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Jacek Nabiałek

Czestochowa University of Technology, Department of Polymer Processing and Production Management, al. Armii Krajowej 19c, 42-201 Częstochowa, Poland
** Corresponding author. E-mail: nabialek@ipp.pcz.pl*

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MODELING OF FIBER ORIENTATION DURING INJECTION MOLDING PROCESS OF POLYMER COMPOSITES

Polymer composites with fibers are widely used as construction materials. Different fibers are used (eg. fiberglass). One method of forming composite materials is injection molding. The paper presents chosen results of investigations on polymer flow during the mould cavity filling phase of the injection molding process. The process is characterized by high dynamics, which causes several technological difficulties, both during injection mould design and during product implementation to the production stage. Deep understanding of the phenomena which occur during filling an injection mould may lead to a more effective design of the processing tools and shortening of the time for the implementation and production time. In the paper the theoretical basis for modeling fiber orientation in an injected polymer composite is described. The orientation and distribution of fibers have a substantial influence on the mechanical properties of a molded part. A computer simulation of the injection molding of a polypropylene composite with glass fiber (PP + 20% glass fiber, Aqualoy 125B, A Schulman NA) is conducted. Special attention is given to the results concerning the orientation of the fiber during processing. Selected results of the computer simulation of the flow velocity distribution of the composite, Poisson's coefficient and fiber orientation tensor across the molded part and selected cross-sections are presented. Significant discrepancies in the orientation of the fibers, depending on the nature of the flow of the injected composite are affirmed. These disparities affect the lack of uniformity of the mechanical strength of the molded part. The author plans to extend the scope simulation research to determine the effect of processing conditions on fiber orientation.

Keywords: **polymer composites, fiber orientation, injection molding process, computer simulations**

MODELOWANIE ORIENTACJI WŁÓKIEN PODCZAS WTRYSKIWANIA KOMPOZYTÓW POLIMEROWYCH

Kompozyty polimerowe z włóknami szklanymi są szeroko stosowane jako materiały konstrukcyjne. Stosowane są różne włókna (m.in. włókna szklane). Jedną z metod formowania wyrobów kompozytowych jest wtryskiwanie. W pracy przedstawiono wybrane wyniki badań przepływu polimeru podczas wypełniania gniazda formy w procesie wtryskiwania. Proces ten charakteryzuje się dużą dynamiką, przez co stwarza szereg trudności technologicznych zarówno podczas projektowania form wtryskowych, jak i na etapie wdrożenia wytworu do produkcji. W pracy opisano teoretyczne podstawy modelowania orientacji włókien we wtryskiwanym kompozycie polimerowym. Orientacja i dystrybucja włókien wtryskowej mają zasadniczy wpływ na właściwości mechaniczne w wypraski. Przeprowadzono symulację komputerową procesu wtryskiwania kompozytu polipropylenu z włóknem szklanym (PP + 20% włókna szklanego, Aqualoy 125B, A Schulman NA). Szczególną uwagę zwrócono na wyniki dotyczące orientacji włókien podczas przetwórstwa. Przedstawiono wybrane wyniki symulacji komputerowej rozkładu prędkości przepływu kompozytu, współczynnika Poissona oraz tensora orientacji włókien w całej wyprasce i wybranych przekrojach poprzecznych. Stwierdzono duże rozbieżności orientacji włókien w zależności od charakteru przepływu wtryskiwanego kompozytu. Rozbieżności te decydują o braku jednorodności wytrzymałości mechanicznej wypraski. Autor planuje rozszerzyć zakres badań symulacyjnych w celu określenia wpływu warunków przetwórstwa na orientację włókien.

Słowa kluczowe: **kompozyty polimerowe, orientacja włókien, proces wtryskiwania, symulacje komputerowe**

THEORETICAL BASIS FOR FIBER ORIENTATION PREDICTION

The numerical prediction of three-dimensional fiber orientation during mold filling is based on an equation of motion for rigid particles in a fluid suspension. The analysis consists of two identifiable terms:

- hydrodynamic term,
- interaction term.

The hydrodynamic influence on particle motion is described by Jeffery's [1] equation assuming an infinite aspect ratio. This theory strictly applies to diluted suspensions but has been shown to provide useful qualitative agreement with experimental data.

The interaction term was proposed by Folgar and Tucker [2] and is incorporated to model the randomizing effect of the mechanical interactions between fibers. It has the form of a diffusion term with the frequency of interaction being proportional to the magnitude of the strain rate. The effect of the interaction term is to reduce highly-aligned orientation states predicted by Jeffery's model for some flow conditions, providing improved agreement with the experimental observations.

The calculation of three-dimensional fiber orientation is performed concurrent with the mold filling analysis on the same finite element mesh. Each triangular element may be considered as consisting of several layers subdividing the local molding thickness. Each layer is identified by a grid point through which it passes. The midplane of the molding passes through grid point 1. An orientation solution is calculated in each layer for each element in the mesh. In this way, it is possible to observe the variation in orientation distribution on a set of planes parallel to the mold surface through the cross-section of the molding.

The three-dimensional orientation solution for each element is described by a second order tensor (1). For graphical representation, the eigenvalues and eigenvectors of the orientation tensor are generated. The eigenvectors indicate the principal directions of fiber alignment and the eigenvalues give the statistical proportions (0 to 1) of fibers aligned with respect to those directions. This information is used to define an orientation ellipsoid which fully describes the alignment distribution of fibers for each element. A general orientation ellipsoid is shown in Figure 1.

$$a_{ij} = \begin{bmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{bmatrix} \rightarrow \begin{bmatrix} \lambda_1 & 0 & 0 \\ 0 & \lambda_2 & 0 \\ 0 & 0 & \lambda_3 \end{bmatrix}; \begin{bmatrix} e_1 & e_2 & e_3 \end{bmatrix} \tag{1}$$

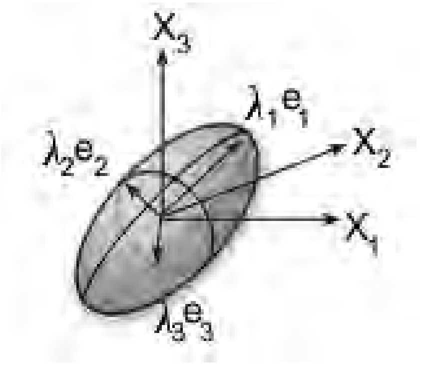


Fig. 1. General orientation ellipsoid which fully describes alignment distribution of fibers for each element

Rys. 1. Ogólna orientacja elipsoidy definiującej uporządkowanie rozkładu włókien dla każdego elementu

For display purposes, this 3D ellipsoid is projected onto the plane of each element to produce a plane ellipse. This creates a useful representation of the orientation distribution, since the gap-wise orientation components eliminated by the projection are usually small. In this representation, a near random distribution is displayed as an ellipse tending to a circle while for a highly aligned distribution, the ellipse degenerates to a line.

DESCRIPTION OF ORIENTATION TENSOR

The second order orientation tensor a_{ij} provides an efficient description of fiber orientation in injection moldings. The tensor has nine components, with the suffixes for the tensor terms being:

- In flow direction.
- Transverse to flow direction.
- In thickness direction.

Typically these axes apply:

- X-Y (or 1-2) flow plane.
- Z-axis in thickness direction, out of 1-2 flow plane.

The original nine components reduce to five independent components, due to:

- tensor symmetry $a_{ij} = a_{ji}$, and
- normalization condition $(a_{11} + a_{22} + a_{33} = 1)$.

These three major orientation components have been included in the orientation considerations:

- a_{11}, fiber orientation in flow direction, varying from 0 to 1.0.
- a_{22}, fiber orientation transverse to flow, varying from 0 to 1.0.
- a_{33}, tilt of orientation in the 1-3 plane, varying from –0.5 to 0.5.

The flow direction orientation term, a_{11}, contains most of the quantitative information about the microstructure and is most sensitive to flow, processing and material changes. A composite material of interest may be considered as particles or fibers suspended within a viscous medium. There may be mechanical and/or hydrodynamic interactions between the fibers. The suspension may be dilute, semi-concentrated or concentrated, as discussed below:

- A dilute suspension is one in which the fibers are never close to one another and do not interact.
- A semi-concentrated suspension would have no mechanical contact between the fibers, but hydrodynamic interactions become significant.
- In a concentrated suspension, the fiber orientation behavior becomes very complex, since both mechanical and hydrodynamic fiber interactions apply.

Jeffery first modeled the motion of a single fiber immersed in a large body of incompressible Newtonian fluid. Jeffery's model applies only to suspensions that are so dilute that any inter-fiber interactions (even hydrodynamic interactions) are negligible. An important measure for assessing suspension concentration is the average distance between the fibers.

Considering fibers of diameter d and length L, with an aspect ratio $\frac{L}{d}$, a fiber concentration by volume c (or volume fraction V_f) and having a uniform length distribution, a typical concentration classification scale is:

- Dilute $c << \left(\frac{d}{L}\right)^2$.
- Semi-concentrated $\left(\frac{d}{L}\right)^2 < c < \left(\frac{d}{L}\right)$.
- Concentrated $c > \frac{d}{L}$.

For example, if $\frac{L}{d}$ is 10 (a small value for reinforcing fibers in a composite), then the fiber concentration must be much less than 1 % by volume for Jeffery's equation to apply.

For commercial materials, the fiber aspect ratio $\frac{L}{d}$ is often 20 or more, so the values for the above concentrations are:

- Dilute, c << 0.025.
- Semi-concentrated, 0.0025 < c < 0.05.
- Concentrated, c > 0.05

These classification scale cutoffs would typically translate to about 0.5 and 10% by weight. Most commercial composites contain 10-50% fibers by weight, which can be regarded as being concentrated suspensions. For semi-concentrated suspensions, a model has been proposed by Dinh and Armstrong [3]. The orientation of the fiber follows the bulk deformation of the fluid with the exception that the particle cannot stretch. For concentrated suspensions, a term, called "the interaction coefficient" (or C_I), has been incorporated in the phenomenological model for fiber orientation proposed by Folgar and Tucker [2, 3]:

- Interactions among fibers tend to randomize the orientation.
- The term takes the same form as a diffusion term and since interactions only occur when the suspension is deforming, the effective diffusivity is proportional to the strain rate.
- The dimensionless C_I term determines the strength of the diffusion term.

Adding the rotary diffusion term to account for fiber interactions has been found to improve the orientation predictions, since Jeffery's equation alone does not give qualitatively accurate predictions for fiber orientation. Until now, the Folgar-Tucker model has been the best available for fiber orientation modeling in concentrated suspensions. The model has been given in this form by Advani and Tucker:

$$\frac{\partial a_{ij}}{\partial t} + v_k \frac{\partial a_{ij}}{\partial x_k} = -\frac{1}{2}\left(w_{ik} a_{kj} - a_{ik} w_{kj}\right) + \frac{1}{2}\lambda\left(\dot{\gamma}_{ik} a_{kj} + a_{ik}\dot{\gamma}_{kj} - 2\dot{\gamma}_{kl} a_{ijkl}\right) + 2C_I\dot{\gamma}\left(\delta_{ij} - \alpha\, a_{ij}\right) \qquad (2)$$

where: α - equals 3 for 3D and 2 for planar (2D) orientation, v_k - is the velocity component, $\frac{1}{2}w_{ij}$ - is the vorticity and $\frac{1}{2}\dot{\gamma}_{ij}$ is the deformation rate tensors, λ - is a constant that depends on the geometry of the particle, δ_{ij} - is a unit tensor, C_I - is the interaction coefficient.

FIBER ORIENTATION MODEL CLOSURE

The tensor form of the fiber orientation model from Advani and Tucker is not yet a suitable derivative for a second order orientation tensor, because it contains the fourth order tensor a_{ijkl}. The derivative for a fourth order tensor contains a sixth order orientation tensor and so on. The only way to develop a suitable derivative is to approximate the fourth order tensor in terms of a second order tensor. This approximation is called a „closure approximation”. Various approximations have been tested by Advani and Tucker. However, the presence of the approximation itself may introduce some errors/a degree of error into the simulation results. Hence the closure approximation is the most challenging problem associated with this model. No value of can make the fiber orientation model expression fit all the orientation model components.

Examination of the Advani and Tucker fiber orientation model form indicates two ways to control the fiber orientation prediction accuracy:

- Find a more accurate closure.
- Find a new interaction model that considers the closure error.

While the first method would be preferred, no closure has been found to satisfactorily cover the range of shearing and stretching flows for a multi-decade range of. The effect of the closure approximation is to predict a too much out-of-plane orientation. This result has been addressed by the fiber orientation model form proposed by Moldflow software.

The fiber orientation tensor result shows the probability of fiber alignment in the specified principal direction. A high probability of fiber alignment in the specified principal direction will be indicated by a value of close to 1 on the result scale, whereas a low probability is indicated by a value close to 0. The fiber orientation tensor in the first principal direction is the most useful result to view. The first principal direction is close to the material flow direction in most cases, but it may not always coincide with the flow direction. The fiber orientation tensor is expressed in the global coordinate system, and is also used to calculate the mechanical/thermal property as well as the residual stress in the cavity.

COMPUTER SIMULATIONS

The computer simulation consisted in several numerical analyses in order to perform computer modeling of the injection process for the chosen composite (PP + 20% glass fiber, Aqualoy 125B, A Schulman NA). For the investigations, the professional software Autodesk Moldflow Insight 2011 has been used. In order to perform a correct analysis, the input of an amount of data became necessary. In order to model the rheologic properties of the plastic, the seven-parameters model Cross-WLF has been employed [4-12]. The chosen rheologic model is rather complicated, but ensures very good imaging of the composite properties.

In Figure 2, the model FEM of the part used for the investigations has been presented. Additionally, the gating system for the mould was modeled. After the input of material data and processing conditions, the numerical calculations were performed.

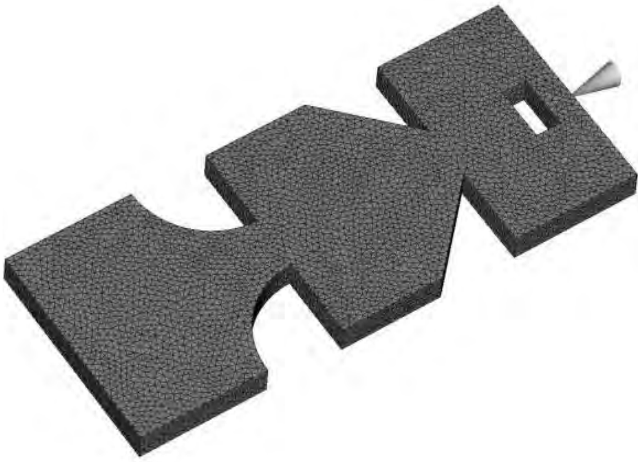


Fig. 2. Part model with FEM mesh

Rys. 2. Wypraska z nałożoną siatką MES

In Figures 3-6, selected results of the numerical analysis have been presented.

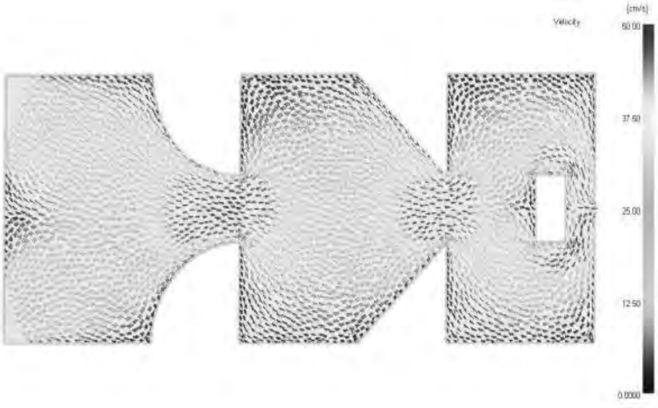
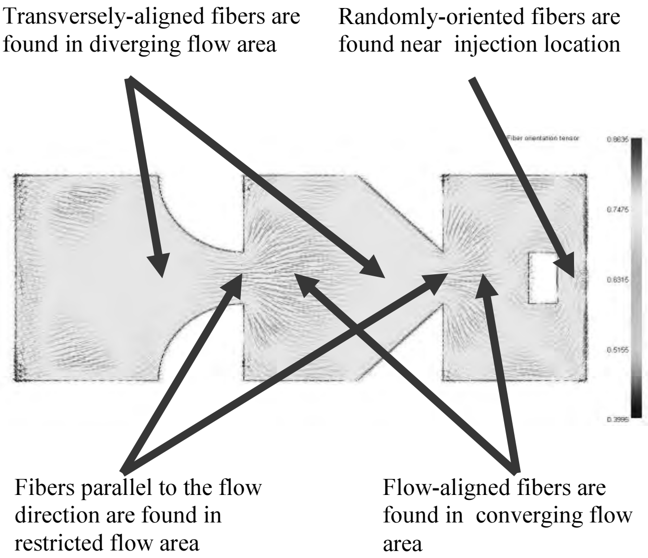


Fig. 3. Velocity distribution at end of cavity filling

Rys. 3. Rozkład prędkości w końcowej fazie wypełniania gniazda formującego



Transversely-aligned fibers are found in diverging flow area

Randomly-oriented fibers are found near injection location

Fibers parallel to the flow direction are found in restricted flow area

Flow-aligned fibers are found in converging flow area

Fig. 4. Fiber orientation tensor

Rys. 4. Tensor orientacji włókien

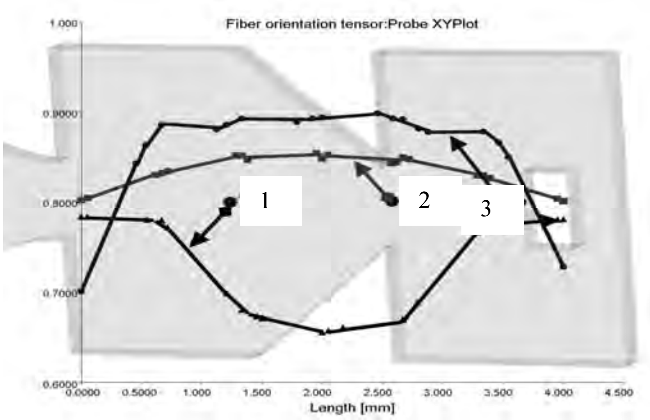


Fig. 5. Fiber orientation tensor at selected points (1, 2, 3) of molded part (plot by thickness of part - 4 mm)

Rys. 5. Tensor orientacji włókien w wybranych punktach (1, 2, 3) wypraski (wykres po grubości wypraski - 4 mm)

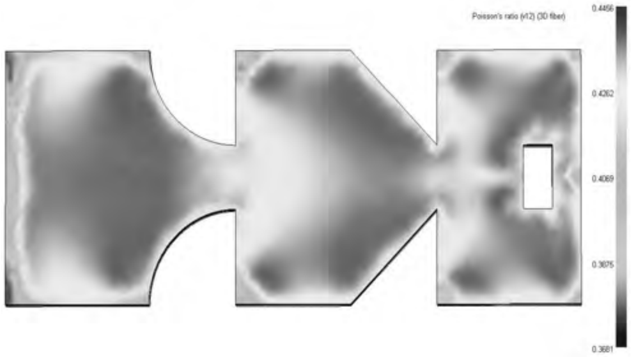


Fig. 6. Poisson's ratio distribution (v12)

Rys. 6. Rozkład współczynnika Poissona (płaszczyzna 12)

CONCLUSIONS

After performing the investigations and the analysis of their results, the following conclusions were drawn:

1. Modeling of fiber orientation during injection molding process allows one to determine the mechanical properties of the injected part.
2. Fiber orientation in an injected composite has a significant influence on the mechanical strength of different areas of the injected part.
3. The author plans to extend the scope simulation research to determine the effect of processing conditions on fiber orientation.
4. Looking for new test methods is done in order to thoroughly investigate unexplained or disputable phenomena occurring during chosen manufacturing processes. Such investigations are performed in order to find out about these phenomena, to analyse them and to use them for optimisation and cost reduction during manufacturing.

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