Simulation of single screw extrusion of wood plastic composites based on the on-line pressure measurements

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Abstract: Simulation and experimental tests of single screw extrusion of wood plastic composite (WPC) based on the polypropylene (PP) matrix were carried out. The rheological properties of the composite were determined on the basis of measurements of the pressure and material flow rate during extrusion. Recently developed computer model for simulating the single screw extrusion of wood plastic composites was applied which has been modified by extending its computing capabilities to calculations based on the power law rule. This computer model allows two-variant modeling the material melting depending on the wood flour content. The results of simulation were verified experimentally, and it was found that the results of simulations and measurements were in a good agreement. Smaller discrepancies were observed in the case of the use of one-dimensional model of melting.

Keywords: single screw extrusion, wood plastic composites, modeling.

Symulacja wytłaczania jednoślimakowego kompozytów polimerowo-drzewnych na podstawie pomiaru ciśnienia *on-line*

Streszczenie: Wykonano badania symulacyjne i doświadczalne wytłaczania za pomocą wytłaczarki jednoślimakowej kompozytu polimerowo-drzewnego na osnowie polipropylenu (PP). Na podstawie pomiarów ciśnienia i natężenia przepływu podczas wytłaczania określono właściwości reologiczne kompozytu i opisano je prawem potęgowym. Badania symulacyjne wykonano z wykorzystaniem nowo opracowanego modelu komputerowego wytłaczania kompozytów drzewnych, rozwiniętego w tej pracy na potrzeby modelowania z wykorzystaniem prawa potęgowego. Model ten umożliwia dwuwariantowe modelowanie uplastyczniania kompozytu w zależności od zawartości mączki drzewnej. Na drodze weryfikacji stwierdzono dobrą zgodność wartości obliczonych i uzyskanych doświadczalnie. Mniejsze rozbieżności wystąpiły wypadku zastosowania jednowymiarowego modelu uplastyczniania.

Słowa kluczowe: wytłaczanie jednoślimakowe, kompozyty polimerowo-drzewne, modelowanie.

Wood plastic composites (WPC) are composed of thermoplastics and wood flour. They are resistant to weather, especially moisture, and are widely used in the economy, successfully replacing wood. Composites based on the polypropylene (PP), high density polyethylene (HDPE) and poly(vinyl chloride) (PVC) are commonly used [1–4].

The state of the art of rheology and processing of WPC is not well-established yet. The fundamental books of Oksman and Sain [2], and Klyosow [3] as well as the review papers of Li and Wolcott are of primary importance [5–7]. Important contributions have been also delivered by Xiao and Tzoganakis [8–11], and Vlachopoulos and Hristov [12–14]. And, some recent papers are worth of mentioning [15, 16].

Wood plastic composites are non-Newtonian substances. Their viscosity decreases with an increase of shear rate and temperature, and increases with an increase of wood flour content. These composites may exhibit a yield stress and slippage during the flow. A slip velocity increases with an increase of shear rate, which may lead to a plug flow. An increase in wood flour content promotes the phenomenon of plug flow. A comprehensive analysis of the state of the art of rheology and processing of wood plastic composites has been recently presented [17].

Rheological properties are of fundamental importance in processing of plastics, and designing plastic processing [18, 19]. Neat polymeric materials are relatively well known, and their material data are usually available in the material databases, *e.g.*, CAMPUS [20], Autodesk-Moldflow [21] and Moldex-3D [22]. Rheological data are usually limited to the mass flow rate index (*MFR*) or viscosity curves, *e.g.*, CAMPUS [20]. Autodesk-Moldflow [21] and Moldex-3D [22] additionally contain the parameters of rheological models, *e.g.*, Cross-WLF model.

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Rheological measurements are in general difficult, time-consuming, and expensive. And, these laboratory measurements are usually performed under the thermomechanical flow conditions (temperature, pressure, shear rate, shear stress) different from the conditions of the actual processing. Therefore, the tests are sought for simplified determination of rheological properties of polymers as well as the tests performed under processing conditions, *i.e.*, in-line or on-line measurements [23, 24].

In this paper, the problem of determining the rheological properties of wood plastic composites has been undertaken. Because the rheological data of these materials are not able to be obtained from the open material databases, *e.g.* [20–22] and the published literatures, *e.g.* [2, 3, 25].

Rheological properties of polymeric materials, including composites and polymer blends are the basis for modeling the processing of these materials. The lack of rheological data is a serious limitation for modeling and practical application of these materials in the industry [26, 27]. The authors indicate this problem when modeling extrusion of neat polymers, *e.g.*, flood fed single screw extrusion [28], starve fed single screw extrusion [29–32], as well as extrusion of wood plastic composites [17, 33, 34].

In this paper, the rheological tests of WPC based on the on-line measurements have been performed. Viscosity has been determined by measuring the extrusion output and the pressure in an extrusion die. The power law model has been used to model viscosity dependence on the shear rate and temperature. Using this model, the extrusion process of WPC has been simulated and validated experimentally.

EXPERIMENTAL PART

Materials

A wood plastic composite on the polypropylene (PP) matrix was used with a content of 50 wt % wood flour (WF). The wood flour came from deciduous trees, a the fibers had a size of about 0.4 mm. The density of the molten composite and the mass flow rate (*MFR*) index were equal to ϱ_m = 0.99 g/cm^3 and *MFR* = 4.0 g/10 min (190 °C, 10.00 kg), respectively.

Viscosity determination

Viscosity curves of the tested material were determined using a high pressure capillary rheometer Rheograph 6000 (Goettfert). The measurements were carried out in the range of shear rate and temperature 5–3500 s^{-1} and 175–195 °C, respectively. Rabinowitsch and Bagley corrections were applied in rheological calculations.

The viscosity curves were modeled using rheological equation of Klein which is represented by:

$$\lg \eta = A_0 + A_1\dot{\gamma} + A_{11}\lg^2\dot{\gamma} + A_{12}T\lg\dot{\gamma} + A_2T + A_{22}T^2 \quad (1)$$

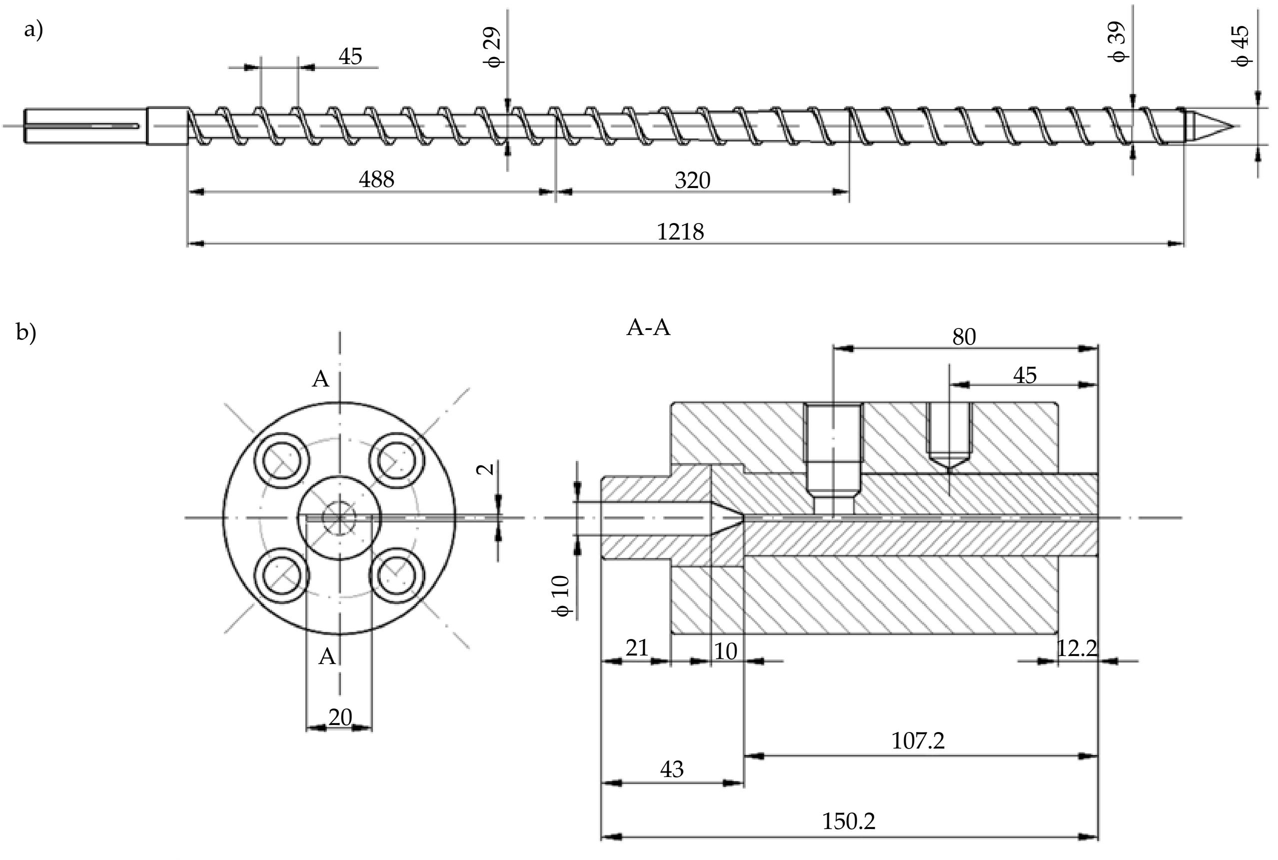

Fig. 1. Geometry of the screw and the die: a) screw, b) forming mouthpiece

where: η – viscosity, $\dot{\gamma}$ – shear rate, T – temperature; A_0, A_1, A_{11}, A_{12}, A_2, A_{22} – parameters of the model, A_0 = 12.469780638, A_1 = -0.8345507, A_{11} = -0.017832191, A_{12} = 0.001331159, A_2 = -0.008413991, A_{22} = -0.000025745.

Experimental

Experimental tests of the single screw extrusion process were carried out. A classical three-zone screw and a special measuring die (without breaker plate) for extruding flat profiles were used. The geometrical scheme of the screw is shown in Fig. 1a. The screw has a diameter D = 45 mm and a length/diameter ratio L/D = 27. The geometrical scheme of the measuring part of the die, which enables pressure measurements, is shown in Fig. 1b. The forming mouthpiece has a cross-section of dimensions (width and height) $W \times H$ = 20 × 2 mm. Pressure and flow rate were measured.

The tests were carried out at three rotational speeds of the screw, N = 30 rpm, N = 50 rpm, and N = 70 rpm. Each time, the polymer flow rate was measured, as well as the pressure in the extruder barrel (three sensors) and in the measuring die. The following temperature conditions were used in the subsequent zones of the barrel: T_{I} = 180 °C, T_{II} = 180 °C, T_{III} = 190 °C, T_{IV} = 190 °C, and in the die T_{DIE} = 190 °C.

Computations

The rheological characteristics of the tested material was determined on the basis of pressure measurement in the die.

The basis of the calculation procedure is the analysis of the flow in the flat channel (between two parallel plates) which is schematically shown in Fig. 2.

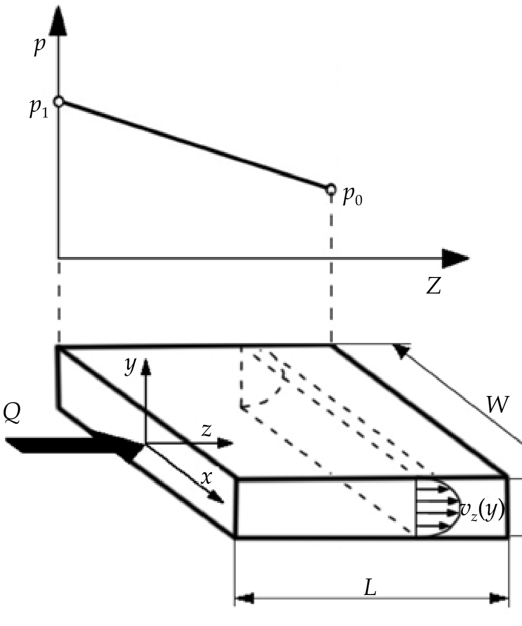

Fig. 2. Scheme of computations: Q – flow rate, p – pressure, W, H, L – channel dimensions, v_z – velocity

Viscosity is defined as:

$$\eta = \frac{\tau_w}{\dot{\gamma}_w} \tag{2}$$

where: η – viscosity, τ_w – shear stress at the channel wall, $\dot{\gamma}_w$ – shear rate at the channel wall.

Shear stress at the wall in the flat channel is expressed as:

$$\tau_w = \tau_{yz}(y = H/2) = -\frac{\Delta p H}{2L} \tag{3}$$

where: Δp – pressure difference, $\Delta p = p_1 - p_0$, p_1 – measured pressure, p_0 – atmospheric pressure, H – channel height, L – channel length.

Shear rate at the wall in the flat channel is expressed as:

$$\dot{\gamma}_w = \frac{\mathrm{d}v_z}{\mathrm{d}y}(y = H/2) = \frac{6Q}{WH^2} \tag{4}$$

where: Q – volumetric flow rate, W – channel width, H – channel height.

An effect of the side walls of the channel on the relationship between a flow rate and a pressure gradient can be expressed by the shape coefficient as follows:

$$\Delta p = \frac{12\eta QL}{WH^3}\frac{1}{f_p} \tag{5}$$

where: Δp – pressure difference, Q – volumetric flow rate, η – viscosity, W, H, L – channel dimensions, $f_p = f_p(H/W)$ – shape coefficient.

The power law model was used for rheological description of the composite under study. This model is expressed as:

$$\tau = m\dot{\gamma}^n \tag{6}$$

where: m – consistency coefficient, Pa · s^n, n – flow exponent (dimensionless).

Using this model, viscosity can be expressed as:

$$\eta = m\dot{\gamma}^{n-1} \tag{7}$$

and after logarithmization:

$$\lg \eta = \lg m + (n-1)\lg \dot{\gamma} \tag{8}$$

Using linear regression, parameters of the power law model, consistency coefficient m and flow exponent n, can be calculated from this equation.

The viscosity dependence on the temperature can be expressed as:

$$\eta(T) = \eta_r \exp[-b(T - T_r)] \tag{9}$$

where: $\eta(T)$ – viscosity at the temperature T, η_r – reference viscosity at the reference temperature T_r, b – material constant, T – temperature.

The material constant b can be expressed and calculated as:

$$b = -\frac{\ln\eta(T) - \ln\eta_r}{T - T_r} \quad (10)$$

Using Equation (1), you can determine the parameter *b*, when you know the viscosity η at two different temperatures *T* and T_r.

Simulations

Extrusion simulations were carried out using a computer model recently developed for modeling the single screw extrusion of WPC [34]. This is the global extrusion model which consists of elementary models of solid conveying, melting, melt conveying and melt flow in the die. In this study, the computer program has been rebuilt to allow using a power law model as the rheological model of the processed material.

In this computer program, melting model is dependent on the wood flour content, and this allows one-dimensional modeling or two-dimensional modeling. Two-dimensional model is used for a lower WF content (*e.g.*, less than 50 wt %), and this is a classical Tadmor melting model with an accumulation of the molten polymer (melt pool) at the pushing flight of the screw [35]. In this case, the width of the solid polymer reduces when melting progresses. One-dimensional model is used for a higher WF content. In this case, the melt pool is not formed at the pushing flight of the screw, but the molten polymer penetrates into the unmolten solid layer. Melting proceeds from the barrel to the core of the screw, and the height of the solid reduces.

A one-dimensional melting model was obtained on the basis of the heat balance on the interface of the solid and melt, and of the mass balance in the melt and solid. To do these, the velocity and temperature profiles in the melt film and the temperature profile in the solid were determined. According to the heat balance, the heat flux used for the material melting is equal to the difference between the heat flux from the melt film into the melt/solid interface and the heat flux from the interface into the solid bed.

Melt conveying is calculated using 3-D FEM based screw pumping characteristics represented by regression models which ensures good accuracy of calculations at a reasonable time of that [29]. This approach was applied in our previous studies in modeling the single screw extrusion, including conventional screw elements [29] as well as non-conventional elements [30, 31]. It is important to know that each screw configuration requires different regression model.

In the classical (flood fed) single screw extrusion process, the extrusion output is not determined by the operator, but results from an operation of the extruder-die system. The calculations begin by assuming a certain initial value of the extrusion output, *e.g.*, equal to the drag flow rate. Then the process is simulated (in the screw channel and at the die), and the pressure at the end of the die is compared with the atmospheric pressure. In dependence on the result (negative or positive difference) the extrusion output is changed (increased or decreased), and calculations are iterated until the convergence is obtained.

Simulations were carried out in the range of experiment conditions, *i.e.*, screw speed and temperature conditions. The viscous flow properties of the WPC material were described by the power law model. The parameters of the power law were obtained from the on-line measurements.

RESULTS AND DISCUSSION

Experimental

The results of measurements of the throughput (*i.e.*, the mass flow rate) and the pressure in the die and in the subsequent sections of the barrel are presented in Table 1. An obvious increase of the throughput and pressure was observed with an increase of the screw speed. The flow rate and the die pressure were used to calculate the viscosity according to the procedure outlined in the previous section.

Table 1. Results of the experiment

Screw speed rpm	Throughput kg/h	Die pressure MPa	Barrel pressure MPa
30	10.71	8.4	5.1/9.3/12.0
50	16.26	9.8	6.1/8.2/12.2
70	22.01	10.0	7.6/8.4/12.8

Computations

The results of computations are presented in Table 2. The shear rate at the wall $\dot{\gamma}_w$, the shear stress at the wall τ_w and the viscosity were calculated using Eqs. (4), (3) and (2). The pressure drop Δp was assumed to be equal to the die pressure, the volumetric flow rate was calculated using the melt density, and the shape coefficient $f_p = 0.95$ was applied to correct the pressure difference according to Eq. (5).

Table 2. Results of the computations

Screw speed rpm	Shear rate s^{-1}	Shear stress Pa	Viscosity Pa · s
30	234.8	110 526.3	470.7
50	356.6	128 947.4	361.6
70	482.8	131 578.9	272.6

With the use of these data, the parameters of the power law were determined using linear regression from Eq. (8). And, the following model parameters were obtained: the consistency coefficient $m = 28\,707.8$ Pa · s^n and the flow exponent $n = 0.25$. The results of the on-line viscosity mea-

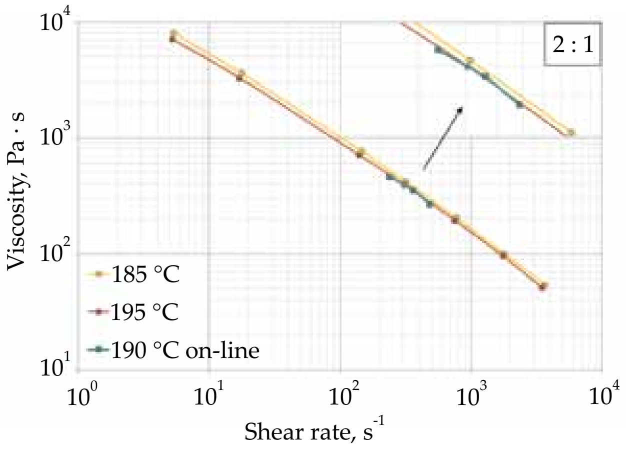

Fig. 3. On-line viscosity measurements against the background of rheological viscosity curves

surements are depicted in Fig. 3, against the background of rheological viscosity curves of the WPC.

The temperature parameter *b* of Eq. (9) was calculated using Eq. (10), and it is equal to 0.015.

Using the data shown in Table 2, the viscosity was also modeled using the Klein Eq. (1), which is the basic rheological model of the computer program used in the study. However, this model does not provide good extrapolation of results beyond the scope of data used for its construction. So, the computer program had to be rebuilt to allow better simulations by using the power law model.

Simulations

The results of melting simulations are shown in Figs. 4–7. Calculations were carried out in two variants, using one-dimensional melting model and two-dimensional model. Figure 4 presents the so-called general characteristics of the extrusion process. This includes the characteristics of the basic process parameters shown on one graph in a dimensionless form. They capture the distribution of pressure and temperature, description of the material melting, power consumption and the degree of filling of the screw channel. In the case of the tested classical extrusion with gravitational feeding, *i.e.*, without dosing, it is equal to 1. The rate of the material melting is determined by the so-called solid bed profile (SBP) which is defined by the ratio of the volume of solid material to the volume of the channel in the volume locally considered. At the beginning of the melting it is equal to 1, and at the end of the melting it is equal to 0.

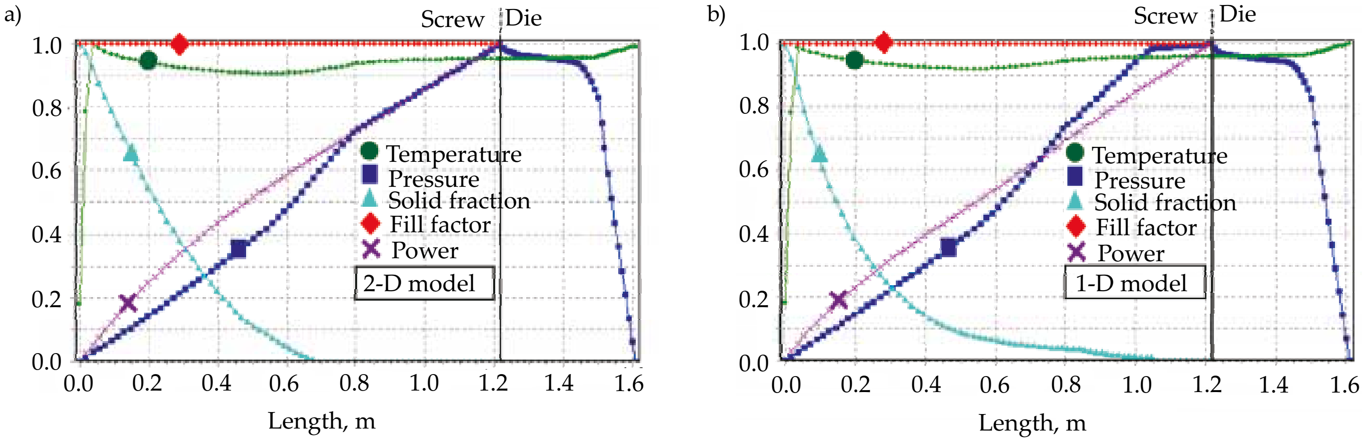

Fig. 4. Dimensionless extrusion process characteristics, *N* = 50 rpm: a) 2-D model, b) 1-D model

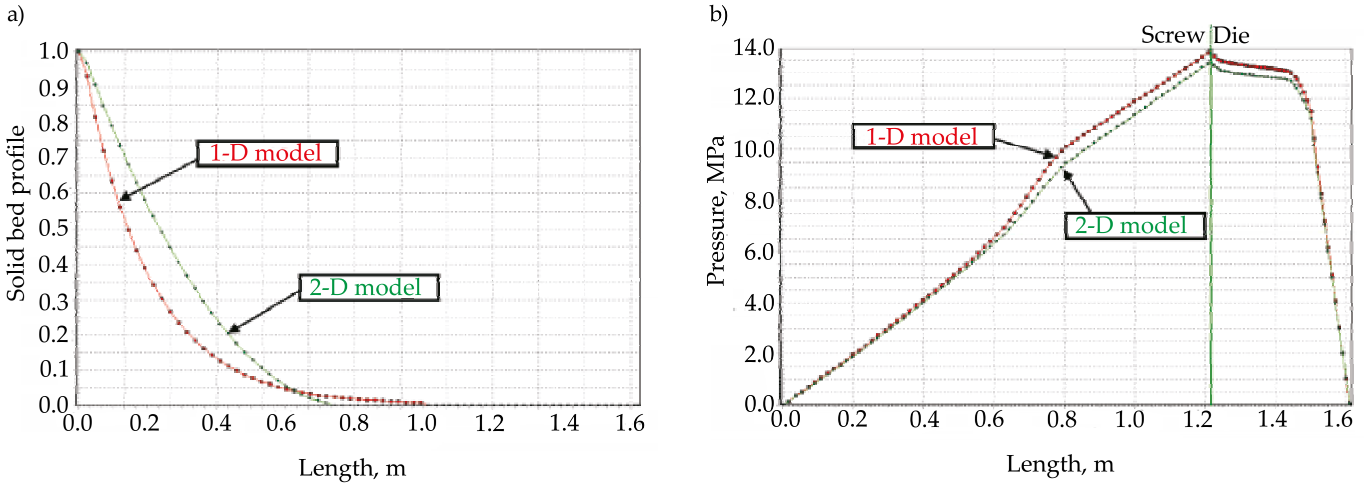

Fig. 5. Process characteristics using 1-D model and 2-D model, *N* = 30 rpm: a) melting course (solid bed profile, SBP), b) pressure profile

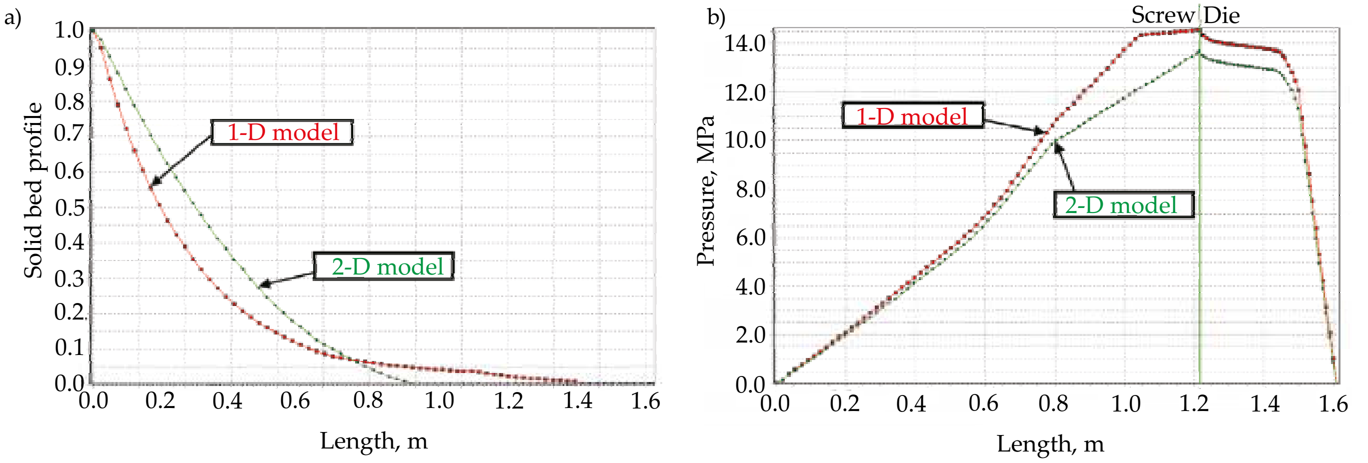

Fig. 6. Process characteristics using 1-D model and 2-D model, *N* = 50 rpm: a) melting course (solid bed profile, SBP), b) pressure profile

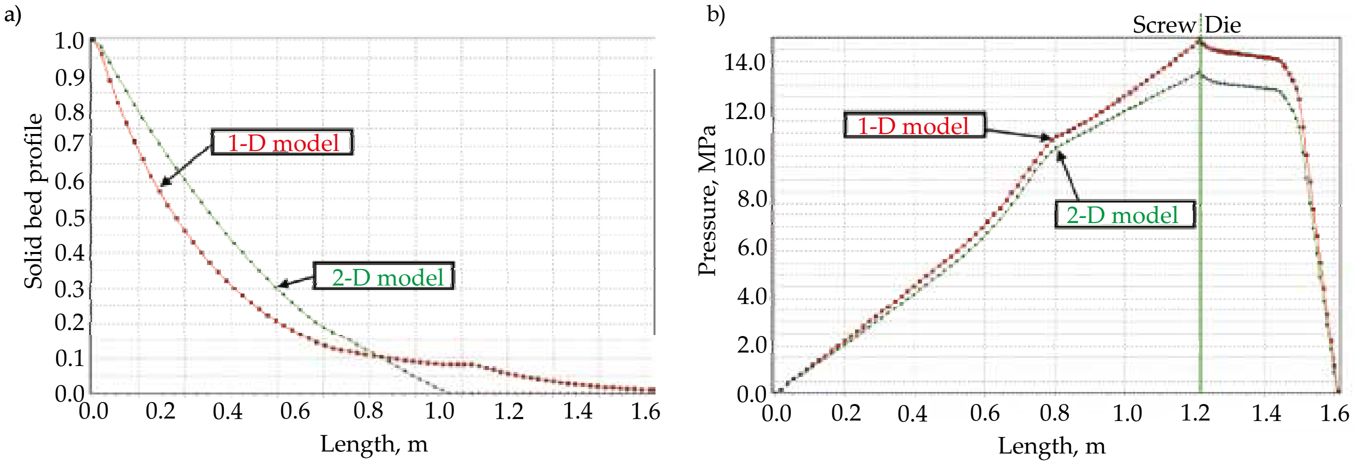

Fig. 7. Process characteristics using 1-D model and 2-D model, *N* = 70 rpm: a) melting course (solid bed profile, SBP), b) pressure profile

Figures 5–7 show the progression of the material melting and the pressure profiles obtained by using two different melting models. In short, the melting derived from the one-dimensional model consists in reducing the thickness of the solid layer of the unmolten material, while the melting derived from the two-dimensional model consists in reducing the width of the solid layer.

Figures 5–7 clearly show that the melting derived from the one-dimensional model proceeds at slower rate. This can be explained by the reduction of energy dissipation along with the process of melting because the thickness of the molten material is then increased. Thus the shear rate in this layer is reduced. However, at the beginning stage the melting derived from the one-dimensional model proceeds faster since the thickness of the molten material is small in this region.

With an increase of the screw speed, the melting proceeds at slower rate because the material stays shorter in the extruder (the residence time is shorter). The type of melting model used has a slight influence on the course of pressure changes in the extruder, although in each case the pressure is higher at the slower melting.

Table 3. Results of the experiment and simulations

Screw speed rpm	Experiment		Simulation 1-D		Simulation 2-D	
	Throughput kg/h	Die pressure MPa	Throughput kg/h	Die pressure MPa	Throughput kg/h	Die pressure MPa
30	10.71	8.4	8.7	8.3	8.6	8.0
50	16.26	9.8	15.8	8.5	14.5	8.1
70	22.01	10.0	23.3	8.8	20.5	8.1

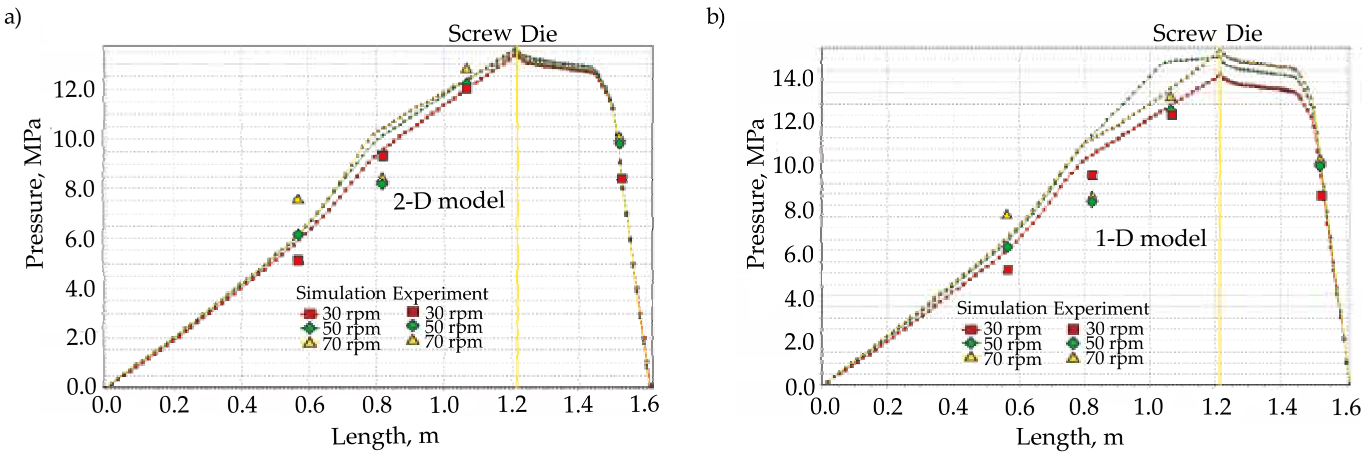

Fig. 8. Simulation validation, pressure profile: a) 2-D model, b) 1-D model

Validations

The results of experimental verification of the extrusion simulations are presented in Table 3 and Fig. 8.

Table 3 shows that the discrepancies in the results of calculations and measurements are not large and are of the order of 10 %, not exceeding in extreme cases 20 %. Interestingly, if the one-dimensional model is used, the convergence of results is greater. This can be explained by the fact that one-dimensional model corresponds more to the material with the content of 50 wt % wood flour. Figure 8 shows that the pressure profile is also well predicted.

CONCLUSIONS

The problem of determining the rheological properties of wood plastic composites has been undertaken in this paper, because the rheological data of these materials are not published in the open material databases.

The rheological tests of WPC based on the on-line measurements have been performed. Viscosity has been determined by measuring the extrusion output and the pressure in the extrusion die. The power law model has been used to analyze viscosity dependence on the shear rate and temperature. Using this model, the extrusion process of WPC has been simulated and validated experimentally.

It was concluded that description of rheological properties of the WPC composite by means of the power law ensured smooth extrapolation of the results beyond the scope of measurement data. Recently developed computer model for simulating the single screw extrusion of wood plastic composites was modified by implementing the power law model into the computation code. The results of extrusion simulation tests were validated experimentally, and a good agreement was observed. Two-variant modeling of the material melting depending on the wood flour content was applied. Smaller discrepancies between simulation and experiment were observed, when one-dimensional model for melting was used.

It should be mentioned that present studies are premised on the materials without slipping at walls. This should be considered in the further studies.

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REFERENCES

[1] Bledzki A.K., Reihmane S., Gassan J.: *Polymer-Plastics Technology Engineering* **1998**, *37*, 451. http://dx.doi.org/10.1080/03602559808001373
[2] Oksman Niska K., Sain M.: "Wood-Polymer Composites", Woodhead Publishing Limited, Abington Hall, Cambridge 2008.
[3] Klyosov A.A.: "Wood-Plastic Composites", John Wiley & Sons, New Jersey 2007.
[4] Zajchowski S., Ryszkowska J.: *Polimery* **2009**, *54*, 674.
[5] Li T.Q., Wolcott M.P.: *Polymer Engineering Science* **2005**, *45*, 549. http://dx.doi.org/10.1002/pen.20308
[6] Li T.Q., Wolcott M.P.: *Polymer Engineering Science* **2006**, *46*, 114. http://dx.doi.org/10.1002/pen.20432
[7] Li T.Q., Wolcott M.P.: *Polymer Engineering Science* **2006**, *46*, 464. http://dx.doi.org/10.1002/pen.20505
[8] Xiao K., Tzoganakis C.: *ANTEC Conference Proceedings* **2002**, *38*, 252.
[9] Xiao K., Tzoganakis C.: *ANTEC Conference Proceedings* **2003**, *39*, 197.
[10] Xiao K., Tzoganakis C.: *ANTEC Conference Proceedings* **2003**, *39*, 975.
[11] Xiao K., Tzoganakis C.: *ANTEC Conference Proceedings* **2004**, *40*, 448.
[12] Hristov V., Takacs E., Vlachopoulos J.: *Polymer Engineering Science* **2006**, *46*, 1204. http://dx.doi.org/10.1002/pen.20592
[13] Vlachopoulos J., Hristov V.: "Rheology of Wood Polymer Composites", The Regional PPS Meeting,

B1, Pretoria, RPA 2006.

[14] Santi R.C., Hage E. Jr., Vlachopoulos J., Correa C.A.: *International Polymer Processing* **2009**, *24*, 346. http://dx.doi.org/10.3139/217.2238

[15] Lewandowski K., Piszczek K., Zajchowski S., Mirowski J.: *Polymer Testing* **2016**, *51*, 58. http://dx.doi.org/10.1016/j.polymertesting.2016.02.004

[16] Wilczyński K.J.: *Polimery* **2018**, *63*, 47. http://dx.doi.org/10.14314/polimery.2018.3.5

[17] Wilczyński K., Buziak K., Bartnik M.: *Polimery* **2016**, *61*, 195. http://dx.doi.org/10.14314/polimery.2016.195

[18] Rauwendaal C.: "Polymer Extrusion", Hanser, Munich 2014.

[19] Vlachopoulos J.: "Polymer Rheology and Extrusion", Polydynamics Inc., Ontario 2011.

[20] www.campusplastics.com

[21] www.autodeskmoldflow.com

[22] www.moldex3d.com

[23] Osswald T., Rudolph N.: "Polymer Rheology. Fundamentals and Applications", Hanser Publ., Munich 2015.

[24] Shaw M.T.: "Introduction to Polymer Rheology", Wiley, Hoboken, New Jersey 2012.

[25] Malkin A.Y., Isayev A.I.: "Rheology. Concepts, Methods, and Applications", ChemTec Publ., Toronto 2012.

[26] Ariffin A., Ahmad M.S.B.: *Polymer-Plastics Technology Engineering* **2011**, *50*, 395. http://dx.doi.org/10.1080/03602559.2010.543228

[27] Wilczyński K., Nastaj A., Lewandowski A., Wilczyński K.J.: *Polymer-Plastics Technology Engineering* **2012**, *51*, 626. http://dx.doi.org/10.1080/03602559.2012.659313

[28] Wilczyński K.: *Journal Materials Processing Technology* **2001**, *109*, 308. https://doi.org/10.1016/S0924-0136(00)00821-9

[29] Wilczyński K.J., Nastaj A., Lewandowski A., Wilczyński K.: *Polymer Engineering Science* **2014**, *54*, 2362. http://dx.doi.org/10.1002/pen.23797

[30] Wilczyński K.J., Lewandowski A., Nastaj A., Wilczyński K.: *International Polymer Processing* **2016**, *31*, 82. http://dx.doi.org/10.3139/217.3154

[31] Wilczyński K.J., Lewandowski A., Nastaj A., Wilczyński K.: *Advances Polymer Technology* **2018**, *37*, 2142. http://dx.doi.org/10.1002/adv.21873

[32] Wilczyński K.J., Nastaj A., Wilczyński K.: *Advances Polymer Technology* **2017**, *36*, 23. http://dx.doi.org/10.1002/adv.21570

[33] Wilczyński K., Nastaj A., Lewandowski A., Wilczyński K.J., Buziak K.: *International Polymer Processing* **2015**, *30*, 113. http://dx.doi.org/10.3139/217.3007

[34] Wilczyński K., Buziak K., Wilczyński K.J., Lewandowski A., Nastaj A.: *Polymers* **2018**, *10* (*3*), 295. http://dx.doi.org/10.3390/polym10030295

[35] Tadmor Z.: *Polymer Engineering and Science* **1966**, *6*, 185. http://dx.doi.org/10.1002/pen.760060303

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