_y and v_z, the flow along the length of the screw channel (represented by v_x) is particularly pronounced. In co-rotating extrusion, material flows just along the channel - from one screw to the other. According to accepted boundary conditions (moving screws, stationary cylinder, no slipping on the walls of the screws and cylinder), the v_x component at the surface of the cores is equal to the peripheral speed of cores and the speed on the cylinder wall is equal to zero. The actual flow of material in the extruder over the screw is as if the coordinate system was placed on the surface of the screw core. Thus, taking into account the assumed flow conditions (right turn screws rotating to the left), the material moves in the opposite direction to the direction of the screw rotation, i.e. to the right.

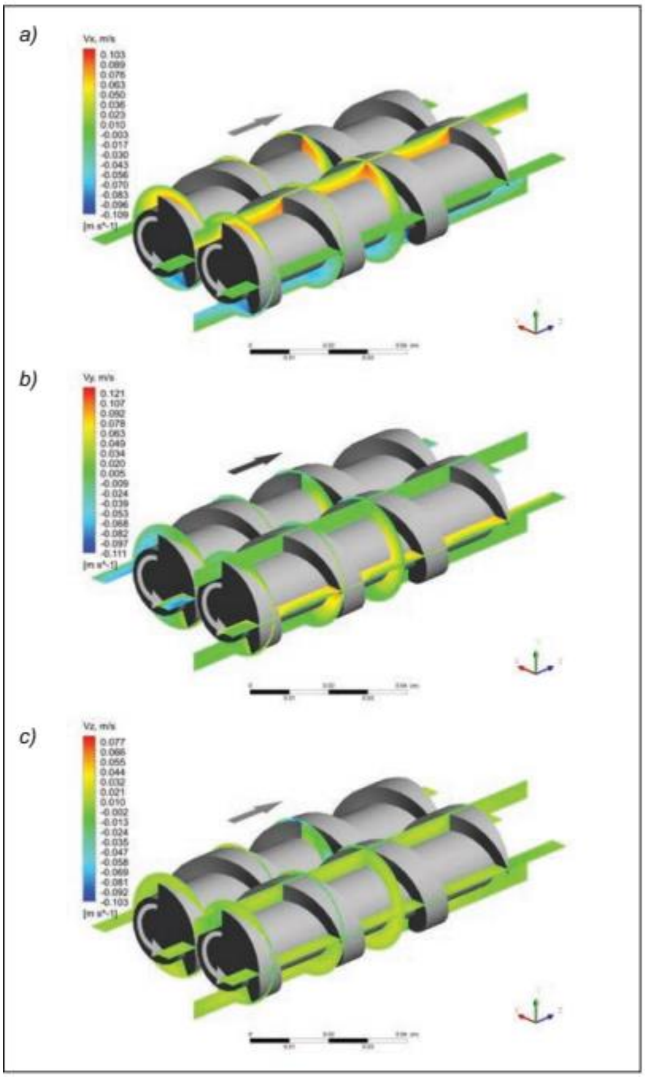

Fig. 4. Distribution of velocity components in a conventional element: *a)* v_x, *b)* v_y, *c)* v_z

Distribution of pressure along the axis of the screws, which is characteristic for the screw flows (saw diagram with intense pressure rise over the coil of the screw and the pressure drop or pressure stagnation in the coil channel) is shown in fig. 5. Due to the assumed flow conditions, it can be seen that its gradient is non-zero and positive. As a result, the pressure flow decreases the flow rate of the material.

Plots in fig. 6 show the effect of flow rate (at constant rotational speed of screws) on the pressure distribution along the length of the screws and the influence of rotational speed of the screws (at constant flow rate) on the pressure distribution. As the flow rate increases, the pressure rises and decreases with increasing rotational speed. At a constant rotational speed of screws *N* = 80 rpm (fig. 6a), i.e. at a constant drag rate, an increase in flow rate from *G* = 4 kg/h to *G* = 12 kg/h occurs as a result of reduced back pressure flow. The gradient pressure (gradient module) decreases with increasing flow rate. With a constant flow rate *G* = 4 kg/h (fig. 6b), the increase in the rotational speed of screws from *N* = 40 rpm to *N* = 120 rpm causes an increase in the drag flow, which means that to maintain a constant flow rate *G* = 4 kg/h, the back pressure flow also must increase. The gradient pressure (gradient module) in this case increases along with the increase of rotational speed of the screws.

Fig. 7 shows the distribution of velocity components vx, vy and vz in the opposite direction of the screw winding, while fig. 8 - pressure distribution along the axis of the screws in this system. The pressure gradient is negative here - the pressure flow supports the drag flow.

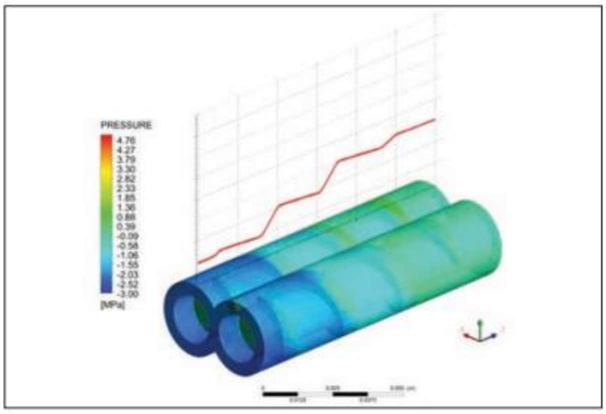

Fig. 5. Distribution of pressure along axis of screws in conventional element

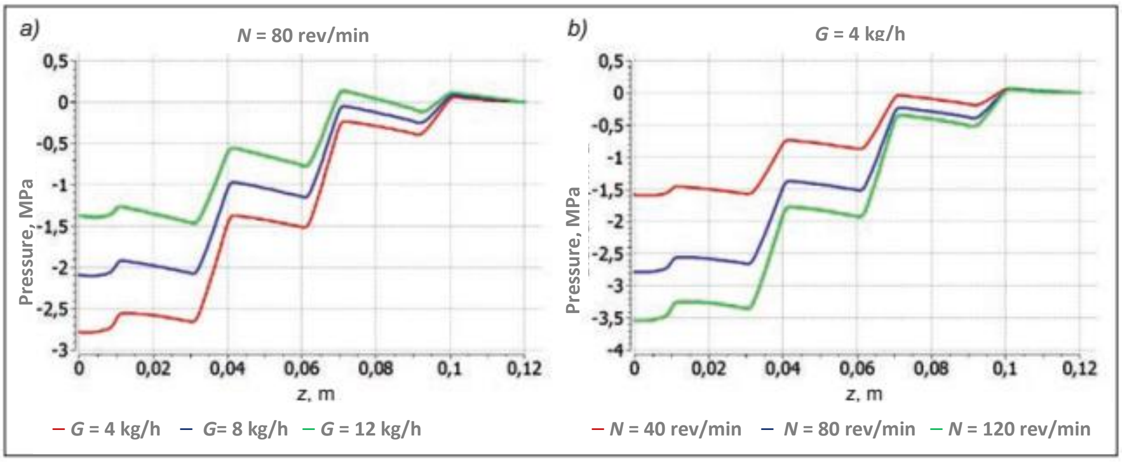

Fig. 6. Effect of flow rate (a) and screw rotational speed (b) on pressure distribution in conventional twin-screw system

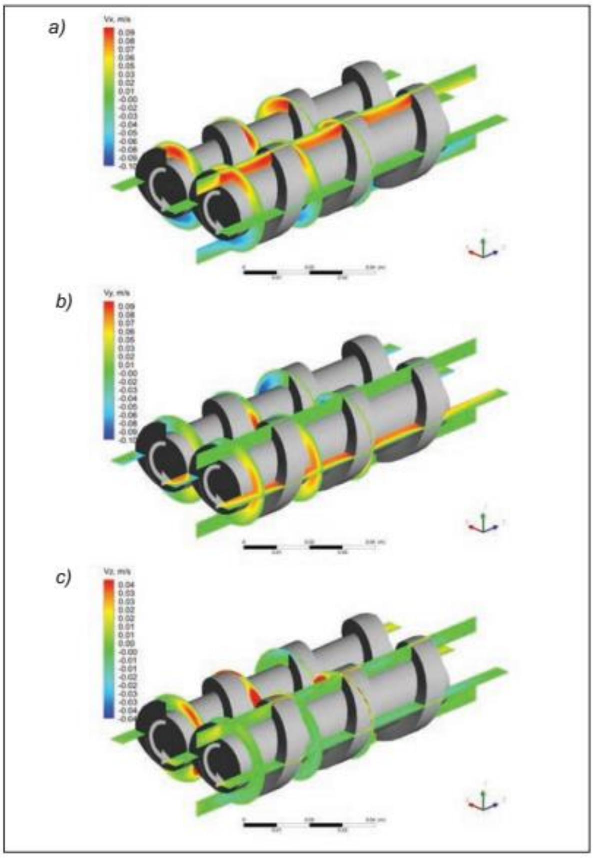

Fig. 7. Speed distribution in unconventional element: a) vx, b) vy, c) vz

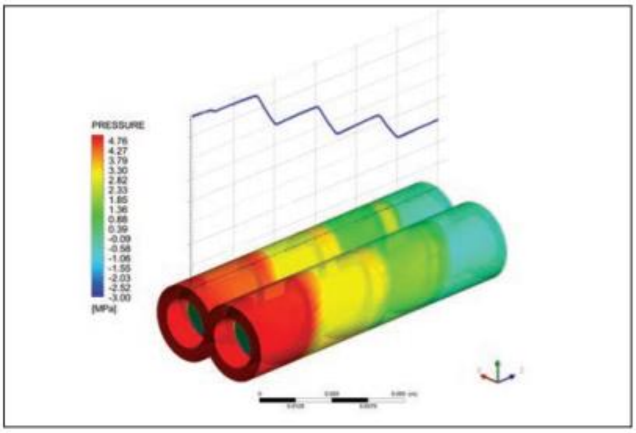

Fig. 8. Distribution of pressure along the axis of the screws in unconventional element

Pressure profiles in the test systems of screws with different pitch lines are shown in fig. 9, and in fig. 10, three-dimensional pressure distributions in these systems. It is noteworthy that when changing the direction of the screw windings from the right (fig. 9a) to the left turn (fig. 9d) and maintaining the same direction of the screws rotation, the pressure gradient changes from positive to negative. The pressure gradient changes with the change in pitch from *t* = 25 mm to *t* = 35 mm are less obvious. The highest gradient value (module) is at *t* = 25 mm, and the smallest - at *t* = 30 mm; at *t* = 35 mm, the gradient has an intermediate value. The pressure gradient dependence on the screw pitch is approximately parabolic.

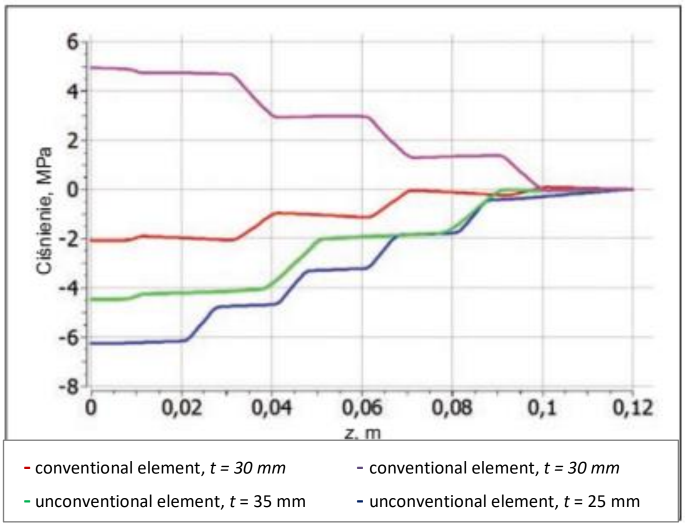

Fig. 9. Pressure profiles in the test systems of screws with different screw pitch

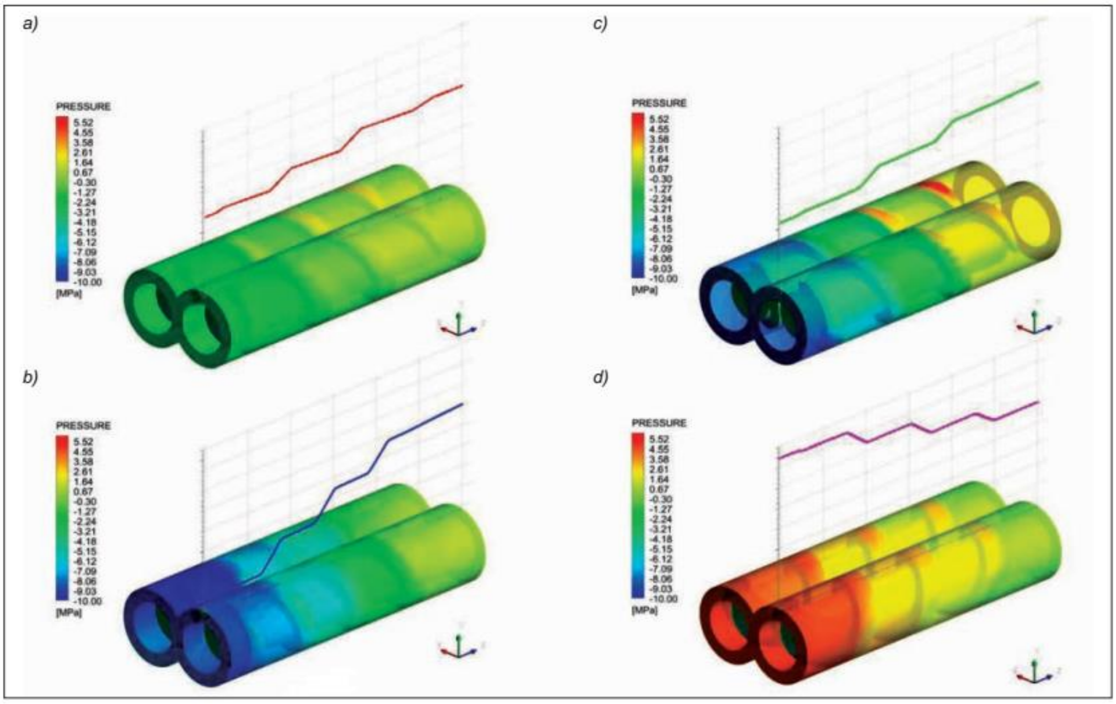

Fig. 10. Three-dimensional pressure distribution: *a)* conventional element, *t* = 30 mm, *b)* element with reduced pitch, *t* = 25 mm, *c)* element with increased pitch, *t* = 35 mm, *d)* element with opposite direction of coil winding *t* = 30 mm

Global modeling of the extrusion process

As previously mentioned, global modeling includes a comprehensive description of the extrusion process including solid state transport, plastics plasticization and plasticized flow (cylinder and extruder head). In this situation, MES calculations do not pass the exam, although they can be used to obtain snail flow characteristics that approximate the selected regression models and then implements the global process model. In addition, global modeling needs to take into account the variability of flow geometry along the flow path of the material to be processed. This is especially important in the case of twin-screw extrusions. The screws in the twin screw extruders are modular in design and form a geometric configuration for the processing process in question. In the modeling of flow in such complex geometrical configurations of screws, it is necessary to formulate the thermo-mechanical flow conditions and boundary flow conditions, among others, input and output parameters in the subsequent areas of analysis.

For example, fig. 11 shows the geometrical configuration of the twin-screw system formed from the screw elements described in this paper. It shows how the flow rate in the extruder is shaped as a suitable stack of drag and pressure flow. In the first three components, the pressure flow is retrograde and reduces the drag flow rate. The pressure gradient is positive in this case, and its value determines the pressure flow. In the fourth element, the pressure flow is supportive and increases the drag flow rate. The pressure gradient is negative and its value also determines the pressure flow. An interesting discussion of the results of the screw modeling was recently presented in [19], indicating frequent misinterpretations of results and a lack of understanding of the kinematic nature of the screw flow.

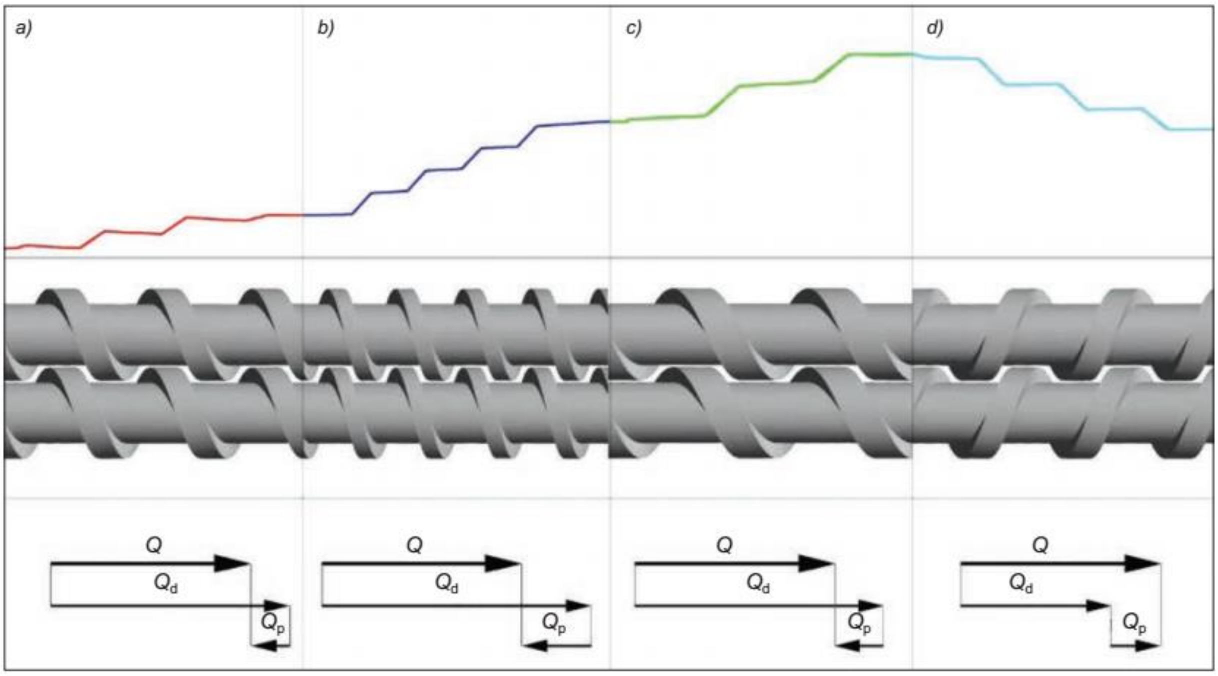

Fig. 11. Global modeling diagram: *a)* conventional element, t = 30 mm, *b)* element with reduced pitch, t = 25 mm, *c)* element with increased pitch, t = 35 mm, *d)* element with opposite direction of coil winding t = 30 mm

Conclusions

The three-dimensional, non-Newtonian modeling of twin-screw extruding involving the use of non-conventional screw systems and the use of ANSYS Polyflow was presented. The problem of global modeling of co-rotating extrusion with the use of dimensionless flow characteristics of screws was described. Such modeling ensures high accuracy of calculations, while at the same time a reasonable time for these analyzes. Numerical calculations were performed using the PLGrid infrastructure.

It was indicated that flow modeling in the complex geometrical configurations of the twin-screw extruders requires appropriate formulation of thermo-mechanical flow conditions and boundary conditions.

The presented modeling methodology allows for a very accurate local flow analysis of the material in the co-rotational extrusion process. This is particularly important in the extrusion of polymeric or polymer composite mixtures - in this case thermo-mechanical flow conditions determine the quality of materials produced and processed.

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