Autodesk® Moldflow® Insight 2012

AMI Fiber Orientation Analysis

Revision 1, 22 March 2012.

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Fiber orientation analysis

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The Fiber orientation Fill+Pack analysis is used to predict the behavior of composite materials. While injection-molded fiber-reinforced thermoplastics constitute a major commercial application of fiber composite (a filler within a polymer matrix) materials, the modeling of the process is more complex than in other flow applications.

A composite material of interest may be considered as particles of fibers suspended within a viscous medium. There may be mechanical and/or hydrodynamic interactions between the fibers. Most commercial composites contain 10-50% fibers by weight, which can be regarded as being concentrated suspensions, where both mechanical and hydrodynamic fiber interactions apply.

In injection-molded composites, the fiber alignment (or orientation) distributions show a layered nature, and are affected by the filling speed, the processing conditions and material behavior, plus the fiber aspect ratio and concentration. Without proper consideration of the fiber behavior, there is a tendency to significantly overestimate the orientation levels. Moldflow's fiber orientation models allow significantly improved orientation prediction accuracy over a range of materials and fiber contents.

The composite's major mechanical properties are derived from the elemental orientation data. There can be a significant variation in mechanical properties with different mold geometry, fiber content and also with the different Fiber orientation models available.

The results from the Fiber orientation analysis can be used later as input for a Stress or Warp analysis, providing more detailed elemental results, and considerably enhanced analysis accuracy.

NOTE: The Fiber orientation analysis is done per the material. Therefore, all you need to do is select a fiber-filled material and ensure that the **Fiber orientation analysis if fiber material** option is selected in the Process Settings Wizard in order to run a Fiber orientation analysis.

Fiber orientation analysis

The Fiber orientation Fill+Pack analysis is used to predict the behavior of composite materials.

Setting up a Fiber orientation analysis

The following table summarizes the setup tasks required to prepare a Fiber orientation analysis (using a Fill or Fill+Pack analysis).

The setup tasks below are for fiber-filled thermoplastic materials.

Setup task	Analysis technology
Selecting an analysis sequence	
Setting up a Fill analysis	

Fiber orientation analysis

Use these dialogs to specify settings for a Fiber orientation analysis.

NOTE: The parameters available to edit will depend on the molding process and mesh type selected.

Fiber Orientation Solver Parameters dialog

Use this dialog to specify the settings for the solver parameters related to Fiber orientation prediction in a Fill or Fill+Pack analysis sequence.

To access this dialog, ensure that you have selected an analysis sequence that includes Fill+Pack , click (**Home tab > Molding Process Setup panel > Process Settings**), if necessary click **Next** one or more times to navigate to the **Fill+Pack Settings** page of the Wizard, select the option **Fiber orientation analysis if fiber material**, then click **Fiber parameters**.

NOTE: All solver parameters have a default value that will be suitable for most analyses.

NOTE: If the shrinkage model for the selected material is set to CRIMS, and the **Use CRIMS** option on the CRIMS Shrinkage Model Coefficients dialog is set to the default (**change solver parameters to be consistent with the CRIMS model**), any changes that you make to the solver parameters above will be overwritten in the analysis. If you want to use non-default settings for these solver parameters, either change the **Use CRIMS** option setting, or select a different shrinkage model.

Calculate fiber orientation using	This option specifies the model used by the Fiber analysis solver to calculate fiber orientation.
Apply fiber inlet condition at	This option specifies whether the fiber orientation calculation begins at the part gate or at the injection location.
Fiber inlet condition	Allows you to specify the inlet boundary condition of the fiber orientation state.

Composite property calculation options	This dialog is used to edit options relating to the prediction of the mechanical properties of the composite, that is, fibers plus polymer matrix.

Composite Property Calculation Options dialog

This dialog is used to edit options relating to the prediction of the mechanical properties of the composite, that is, fibers plus polymer matrix.

When using the Automatic setting, if you use a material that has composite properties or isotropic matrix properties, the Tandon-Weng micro-mechanics model will be used by default. If your material has anisotropic matrix properties, the Mori-Tanaka micro-mechanics model will be used by default.

To access this dialog, ensure that you have selected an analysis sequence that includes Fill+Pack. Then click (**Home tab > Molding Process Setup panel > Process Settings**), if necessary click **Next** one or more times to navigate to the **Fill+Pack Settings** page of the Wizard, select the option **Fiber orientation analysis if fiber material**, click **Fiber parameters**, then click **Composite property calculation options**.

NOTE: The automatic settings are appropriate for most simulations. This dialog has been provided for specialist users conducting research into the fluid mechanics of fiber-filled materials.

TIP: If you have a material that has anisotropic matrix material properties, the Mori-Tanaka micro-mechanics model may provide more accurate shrinkage and warpage predictions.

Closure approximation model	A closure approximation is a formula used to approximate the fourth-order orientation tensor in terms of a second-order tensor.
Fiber-filled property output	Specifies which composite (matrix + fiber) mechanical properties results are to be outputted to the .lsp result file generated by the Fiber orientation solver.
Micro-mechanics model	Micro-mechanics models are the set of models used to predict the elastic properties of short-fiber reinforced composites from the knowledge of the matrix and the fiber elastic properties, fiber content and fiber aspect ratio.
Thermal expansion coefficient model	Specifies the model for predicting the longitudinal and transverse coefficients of thermal expansion of unidirectional fiber reinforced composites, from the knowledge of the matrix and the fiber

	thermal expansion coefficients, fiber content and fiber aspect ratio.

Fiber Interaction Calculation Parameters dialog

This dialog is used to enter specific values for the **Coefficient of interaction (Ci)** and **Thickness moment of interaction coefficient (Dz)** settings that will be used in the calculation of fiber interactions.

To access this dialog, ensure that you have selected an analysis sequence that includes Fill+Pack , click (**Home tab > Molding Process Setup panel > Process Settings**), if necessary click **Next** one or more times to navigate to the Fill+Pack Settings page of the Wizard, select the option **Fiber orientation analysis if fiber material**, click **Fiber parameters**, set the **Calculate fiber interactions using** option to **Moldflow model with specified Ci and Dz values**, then click **Edit settings**.

NOTE: The default settings will be appropriate for most simulations. This dialog has been provided for specialist users conducting research into the fluid mechanics of fiber-filled materials.

Thickness moment of interaction coefficient (Dz)	Specifies the thickness moment of interaction coefficient (Dz) value that will be used in the calculation of fiber interactions.
Coefficient of interaction (Ci)	The fiber interaction coefficient (Ci) is an empirical constant that characterizes the effect of fiber-fiber interaction in concentrated suspensions.

Fiber Orientation Model Parameters dialog

This dialog is used to enter specific values for the **Coefficient of interaction (Ci)** and **Reduced Strain Closure factor** settings that will be used in the calculation of fiber orientation.

To access this dialog, set the **Calculate fiber orientation using** option to **RSC model with specified Ci**, then click **Edit settings**.

NOTE: The default settings will be appropriate for most simulations. This dialog has been provided for specialist users conducting research into the fluid mechanics of fiber-filled materials.

Coefficient of interaction (Ci)	Specifies the coefficient of interaction (Ci) value that will be used in the calculation of fiber interactions.

Reduced Strain Closure factor	Specifies the Reduced Strain Closure factor, which is used to model slow fiber orientation dynamics.

User-supplied inlet orientation dialog

This dialog is used to specify values for the in-plane fiber orientation components in the flow direction and cross-flow direction vs. normalized thickness, which define the initial fiber orientation profile at the inlet to the cavity.

To access this dialog, set the **Fiber inlet condition** option to **User-supplied inlet orientation**, then click **Edit profile**.

NOTE: The default settings will be appropriate for most simulations. This dialog has been provided for specialist users conducting research into the fluid mechanics of fiber-filled materials.

Fiber orientation prediction theory

2

Fiber orientation prediction involves determining the spatial distribution of fibers, for each element and as a function of location through the part thickness.

While injection molded fiber-reinforced thermoplastics constitute a major commercial application of short fiber composite materials, the modeling of the process is more complex than in other applications as parts are usually thin and shorter fibers are often used. Other aspects such as the three-dimensional orientation of the fibers and the significant orientation variations across the part also contribute to the complexity of the problem.

During the filling of an injection molding die, three flow regions normally exist (*Figure 1: Flow regions during filling* on page 6). These regions are:

- A 3D region near the gate (Region A).
- A lubrication region (Region B), where no significant velocities out of the main flow plane exist and where the majority of the flow is contained.
- A fountain flow region at the flow front (Region C).

(1) Mold wall; (2) Frozen layer.

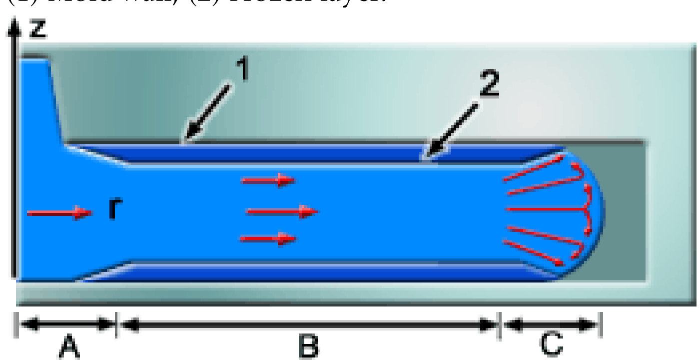


Figure 1: Flow regions during filling

Of the various mold filling simulations developed, most simplify the governing equations using the assumptions:

- Most moldings are thin.
- Flow is approximated to occur in the lubrication region.

During molding, the fiber orientation at a position is controlled by the fluid motion in two different ways:

- Flow-deduced orientation (a kinematic term).

- Flow-convected orientation (an advection term).

When modeling this, the accuracies of these separate terms depend on the accuracy of the determined velocity gradient and orientation gradient respectively.

The effect of flow behavior on fiber orientation is complex, but two rules of thumb have been demonstrated (*Figure 2: Effect of stretching flows on fiber alignment* on page 7):

- Shearing flows tend to align fibers in the direction of flow.
- Stretching flows tend to align fibers in the direction of stretching. For a center-gated disk, the stretching axis is perpendicular to the radial flow direction.

A = Entrance: Random fibers, **B** = Converging flow: Flow aligned fibers, **C** = Diverging flow: Transverse alignment

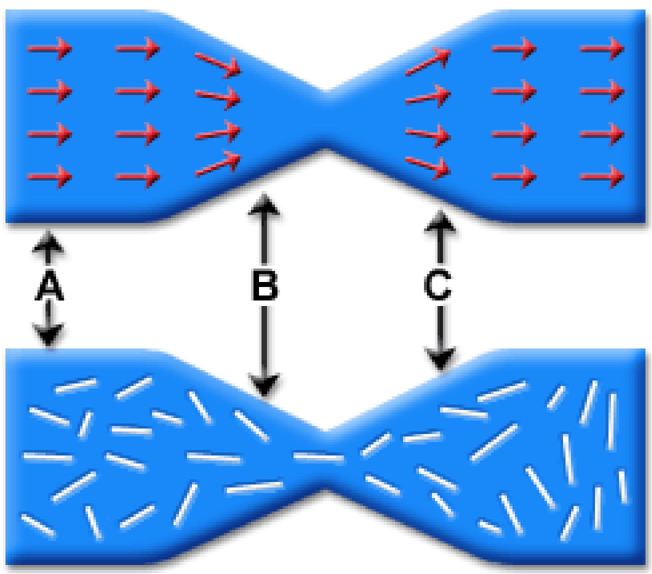


Figure 2: Effect of stretching flows on fiber alignment

It has been found that the orientation of fibers in injection molded composites is layered, with a core created by in-plane fiber motion during mold filling.

For a radial flow case (as in a center-gated disk), there is an in-plane stretching flow and the core layer contains fibers aligned in the stretching direction.

For a case where no stretching applies, as for a strip mold, the orientation set by the flow at the gate is simply convected down the flow length with little change, giving:

- Shell layers on either side of the core, with a flow aligned orientation caused by gapwise shearing.
- Skin layers at the mold surface:
  - when thick frozen layers form during filling.
  - orientation is set by the fountain flow, at a value between that of the core and shell layers.

The number, thickness and type of layers depending on the location in the part and the part geometry. In addition to the above, it is observed that:

- Processing conditions and material behavior do affect the orientation.
- The filling speed is the process parameter that most influences fiber orientation. Faster injection speeds cause thicker core layers and thinner skin layers.
- The fiber average aspect ratio and concentration also influence the fiber orientation. With increased fiber aspect ratio and concentration, the flow-aligned orientation in the shell layer increases.

There are three factors which must be considered by the analysis program for a fiber-filled material. They are:

- The general fluid dynamics of the molten polymer.
- The effects of the molten polymer on the fibers.
- The inter-fiber interactions.

The general fluid dynamics of the molten polymer is dealt with using Autodesk Moldflow's regular Fill+Pack analysis algorithm, but the effects of the molten polymer on the fibers and the interaction of the fibers requires the use of an equation of motion for rigid particles in a fluid suspension.

Theoretical basis for fiber orientation prediction

3

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:

- The hydrodynamic term.
- The interaction term.

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

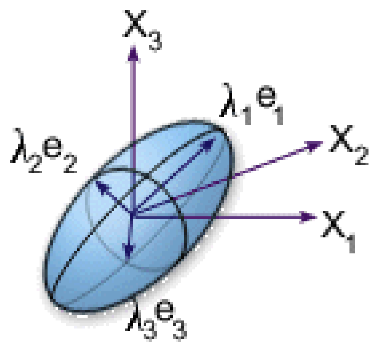
The interaction term has been proposed by Folgar and Tucker and is incorporated to model the randomizing effect of mechanical interactions between fibers. It has the form of a diffusion term with the frequency of interaction being proportional to the magnitude of the strain rate. The effect of the interaction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

Definition and prediction of fiber orientation

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 the grid point through which it passes. The midplane of the molding passes through grid point 1. An orientation solution is calculated at 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. 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 the figure below.

aij⊠=a1⊠a1⊠a1⊠a2⊠a2⊠a2⊠a3⊠a3⊠a3⊠⊠000⊠000⊠;e1e2e3



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 orientation distribution, since the gapwise orientation components eliminated by 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 the orientation tensor

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

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

Typically these axes apply:

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

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

- Tensor symmetry aij⊠=aj⊠ and
- A normalization condition a1⊠+a2⊠+a3⊠=1

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

- a1⊠, fiber orientation in the flow direction, varying from 0 to 1.0.
- a2⊠, fiber orientation transverse to flow, varying from 0 to 1.0.
- a1⊠, tilt of orientation in the 1-3 plane, varying from -0.5 to 0.5.

Note: The flow direction orientation term, a1⊠, contains most of the quantitative information about the microstructure and is most sensitive to flow, processing and material changes.

A fiber orientation model

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 the 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 (*L*/*d*), a fiber concentration by volume (*c*) (or volume fraction Vf) and having a uniform length distribution, a typical concentration classification scale is:

- Dilute c⊠/L2.
- Semi-concentrated $d/L2 < c < d/L$.
- Concentrated $c > d/L$.

For example, if *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 *L*/*d* is often 20 or more, so the values for the above concentrations are:

- Dilute, $c \ll 0.025$.
- 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% to 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. 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 CI), has been incorporated in the phenomenological model for fiber orientation proposed by Folgar and Tucker:

- 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 CI term determines the strength of the diffusion term.

Adding the rotary diffusion term to account for the 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:

∂aij∂t+vk∂aij∂xk=−12([illegible]

where:

- [illegible] equals 3 for 3D and 2 for planar (2D) orientation
- [illegible] is the velocity component
- 12[illegible] is the vorticity tensor, and 12[illegible] is the deformation rate tensor.
- [illegible] is a constant that depends on the geometry of the particle
- [illegible] is a unit tensor
- CI 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 ai[illegible]

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 error into the simulation results. So the closure approximation is the most challenging problem associated with this model. No value of CI 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 CI .

The effect of the closure approximation is to predict too much out-of-plane orientation. This result has been addressed by the fiber orientation model form proposed by Autodesk.

Prediction of composite mechanical properties

4

Fiber orientation is one of the major factors that determines the mechanical (elastic) strength as well as the stiffness of a molded part.

Theories have been developed to predict the mechanical properties of short fiber composites once the fiber orientation distribution in the parts is known.

To calculate the mechanical properties, all the theories follow a two step procedure:

1. The properties of a unidirectional short fiber reinforced material are estimated.
2. These properties are then averaged across the laminates according to the fiber orientation distribution density.

Thus, this methodology independently accounts for the influence of fiber length and fiber orientation.

The Tandon-Weng model serves as the basis for the calculation of the composite material's unidirectional mechanical properties. The Autodesk Moldflow Insight implementation also considers Tucker/Liang's treatment on the Poisson ratio calculation of the Tandon-Weng model.

The properties of the fiber and polymer required as inputs to the analysis are:

- Ef☒ (longitudinal modulus of fiber)
- Ef☒ (transverse modulus of fiber)
- ☒☒☒ (longitudinal Poisson's ratio of fiber)
- Gf☒☒ (longitudinal shear modulus of fiber)
- Ep☒ (longitudinal modulus of polymer)
- Ep☒ (transverse modulus of polymer)
- ☒☒☒ (longitudinal Poisson's ratio of polymer)
- Gp☒☒ (longitudinal shear modulus of polymer)
- lf (average fiber length)
- df (average fiber diameter)
- Vf (volume fraction of fibers)

The following basic mechanical properties are derived for each element in the composite material:

- E1☒ (longitudinal modulus)
- E2☒ (transverse modulus)
- G1☒ (in-plane shear modulus)
- G2☒ (out-of-plane shear modulus)
- ☒☒ (in-plane Poisson's ratio)

- □□ (out-of-of-plane Poisson's ratio)

Longitudinal and transverse moduli

The Tandon Weng model treats the short fiber reinforced composite as a special case of unidirectionally aligned spheroidal inclusions embedded in a finite elastic polymer matrix.

The longitudinal modulus of the uniaxially aligned system can be written as:

E1□=Ep□□□A+Vf□1+2p□□□A2

where A , A1 and A2 are parameters related to those in the Tandon Weng paper.

The transverse modulus of the uniaxially aligned system can be written as:

E2□=Ep□□□A2□A+Vf□2p□□□A3+1−p□□□A4+1+□□□□A5□A

where A , A3 , A4 and A5 are parameters related to those in the Tandon Weng paper.

Shear modulus and Poisson's ratio

The Halpin-Tsai procedures are applied when calculating the longitudinal and transverse shear moduli and Poisson's ratios for the composite material.

These constants can be written as:

G1□=Gp□□□+Vf□1−Vf□ G2□=Gp□□□+□Vf□1−Vf□

where:

□=Gf□□/Gp□□−1Gf□□/Gp□□+1 □=Gf□□/Gp□□−1Gf□□/Gp□□+□
□Kp/Gp□□Kp/Gp□□+2

where Kp is the bulk modulus of the polymer, defined as Kp=Ep□3−6p□□□

The in-plane Poisson's ratio is calculated from the rule of mixtures by:

□□=□□□□Vf+1−Vfp□□□

The out-of-plane Poisson's ratio of the composite is calculated as:

□□=□−4□□2−1□1

Moldflow's fiber orientation models

5

Moldflow's fiber orientation models are based on the Folgar-Tucker orientation equation.

The Folgar-Tucker orientation equation is used for fiber orientation calculations on 3D meshes. The governing equation is:

D⊠aijD⊠t=−12⊠⊠ik⊠akj−aik⊠⊠kj+12⊠⊠⊠ik⊠akj+aik⊠⊠kj−2⊠⊠aijkl⊠⊠kl+2⊠⊠CI⊠⊠⊠(⊠ij−3aij)

Note the following:

- aij is the fiber orientation tensor.
- 12⊠⊠j is the vorticity tensor, and 12⊠⊠j is the deformation rate tensor.
- CI is the fiber interaction coefficient, a scalar phenomenological parameter, the value of which is determined by fitting to experimental results. This term is added to the original Jeffery form to account for fiber-fiber interactions.

This fiber orientation model is further revised for calculations on Midplane and Dual Domain meshes. An extra term called a thickness moment of interaction coefficient (Dz) has been introduced into the model:

D⊠aijD⊠t=−12⊠⊠ik⊠akj−aik⊠⊠kj+12⊠⊠⊠ik⊠akj+aik⊠⊠kj−2aijkl⊠⊠kl⊠2⊠⊠CI⊠⊠j−2+DZaij

The following assumptions and considerations apply for this revised model:

- The Folgar-Tucker model gives acceptable accuracy for the prediction of fiber orientation in concentrated suspensions.
- Hybrid closure is used, as its form is simple and has good dynamic behavior.

Note the following:

- Setting CI = 0.0 sets the model back to the Jeffery form. CI⊠affects the orientation tensor. If CI⊠=0, fibers do not interact with each other; and if the value of CI⊠ becomes very large, fibers becomes less aligned.
- The magnitude of the Dz term sets the significance of the randomizing effect in the out-of-plane direction due to the fiber interaction.
- Setting Dz = 1.0 gives the Folgar-Tucker orientation model for the 3D problem. Setting Dz = 0.0 gives the Folgar-Tucker orientation model for the 2D problem.

However, for injection molding situations, the flow hydrodynamics cause the fibers to lie mainly in the flow plane. Their ability to rotate out-of-plane is severely limited. This mechanism predicts that the randomizing effect of fiber orientation is much smaller in the out-of-plane direction than in the in-plane direction, hence a small Dz value.

- Decreasing this Dz parameter:

- decreases the out-of-plane orientation.
- increases the thickness of the core layer.

- The simulation treats the problem as being symmetric about the midplane.

Empirical CI versus scaled-volume fraction expression

The experimental work of Bay suggests that the interaction model of Folgar and Tucker does apply to injection molding problems. However, how does one know which CI value to apply in fiber orientation modeling?

Experiments by Folgar and Tucker indicated that CI depends on the fiber volume fraction and aspect ratio, but the form of the dependence was unclear.

The flow in a film-gated strip is mainly simple shear. The shell layer (covering 40-90% to the walls from the midplane) should take on the steady-state value for simple shear. This situation would offer a ready way of examining this dependence.

Bay's shell layer orientation results show that the orientation a11 is very sensitive to fiber concentration, suggesting that an empirical relation for the interaction coefficient could be developed. Also, Bay's measurements support the proposal of making the fibers diffuse at a rate proportional to the strain rate.

From Bay's thesis, an expression was presented to provide an empirical relationship for the dependence of the interaction coefficient CI on some fiber details. The expression is a simple exponential a11 term. The data comes from the shell layers of injection molded strips of different materials (PC, PBT, PA66) at 6-7 glass levels for each material. The cases may all be considered concentrated suspensions.

Revised empirical CI expressions

Based on the shell layer orientation results, the applicability of the default CI value from the Bay expression across the range of glass contents has been reviewed.

At the Dz = 1.0 condition (Folgar-Tucker model form), the a11 orientation is over-predicted for all glass contents of both materials. The level of over-prediction reduces as the glass content increases. See the figure below.

A series of Fiber Fill+Pack analysis validation procedures were performed using both an end gated strip and a centrally gated disk. A more detailed consideration of the shell layer a11 orientation of the strip for two materials (PA66 and PBT) and at different glass levels was undertaken and the results compared with Bay's experimental orientation data. The orientation levels were typically 0.8.

Revised empirical expressions for CI versus the scaled volume fraction cL / d at Dz = 0.01 and 1.0 were derived, using the packing phase results.

A more complex procedure applies for intermediate Dz values.

The figure below shows the error in shell layer a11 orientation prediction for both materials at different glass levels for these cases:

- CI = 0 (the Jeffery model).
- Bay empirical expression for CI with Dz = 1.0 (the Folgar-Tucker model).

- For typical injection-molded parts (part thickness <; 2.5 mm), the revised CI model with a low Dz value, such as Dz = 0.01 as a default, as proposed in the past, is shown in the graph below.

  (a) Error; **(b)** % glass (weight); —— C1 = 0.0 (Jeffery Model); - - - Bay C1 (Dz=1.0); ······ Moldflow C1 Model (Dz= 0.01)

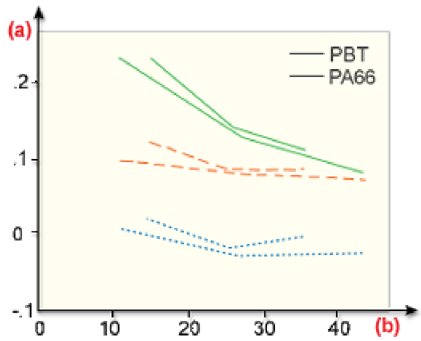


Figure 3: Revised CI model with a low Dz value

- For thick parts (thickness > 2.5 mm), the revised CI model with Dz = 1.0 is used. The value of Dz has been shown to increase monotonically with part thicknesses. This increasing trend is consistent with the expectation that out-of-plane fiber orientation would increase with increasing part thickness.

The following observations can be made:

- The Jeffery and Folgar-Tucker models tend to lead to an over-prediction in the orientation estimates.
- The low Dz model case results in substantially reduced error levels for thin parts (thickness < 2.5 mm).
- The default Bay model with low Dz value provides orientation estimates that lie within the confidence band of the Bay experimental data, for all but the high glass levels.
- The revised model offers a substantially improved orientation prediction over the other model cases, for both materials and across all glass levels considered.

Summary of CI – Dz combinations

The valid data range for the coefficient of interaction, CI, is 0-1.0; however, we have found that using values greater than 0.1 does not improve the predictions compared to experimental results.

The valid data range for the thickness moment of the interaction coefficient, Dz , is 0.0001-1.0.

The interaction coefficient and thickness moment combinations which are allowed with this software release are summarized in the following table:

Coefficient of Interaction, CI	Thickness Moment of the Interaction Coefficient, Dz	Comments
0	0.0001–1.0	■ Jeffery Model; dilute suspension ■ Dz ineffective ■ Also set for volume fraction or fiber length set to zero
0 < CI <= 0.1	1.0	Folgar-Tucker Model
default	Dz <= 1.0, (default = 1.0)	CI derived from empirical expression, according to scaled volume fraction (*cL* / *d*) using terms in mechanical properties and Dz ■ if *d* = 0 execution is aborted ■ if *cL* / *d* = 0, then CI = 0. ■ if 0 < *cL* / *d* < 1.0, then CI = 0.003 ■ if *cL* / *d* > 1, then CI is calculated empirically Basically insensitive where CI < 0.01
User Set (0–0.1)	Dz <= 1.0 (default = 1.0)	Other implementation allowed

Analysis scheme overview for fiber orientation

During the molding process, fiber orientation at a point is controlled by the fluid motion in two different manners: flow-deduced orientation (kinematic term) and flow-convected orientation (advection term).

For the kinematic term, the prediction accuracy depends upon the accuracy of the velocity gradient calculated.

For the advection term, its accuracy is dependent on the calculation of the orientation gradient. Like velocity, the representation of the orientation tensor is also coordinate system dependent. All numerical schemes suitable for the calculation of velocity gradients can be used to calculate the orientation gradient. In the fiber orientation software, the same element system is used to represent the velocity and orientation fields, consequently the same scheme is used to calculate the velocity and orientation gradients.

An outline of the overall fiber orientation scheme is now described. The fiber orientation prediction is coupled with the mold filling simulation.

First, the algorithm initializes for the filling and fiber orientation calculations.

The following loop is then repeated for the analysis until all elements are frozen:

- Determine time step ⊠flow for the Fill+Pack analysis.
- Advance the flow front.
- Calculate the pressure and velocity fields and the strain tensor.
- Calculate the stable time step ⊠adv for the advection term.
- Repeat time step until ∑⊠adv=⊠flow.
- For **each** grid point in **each** element:
  - calculate the advection fiber orientation term until ∑⊠kin=⊠adv.
  - calculate kinematic fiber orientation term.
  - calculate time step ⊠kin, for kinematic term.
  - calculate new fiber orientation during time step ⊠kin.
- Return to the beginning of the loop.

Reduced Strain Closure model

6

The Reduced Strain Closure (RSC) model is an option for calculating fiber orientation when performing a fiber orientation analysis.

The Folgar-Tucker orientation equation is the standard model used for fiber orientation calculations. The governing equation is:

D⊠aijD⊠t=−12⊠ik⊠kj−aik⊠kj+12⊠ik⊠kj+aik⊠kj−2⊠aijkl⊠kl+2⊠CI⊠⊠⊠ij−3aij)

Note the following:

- aij is the fiber orientation tensor.
- 12⊠ij is the vorticity tensor, and 12⊠ij is the deformation rate tensor.
- CI is the fiber interaction coefficient, a scalar phenomenological parameter, the value of which is determined by fitting to experimental results. This term is added to the original Jeffery form to account for fiber-fiber interactions.

However, recent experiments and references indicate that the Folgar-Tucker model over-estimates the change rate of the orientation tensor in concentrated suspensions. To capture the slow orientation dynamics and preserve the objectivity, the RSC model has been developed.[1] This model is based on the concept of reducing the growth rates of the eigenvalues of the orientation tensor by a scalar factor, while leaving the rotation rates of the eigenvectors unchanged. Thus the orientation equation is modified to:

D⊠aijD⊠t=−12⊠ik⊠kj−aik⊠kj+12⊠⊠ik⊠kj+aik⊠kj−2⊠aijkl+(1−⊠)(Lijkl−Mijmn⊠mnkl)]⊠kl+2⊠⊠⊠⊠ij−3aij)

The RSC model differs from the standard Folgar-Tucker model only in that:

1 The diffusion term is reduced by the scalar factor, ⊠

2 The closure term, ⊠ijkl, is replaced by [aijkl+(1−⊠)(Lijkl−Mijmn⊠mnkl)].

The fourth-order tensors, Lijkl and Mijkl, are defined as: Lijkl=Σp=13⊠p⊠eip⊠jp⊠kp⊠lp Mijkl=Σp=13⊠ip⊠jp⊠kp⊠lp

Here, ⊠p is the pth eigenvalue of the orientation tensor aij, and eip is the ith component of the pth eigenvector of the orientation tensor aij.

The scalar factor ⊠ is a phenomenological parameter, and ⊠1 to model the slow orientation dynamics. The smaller the scalar factor ⊠ the slower the orientation tensor develops with flow, and the thicker the orientation core layer becomes. When ⊠= 1, the RSC model is reduced to the original Folgar-Tucker model.

[1] A United States Patent is held on the RSC model by Delphi Technologies, Inc. (Tucker et al., 2007), and Autodesk holds an exclusive license for use of this model.

Reference

J. Wang, J.F. O'Gara, and C.L. Tucker III, An Objective Model for Slow Orientation Dynamics in Concentrated Fiber Suspensions: Theory and Rheological Evidence. *Journal of Rheology*, 52(5):1179-1200 (2008).

Anisotropic Rotary Diffusion model for long-fiber composites

7

The Anisotropic Rotary Diffusion (ARD) model is an option for calculating fiber orientation when performing a fiber orientation analysis using a long-fiber composite material.

Fibers longer than 1 mm are generally considered as long fibers. Usually, the fiber alignment in the flow direction is weaker in long-fiber materials than in short-fiber materials in injection-molded parts. The isotropic diffusion used in the Folgar-Tucker and Reduced Strain Closure models is unable to capture the behavior of fiber-fiber interactions in long-fiber materials and cannot accurately predict all fiber orientation components simultaneously.

The isotropic diffusion was replaced with the anisotropic rotary diffusion (ARD), which is defined on the surface of the unit sphere traced by all orientations of the unit vector, developed by Phelps and Tucker:

DaijDt=−12(akj−aik)+12(kj+aik)j−2ijklkl+[2cij−2ckkaij−5(cikakj+aikckj)+10cklaijkl]

Here, the rotary diffusion tensor cij is assumed as a quadratic function of j and aij and is defined as:

cij=b1j+b2aij+b3aikakj+b4ij+b5kkj2

where each bj is a scalar constant, and its values are determined by matching experimental steady-state orientation and requiring stable orientation. Setting b1=CI and bj=0(j=2, ...,5) reduces the ARD model to the Folgar-Tucker model.

The RSC version of the ARD model (ARD-RSC model) is also developed as:

[illegible]

Reference

Phelps, J. and C. L. Tucker III, An Anisotropic Rotary Diffusion Model for Fiber Orientation in Short- and Long-Fiber Thermoplastics. *Journal of Non-Newtonian Fluid Mechanics* 156(3): 165–176 (2009).

Fiber orientation prediction theory references

8

The models used in fiber orientation prediction have three major groupings: micro-mechanics models, thermal expansion coefficient models, and fiber closure approximation models. Additional general research is also considered.

Micro-mechanics models

Micro-mechanics models are the set of models used to predict the elastic properties of short-fiber reinforced composites from the knowledge of the matrix and the fiber elastic properties, fiber content, and fiber aspect ratio.

Model	Reference
Halpin-Tsai	J.C. Halpin and J.L. Kardos, The Halpin-Tsai Equations: A review, *Polym. Eng. Sci.*, 16(5), 345-352 (1976).
Tandon-Weng	G.P. Tandon and G.J. Weng, The Effect of Aspect Ratio of Inclusions on the Elastic properties of Unidirectionally Aligned Composites, *Polym. Compos.*, 5(4), 327-333 (1984).
Krenchel	H. Krenchel, *Fiber Reinforcement*. Stockholm, Akademisk Vorlag, 1964.
Cox	H.L. Cox, The Elasticity and Strength of Paper and Other Fibrous Materials, *British J. Appl. Phys.*, 3, 72-79 (1952).
Mori-Tanaka	Tucker, C. L. and Liang, E., Stiffness predictions for unidirectional short fiber composites: review and evaluation. *Compos. Sci. Technol.*, 59, 655-71 (1999)
Ogorkiewicz-Weidmann-Counto	R.M. Ogorkiewicz and G.W. Weidmann, Tensile Stiffness of a Thermoplastic Reinforced with Glass Fibers or Spheres, *J. Mech. Sci.*, 16, 10 (1974). V.J. Counto, The Effect of the Elastic Modulus of the Aggregate on the Elastic Modulus Creep and Creep Recovery of Concrete, *Mag. Concrete Res.*, 16, 129 (1964).

Thermal expansion coefficient models

Thermal expansion coefficient models are the set of models for predicting the longitudinal and transverse coefficients of thermal expansion of unidirectional fiber reinforced composites from the knowledge of the matrix and the fiber thermal expansion coefficients, fiber content and fiber aspect ratio.

Model	Reference
Schapery	R.A. Schapery, Thermal Expansion Coefficients of Composite materials Based on Energy Principles, *J. Compos. Mater.*, 2 (3), 380-404 (1968).
Chamberlain	D.E. Bowles and S.S. Tompkins, Prediction of Coefficients of Thermal Expansion for Unidirectional Composites, *J. Comps. Mater.*, 23, 370-388 (1989).
Rosen-Hashin	B.W. Rosen and Z. Hashin, Effective Thermal Expansion Coefficients and Specific Heat of Composite Materials, *Int. J. Eng. Sci.*, 8, 157-173 (1970).

Fiber closure approximation models

Closure approximation is a formula that approximates the fourth-order orientation tensor in terms of a second-order tensor. A variety of different forms of closure approximations have been proposed.

Model	Reference
Hybrid	S.G. Advani and C.L. Tucker, The Use of Tensors to Describe and Predict Fiber Orientation in Short Fiber Composites, *J. Rheol.*, 31, 751-784 (1987).
Orthotropic 1	Moldflow Bi-linear model based on J.S. Cintra and C.L. Tucker, Orthotropic Closure Approximations for Flow-induced Fiber Orientation, *J. Rheol.*, 39, 1095-1122 (1995).
Orthotropic 2	ORF (orthotropic fitted), see J.S. Cintra and C.L. Tucker, Orthotropic Closure Approximations for Flow-induced Fiber Orientation, *J. Rheol.*, 39, 1095-1122 (1995).
Orthotropic 3	Moldflow Bi-quadratic model based on J.S. Cintra and C.L. Tucker, Orthotropic Closure Approximations for Flow-induced Fiber Orientation, *J. Rheol.*, 39, 1095-1122 (1995).
Orthotropic 4	ORL (orthotropic, fitted for low Ci), see J.S. Cintra and C.L. Tucker, Orthotropic Closure

Model	Reference
	Approximations for Flow-induced Fiber Orientation, *J. Rheol.*, 39, 1095-1122 (1995).

General

Jeffery, G.B., The Motion of Ellipsoidal Particles Immersed in Viscous Fluid, *Proc. Roy. Soc.*, A102, p.161 (1922).

J.C. Halpin and J.L. Kardos, The Halpin-Tsai Equations: A review, *Polym. Eng. Sci.*, 16(5), 345-352 (1976).

Folgar, F.P. and C.L. Tucker, Orientation Behavior of Fibers in Concentrated Suspensions, *J. Reinf. Plas. Compos.*, 3, p.98 (1984).

Dinh, S.M. and Armstrong, R.C., A Rheological Equation of State for Semi-Concentrated Fiber Suspensions. *J. Rheol.*, 28, p207 (1984).

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J. Wang, J.F. O'Gara, and C.L. Tucker III, An Objective Model for Slow Orientation Dynamics in Concentrated Fiber Suspensions: Theory and Rheological Evidence. *Journal of Rheology*, 52(5):1179-1200 (2008).

Phelps, J. and C. L. Tucker III, An Anisotropic Rotary Diffusion Model for Fiber Orientation in Short- and Long-Fiber Thermoplastics. *Journal of Non-Newtonian Fluid Mechanics* 156(3): 165–176 (2009).