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Numerical Treatment of Finite Rotation for a Cylindrical Particle

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A problem for a rotation of a rigid cylindrical body in a medium is analyzed based on the laws of dynamics. The resistance moment is taken into account. For the numerical solution equations governing the rotary motion are formulated in terms of the right angular velocity and the rotation vector. The equations are solved numerically applying the Runge-Kutta method. The results illustrate the time variation of the unit vector spanned on the longitudinal axis of the body. By neglecting the moment of viscous friction the numerical results agree well with the classical analytical solution.

1 Introduction

During the last years many industries have more and more been interested in construction materials, that are, compared with metals or ceramics, lightweight and easy to process. Such materials are, for example, fiber reinforced thermoplastics (fiber length about 0.1 - 1 mm, fiber diameter about 0.01 mm, fiber volume fraction 15 - 40 %). They have, compared with pure polymeric materials, improved mechanical properties. Load transmitting, thin-walled structures can, like components made of pure polymers, be manufactured by injection molding, see Michaeli (1999). Because of highly automated production, short cycle time and low production costs this manufacturing process is of particular interest.
During the filling stage of the injection molding process a microstructure of preferred fiber orientation forms, that is dominated by the flow. It leads to an anisotropy of the mechanical properties (Yasuda et al. (2002)). In order to be able to predict the structural behavior (such as stiffness, strength, shrinkage, warpage) of an injection molded component, it is necessary to know the fiber orientation at every point (VerWeyst et al. (1999)). It is known from experiments that it is usually not constant (Bay and Tucker (1992) and Whiteside et al. (2000)), but it is influenced by various factors like the processing conditions or the geometry of the mold cavity.
During the design of a construction component it is important to predict its strength and stiffness. Therefore one needs a simulation software with which it is possible to demonstrate the formation of the fiber orientation during the filling stage. Thus the characterization of the flow as well as of the developing microstructure and the resulting anisotropy is of special interest for the design of components.
This paper deals with the rotational motion of one single particle that is surrounded by a medium. The numerical treatment of a finite rotation is nontrivial and numerous contributions have been made in the framework of continuum mechanics (e. g. Menzel et al. (2004)). The determination of the rotation of one particle is the first step in the creation of a model to simulate the formation of the fiber orientation during the injection molding process. In order to develop such a model for a suspension a field problem has to be solved (see e. g. Altenbach et al. (2003)).
The scope of this paper therefore is to formulate and discuss the governing equations describing the motion of a single cylindrical particle under the consideration of the resistance and the friction moment. In addition, we discuss an efficient algorithm of this problem and compare our results with the classical solutions.

2 Basic Equations

The object of this paper is to present a solution technique with which one can determine the orientation of a single particle that is suspended in a viscous fluid. The particle is regarded as a rigid body. The actual position of each point of a body, in relation to a frame of reference, is specified with the help of its position vector. In Figure 1 $\boldsymbol{r}_Q$ and $\boldsymbol{r}$ are the position vectors of the reference point Q and of a point P in the initial position (time t_0) and $\boldsymbol{R}_Q(t)$ and $\boldsymbol{R}(t)$ are the time-dependent position vectors of the actual time ($t > t_0$).
Each material point has three degrees of freedom. For the motion of a rigid body six degrees of freedom must be considered (see e. g. Gummert and Reckling (1994)). The basic equation with which the motion may be described is the fundamental theorem of the kinematics of rigid bodies, that takes the form

$$\boldsymbol{R}(t) = \boldsymbol{R}_Q(t) + \boldsymbol{P}(t) \cdot (\boldsymbol{r} - \boldsymbol{r}_Q) \tag{1}$$

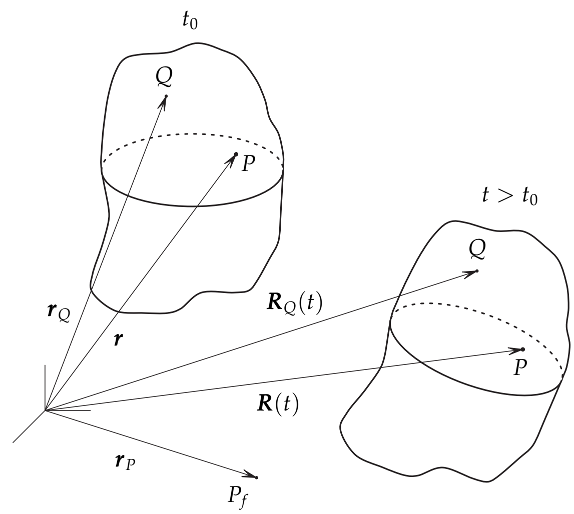

Figure 1. Reference and Actual Position of the Points of a Rigid Body

with $\boldsymbol{P}(t)$ being the rotation tensor. In order to create a particle model the balance equations of the momentum $\boldsymbol{K}_1$ and of the angular momentum $\boldsymbol{K}_2$ have to be set up:

$$\frac{d}{dt}\boldsymbol{K}_1 = \boldsymbol{F}, \qquad \frac{d}{dt}\boldsymbol{K}_2 = \boldsymbol{M}. \tag{2}$$

The momentum and the angular momentum follow from the equation of the kinetic energy K of a body that is known from the Eulerian mechanics

$$K = m\left(\frac{1}{2}\boldsymbol{v}\cdot\boldsymbol{v} + \boldsymbol{v}\cdot\boldsymbol{B}\cdot\boldsymbol{\omega} + \frac{1}{2}\boldsymbol{\omega}\cdot\boldsymbol{C}\cdot\boldsymbol{\omega}\right). \tag{3}$$

In equation (3) $\boldsymbol{B}$ and $\boldsymbol{C}$ are tensors of inertia, m the mass of the body, $\boldsymbol{v}$ its translatory and $\boldsymbol{\omega}$ its angular velocity. Momentum and angular momentum are defined as follows

$$\boldsymbol{K}_1 = \frac{\partial K}{\partial \boldsymbol{v}}, \qquad \boldsymbol{K}_2 = [\boldsymbol{R}(t) - \boldsymbol{r}_P] \times \frac{\partial K}{\partial \boldsymbol{v}} + \frac{\partial K}{\partial \boldsymbol{\omega}} \tag{4}$$

with $\boldsymbol{r}_P$ being the position vector of a fixed point P_f in the reference frame, see Figure 1. From the first equation of (4) and equation (3)

$$\boldsymbol{K}_1 = m(\boldsymbol{v} + \boldsymbol{\omega}\cdot\boldsymbol{B}) \tag{5}$$

can be derived. Concerning tensor $\boldsymbol{B}$ the following equation is valid:

$$\boldsymbol{B}(t) = \boldsymbol{P}(t)\cdot\boldsymbol{B}_0\cdot\boldsymbol{P}^T(t), \qquad \boldsymbol{B}_0 = m(\boldsymbol{r}_S - \boldsymbol{r}_Q)\times\boldsymbol{E}. \tag{6}$$

$\boldsymbol{E}$ is the second rank unit tensor and $\boldsymbol{r}_S$ is the position vector of the center of mass. If the reference point is located in the center of mass (i. e. $\boldsymbol{r}_S = \boldsymbol{r}_Q$), $\boldsymbol{B}$ becomes the zero tensor $\boldsymbol{0}$ and the momentum is

$$\boldsymbol{K}_1 = m\boldsymbol{v}. \tag{7}$$

From the second equation of (4) one obtains the following equation for the angular momentum:

$$\boldsymbol{K}_2 = (\boldsymbol{R}_Q - \boldsymbol{r}_P)\times\boldsymbol{K}_1 + \boldsymbol{B}\cdot\boldsymbol{v} + \boldsymbol{C}\cdot\boldsymbol{\omega} \tag{8}$$

and, accordingly with $\boldsymbol{B} = \boldsymbol{0}$,

$$\boldsymbol{K}_2 = (\boldsymbol{R}_Q - \boldsymbol{r}_P)\times\boldsymbol{K}_1 + \boldsymbol{C}\cdot\boldsymbol{\omega}. \tag{9}$$

If the translatory velocity is equal to zero ($\boldsymbol{v} = \boldsymbol{0}$), the momentum is also zero ($\boldsymbol{K}_1 = \boldsymbol{0}$) and the angular momentum is reduced to

$$\boldsymbol{K}_2 = \boldsymbol{C} \cdot \boldsymbol{\omega}. \tag{10}$$

The tensor $\boldsymbol{C}$ is time dependent

$$\boldsymbol{C}(t) = \boldsymbol{P}(t) \cdot \boldsymbol{C}_0 \cdot \boldsymbol{P}^T(t) \tag{11}$$

and $\boldsymbol{C}_0$ is the reference tensor of inertia. In order to calculate $\boldsymbol{C}_0$ consider a rigid body occupying a volume V. The moment of momentum for the body is calculated as follows:

$$\boldsymbol{K}_2 = \int\limits_V \varrho \left[\boldsymbol{R}(t) - \boldsymbol{r}_P\right] \times \boldsymbol{v}\, dV, \tag{12}$$

where ϱ is the mass density of the body. Using Euler's formula (Hamel (1949)) for the velocity distribution in a rigid body

$$\boldsymbol{v}(t) = \boldsymbol{v}_Q(t) + \boldsymbol{\omega}(t) \times \left[\boldsymbol{R}(t) - \boldsymbol{R}_Q(t)\right] = \boldsymbol{v}_Q(t) + \boldsymbol{\omega}(t) \times \boldsymbol{P}(t) \cdot (\boldsymbol{r} - \boldsymbol{r}_Q) \tag{13}$$

as well as equations (11) and (12) one can obtain

$$\boldsymbol{C}(t) = \boldsymbol{P}(t) \cdot \left\{ \varrho \int\limits_V \left[(\boldsymbol{r} - \boldsymbol{r}_Q)^2 \boldsymbol{E} - (\boldsymbol{r} - \boldsymbol{r}_Q) \otimes (\boldsymbol{r} - \boldsymbol{r}_Q) \right] dV \right\} \cdot \boldsymbol{P}^T(t). \tag{14}$$

By comparing equation (11) with equation (14) the tensor $\boldsymbol{C}_0$ in equation (11) can be determined as

$$\boldsymbol{C}_0 = \varrho \int\limits_V \left[(\boldsymbol{r} - \boldsymbol{r}_Q)^2 \boldsymbol{E} - (\boldsymbol{r} - \boldsymbol{r}_Q) \otimes (\boldsymbol{r} - \boldsymbol{r}_Q) \right] dV. \tag{15}$$

The reference point Q of the particle can arbitrarily be chosen without loss of generality. The simplest case is that the reference point is selected in the center of mass. The origin of the co-ordinate system is also placed in this point, i. e. $\boldsymbol{r}_Q = \boldsymbol{0}$. With these assumptions equation (15) is reduced to

$$\boldsymbol{C}_0 = \varrho \int\limits_V \left(r^2 \boldsymbol{E} - \boldsymbol{r} \otimes \boldsymbol{r} \right) dV, \qquad r^2 = \boldsymbol{r} \cdot \boldsymbol{r}. \tag{16}$$

In what follows we consider a cylindrical body with the radius R and the height H. In this case tensor $\boldsymbol{C}_0$ is transversally isotropic and takes the form

$$\begin{aligned} \boldsymbol{C}_0 &= \lambda\, \boldsymbol{m}_0 \otimes \boldsymbol{m}_0 + \mu (\boldsymbol{E} - \boldsymbol{m}_0 \otimes \boldsymbol{m}_0), \\ \lambda &= \varrho \frac{\pi}{2} R^4 H, \qquad \mu = \varrho \frac{\pi}{12} \left(3R^4 H + R^2 H^3 \right) \end{aligned} \tag{17}$$

where λ and μ are the moments of inertia. Considering $V = \pi R^2 H$ and $\varrho = mV$ one gets

$$\lambda = \frac{m}{2} R^2, \qquad \mu = \frac{m}{12} \left(3R^2 + H^2 \right). \tag{18}$$

3 Frictionless Motion of a Rigid Body. Classical Solution

Zhilin gives in Zhilin (2001) the classical analytical solution of the equation of motion of a rigid body in the gravitational field. In the following the main results are briefly discussed. Its tensor of inertia $\boldsymbol{C}_0$ is transversally isotropic and in the reference position (i. e. at the time $t = 0$) given by

$$\boldsymbol{C}_0 = \lambda\, \boldsymbol{m}_0 \otimes \boldsymbol{m}_0 + \mu (\boldsymbol{E} - \boldsymbol{m}_0 \otimes \boldsymbol{m}_0), \tag{19}$$

where $\boldsymbol{m}_0$ is the unit vector of the longitudinal axis of the body in its initial position. It is assumed that friction between the body and its surrounding does not exist. The momentum $\boldsymbol{K}_1$ and the angular momentum $\boldsymbol{K}_2$ of the body take the form

$$\boldsymbol{K}_1 = m\,\dot{\boldsymbol{R}}_m(t), \qquad \boldsymbol{K}_2 = \boldsymbol{R}_m(t) \times m\,\dot{\boldsymbol{R}}_m(t) + \boldsymbol{L}, \qquad \boldsymbol{L} = \boldsymbol{P}(t) \cdot \boldsymbol{C}_0 \cdot \boldsymbol{P}^T(t) \cdot \boldsymbol{\omega}(t) \tag{20}$$

with $\dot{\boldsymbol{R}}_m \equiv \frac{d}{dt}\boldsymbol{R}_m$, $\boldsymbol{R}_m$ being the time dependent position vector of the center of mass. For the given angular velocity the rotation tensor can be determined from the Poisson equation

$$\dot{\boldsymbol{P}} = \boldsymbol{\omega} \times \boldsymbol{P}. \tag{21}$$

The first and the second law of dynamics are presented in the following. The momentum balance equation is given by

$$\frac{d}{dt}\left(m\,\dot{\boldsymbol{R}}_m\right) = -\,G\,\frac{Mm}{R^3}\,\boldsymbol{R}_m, \tag{22}$$

where G is the universal gravitational constant ($G = 6,67259 \cdot 10^{-11}\,m^3 \cdot kg^{-1} \cdot s^{-2}$). Equation (22) has four integrals (one scalar and one vectorial). The scalar integral represents the conservation of energy of the translatory motion. It is obtained by the scalar product of both sides of equation (22) with vector $\dot{\boldsymbol{R}}_m$ as follows

$$\frac{d}{dt}\left[\frac{m}{2}\,\dot{\boldsymbol{R}}_m \cdot \dot{\boldsymbol{R}}_m\right] = \frac{d}{dt}\left[G\,\frac{Mm}{R}\right] \qquad \Rightarrow \frac{1}{2}\,m\,\dot{\boldsymbol{R}}_m \cdot \dot{\boldsymbol{R}}_m - G\,\frac{Mm}{R} = \varepsilon_T = \text{const.} \tag{23}$$

In equation (23) ε_T is the energy of the translatory motion of the body. The vectorial integral represents the conservation of the moment of momentum. It is obtained by the vector product of both sides of equation (22) with vector $\boldsymbol{R}_m$ as follows:

$$m\,\boldsymbol{R}_m \times \ddot{\boldsymbol{R}}_m = -G\,\frac{Mm}{R^3}\,\boldsymbol{R}_m \times \boldsymbol{R}_m = \boldsymbol{0} \tag{24}$$

$$\boldsymbol{R}_m \times m\,\dot{\boldsymbol{R}}_m = \boldsymbol{H} = \text{const} \qquad \Rightarrow \qquad \boldsymbol{R}_m \cdot \boldsymbol{H} = 0. \tag{25}$$

With the help of the balance equation for the angular momentum

$$\frac{d}{dt}\left[\boldsymbol{R}_m(t) \times m\,\dot{\boldsymbol{R}}_m(t) + \boldsymbol{P}(t) \cdot \boldsymbol{C}_0 \cdot \boldsymbol{P}^T(t) \cdot \boldsymbol{\omega}(t)\right] = \boldsymbol{0} \tag{26}$$

and equation (25) the following expression can be obtained:

$$\boldsymbol{P}(t) \cdot \boldsymbol{C}_0 \cdot \boldsymbol{P}^T(t) \cdot \boldsymbol{\omega}(t) = \boldsymbol{L} = \text{const.} \tag{27}$$

Rearranging equation (27) yields

$$\boldsymbol{\omega}(t) = \boldsymbol{P}(t) \cdot \boldsymbol{C}_0^{-1} \cdot \boldsymbol{P}^T(t) \cdot \boldsymbol{L}. \tag{28}$$

Equation (28) must be solved together with the Poisson equation (21) in order to find the rotation tensor. The initial conditions for the rotation tensor $\boldsymbol{P}$ and the angular velocity $\boldsymbol{\omega}$ must be given, for example, in the following form:

$$\boldsymbol{P}(0) = \boldsymbol{E}, \qquad \boldsymbol{\omega}(0) = \boldsymbol{\omega}_0 \qquad \Rightarrow \qquad \boldsymbol{L} = \boldsymbol{C}_0 \cdot \boldsymbol{\omega}_0. \tag{29}$$

The energy of the rotary motion ε_R is calculated by

$$\varepsilon_R = \frac{1}{2}\,\boldsymbol{\omega}(t) \cdot \boldsymbol{P}(t) \cdot \boldsymbol{C}_0 \cdot \boldsymbol{P}^T(t) \cdot \boldsymbol{\omega}(t) = \frac{1}{2}\,\boldsymbol{L} \cdot \boldsymbol{\omega}(t) = \frac{1}{2}\,\boldsymbol{L} \cdot \boldsymbol{P}(t) \cdot \boldsymbol{C}_0^{-1} \cdot \boldsymbol{P}^T(t) \cdot \boldsymbol{L}. \tag{30}$$

By differentiating equation (30) with respect to time and considering equations (28) and (21) one can show that the energy of the rotary motion is conserved.

The rotation tensor may be specified by the Euler theorem (e. g. Zhilin (1996))

$$\boldsymbol{Q}[\psi(t)\boldsymbol{n}(t)] \equiv [1-\cos\psi(t)]\,\boldsymbol{n}(t)\otimes\boldsymbol{n}(t)+\cos\psi(t)\boldsymbol{E}+\sin\psi(t)\boldsymbol{n}(t)\times\boldsymbol{E}, \tag{31}$$

where the unit vector $\boldsymbol{n}$ stands for the rotation axis and $-\pi < \psi < \pi$ for the angle of rotation. The rotation tensor contains nine components, but only three of them are independent (Gummert and Reckling (1994)). In equation (31) the independent quantities are two components of the vector $\boldsymbol{n}$ and the angle ψ.
Each rotation can be expressed as a composition of rotations of the type (31) (Zhilin (2001)). In the case of the free rotation of a transversely isotropic body we have

$$\boldsymbol{P}(t) = \boldsymbol{Q}\left[\psi(t)\boldsymbol{n}\right]\cdot\boldsymbol{Q}\left[\varphi(t)\boldsymbol{m}_0\right], \qquad \boldsymbol{n} \equiv \frac{\boldsymbol{L}}{|\boldsymbol{L}|} = \text{const}, \tag{32}$$

where φ is the angle of the own rotation around the axis of isotropy of the body and ψ is called the angle of precession around the constant vector $\boldsymbol{L}$. Inserting equation (32) into equation (30) yields

$$\begin{aligned} \varepsilon_R &= \frac{1}{2}\boldsymbol{L}\cdot\boldsymbol{\omega}(t) = \frac{1}{2}\boldsymbol{L}\cdot\boldsymbol{Q}(\psi\boldsymbol{n})\cdot\boldsymbol{Q}(\varphi\boldsymbol{m}_0)\cdot\boldsymbol{C}_0^{-1}\cdot\boldsymbol{Q}^T(\varphi\boldsymbol{m}_0)\cdot\boldsymbol{Q}^T(\psi\boldsymbol{n})\cdot\boldsymbol{L} \\ &= \frac{1}{2}\boldsymbol{L}\cdot\boldsymbol{C}_0^{-1}\cdot\boldsymbol{L} = \text{const.} \end{aligned} \tag{33}$$

The angular velocity is calculated by

$$\boldsymbol{\omega} = \dot{\psi}\boldsymbol{n} + \dot{\varphi}\,\boldsymbol{Q}(\psi\boldsymbol{n})\cdot\boldsymbol{m}_0. \tag{34}$$

Taking into consideration the equality

$$\boldsymbol{n}\cdot\boldsymbol{Q}(\psi\boldsymbol{n}) = \boldsymbol{n} \tag{35}$$

the angular velocity takes the form

$$\boldsymbol{\omega} = \boldsymbol{Q}(\psi\boldsymbol{n})\cdot\left(\dot{\psi}\boldsymbol{n}+\dot{\varphi}\boldsymbol{m}_0\right). \tag{36}$$

Inserting equations (32) and (36) into equation (28) and calculating the left dot product of the resulting equation with $\boldsymbol{Q}^T(\psi\boldsymbol{n})$ yields the following expression

$$\dot{\psi}\boldsymbol{L} + L\dot{\varphi}\boldsymbol{m}_0 = L\boldsymbol{C}_0^{-1}\cdot\boldsymbol{L} = L\boldsymbol{\omega}_0, \qquad L = \sqrt{\mu^2\omega_0^2+(\lambda^2-\mu^2)(\boldsymbol{m}_0\cdot\boldsymbol{\omega})^2} \tag{37}$$

with L being the magnitude of the vector $\boldsymbol{L}$. The solution of equation (37) is given by

$$\psi = \frac{tL}{\mu}, \qquad \varphi = \frac{t(\mu-\lambda)}{\mu}(\boldsymbol{m}_0\cdot\boldsymbol{\omega}_0) = \frac{t(\mu-\lambda)}{\lambda\mu}(\boldsymbol{m}_0\cdot\boldsymbol{L}). \tag{38}$$

4 Moment of Friction

In order to describe the motion of the particle, the particle-medium-interaction must be known. We make the following assumptions: (1) The particle under consideration is moment-free supported in its center of mass. From this assumption follows that the interaction between the particle and the medium is described by a moment. (2) Brenner supposes in (Brenner (1964)) that the medium is undisturbed in a large distance from the particle. The hydrodynamic moment, exerted on the particle in a viscous fluid, can, according to Brenner, be presented as follows:

$$\boldsymbol{M} = -\left[\boldsymbol{G}\cdot(\boldsymbol{\omega}-\boldsymbol{\phi}) + {}^{(3)}\boldsymbol{C}\cdot\cdot\boldsymbol{D}\right], \quad \boldsymbol{\phi} = \frac{1}{2}\nabla\times\boldsymbol{v}, \quad \boldsymbol{D} = \frac{1}{2}\left(\nabla\boldsymbol{v}+(\nabla\boldsymbol{v})^T\right), \tag{39}$$

where $\boldsymbol{v}$ is the velocity of the undisturbed flow, $\boldsymbol{G}$ and ${}^{(3)}\boldsymbol{C}$ are the second and third rank resistance tensors that depend on the viscous properties of the fluid and the geometry of the particle. We limit our considerations to the case that the undisturbed flow is at rest. Disturbances, that are caused by the particle itself, will here not be discussed. From that follows, that in equation (39) $\boldsymbol{D} = \boldsymbol{0}$ and $\boldsymbol{\phi} = \boldsymbol{0}$, and therefore that the moment is a linear function of the angular velocity $\boldsymbol{\omega}$ taking the form

$$\boldsymbol{M}(t) = -\boldsymbol{P}(t) \cdot \boldsymbol{G}_0 \cdot \boldsymbol{P}^T(t) \cdot \boldsymbol{\omega}(t). \tag{40}$$

We call $\boldsymbol{M}$ resistance moment and $\boldsymbol{G}_0$ resistance tensor. Since the particle is assumed to be a cylinder with transverse isotropy, the resistance tensor can be presented as follows:

$$\boldsymbol{G}_0 = \alpha\, \boldsymbol{m}_0 \otimes \boldsymbol{m}_0 + \beta\, (\boldsymbol{E} - \boldsymbol{m}_0 \otimes \boldsymbol{m}_0) \tag{41}$$

with $\boldsymbol{m}_0$ being the unit vector of the symmetry axis of the particle. The constants α and β describe the influence of the surrounding medium on the particle rotation. They depend on the geometry and the surface properties of the particle and on the fluid.

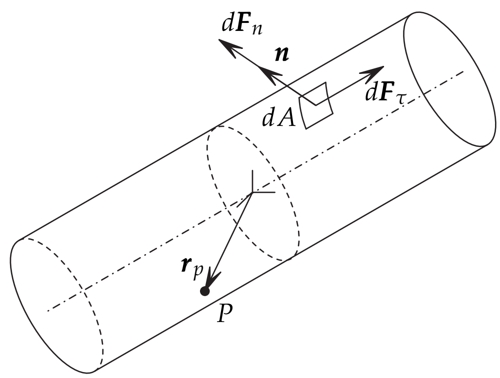

Figure 2. Cylindrical Particle

In Figure 2 a cylindrical particle is presented. In this figure dA is a differential element on the surface. Let $\boldsymbol{n}$ be the outer normal unit vector of the surface. We assume that the resultant force exerted on dA can be presented as follows:

$$d\boldsymbol{F} = \boldsymbol{f}\, dA, \tag{42}$$

where $\boldsymbol{f}$ is the force intensity. The interaction force consists of a tangential and a normal part

$$d\boldsymbol{F}_\tau = \boldsymbol{f}_\tau\, dA, \qquad d\boldsymbol{F}_n = \boldsymbol{f}_n\, dA. \tag{43}$$

The resistance moment can then be calculated by means of

$$\boldsymbol{M} = \int_A \boldsymbol{r}_p \times (\boldsymbol{f}_\tau + \boldsymbol{f}_n)\, dA. \tag{44}$$

The translatory velocity of a point P may in analogous manner be divided into a normal and a tangential part:

$$\boldsymbol{v}_p = \boldsymbol{v}_n + \boldsymbol{v}_\tau = \boldsymbol{v}_p \cdot \boldsymbol{n} \otimes \boldsymbol{n} + \boldsymbol{v}_p \cdot (\boldsymbol{E} - \boldsymbol{n} \otimes \boldsymbol{n})\,. \tag{45}$$

For the intensities $\boldsymbol{f}_\tau$ and $\boldsymbol{f}_n$ we assume a linear dependence on the velocities, i. e.

$$\boldsymbol{f}_\tau = -\zeta \boldsymbol{v}_\tau = -\zeta \boldsymbol{v}_p \cdot (\boldsymbol{E} - \boldsymbol{n} \otimes \boldsymbol{n}), \qquad \boldsymbol{f}_n = \begin{cases} -\xi\, \boldsymbol{v}_p \cdot \boldsymbol{n} \otimes \boldsymbol{n} & , \quad \boldsymbol{v}_p \cdot \boldsymbol{n} > 0 \\ \boldsymbol{0} & , \quad \boldsymbol{v}_p \cdot \boldsymbol{n} \leq 0 \end{cases}. \tag{46}$$

ζ and ξ are the coefficient of friction and resistance, respectively. The resistance force does not act on the whole surface, but only on a part of it. In order to calculate the partial area on which the resistance force acts, the inequality $\boldsymbol{v}_p \cdot \boldsymbol{n} > 0$ must be solved. With the angular velocity $\boldsymbol{\omega}$ the velocity $\boldsymbol{v}_p$ may be specified as

$$\boldsymbol{v}_p(\boldsymbol{r}_p) = \boldsymbol{\omega} \times \boldsymbol{r}_p. \tag{47}$$

Using cylindrical coordinates r, φ, z, every point on the surface is described by the position vector

$$\boldsymbol{r}_p(z, \varphi) = r\boldsymbol{e}_r + z\boldsymbol{m}_0, \tag{48}$$

where $\boldsymbol{m}_0$ is the unit vector of the longitudinal axis of the cylinder in the initial configuration. The unit normal vector $\boldsymbol{n}$ and the position vector $\boldsymbol{r}_p$ are different for the lateral and the upper (lower) top surface. In the case of the lateral surface $\boldsymbol{n} = \boldsymbol{e}_r$ and $\boldsymbol{r}_p = R\boldsymbol{e}_r + z\boldsymbol{m}_0$ with R being the radius of the cylinder. The points of the upper (lower) top surface are described by means of $\boldsymbol{r}_p = r\boldsymbol{e}_r + Z\boldsymbol{m}_0$, where $Z = \pm H/2$. The normal vector $\boldsymbol{n}$ is equal to the unit vector of the longitudinal axis $\boldsymbol{m}_0$. The inequality $\boldsymbol{v}_p \cdot \boldsymbol{n} > 0$ then becomes

$$z\boldsymbol{e}_r \cdot (\boldsymbol{\omega} \times \boldsymbol{m}_0) > 0 \tag{49}$$

for the lateral surface and

$$r\boldsymbol{e}_r \cdot (\boldsymbol{\omega} \times \boldsymbol{m}_0) < 0 \tag{50}$$

for the upper (lower) top surface, respectively. The cross product $\boldsymbol{\omega} \times \boldsymbol{m}_0$ is the normal vector to the plane spanned on $\boldsymbol{\omega}$ and $\boldsymbol{m}_0$, see Figure 3. The meaning of the above inequalities is obvious. They characterize those parts of the outer surface that are affected by the resistance force. The solution is presented in Fig. 3 for the upper part of the cylinder ($0 \leq z \leq H/2$).

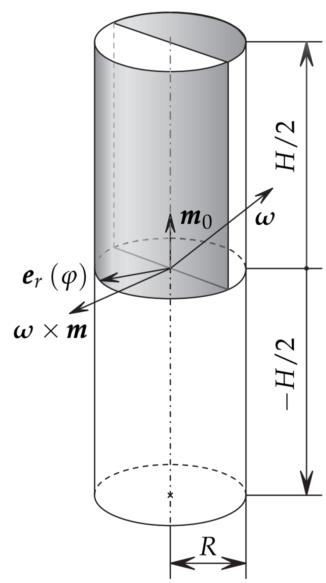

Figure 3. Part of the Surface, where the Resistance Force is Exerted.

Substituting $\boldsymbol{r}_p$, $\boldsymbol{f}_\tau$ and $\boldsymbol{f}_n$ in equation (44) by equations (46) and (48) one gets the constants α and β of the resistance tensor, being

$$\begin{aligned} \alpha &= \pi\zeta\left(R^4 + 2R^3H\right), \\ \beta &= \pi\zeta\left(R^3H + \frac{1}{2}R^2H^2 + \frac{1}{12}RH^3\right) + \pi\xi\left(\frac{1}{2}R^4 + \frac{1}{24}RH^3\right). \end{aligned} \tag{51}$$

5 Equation of Motion in Terms of the Right Angular Velocity and the Rotation Vector

From the balance equation of the angular momentum

$$\frac{d}{dt}\boldsymbol{K}_2 = \boldsymbol{M}, \qquad \boldsymbol{K}_2 = \boldsymbol{P}(t) \cdot \boldsymbol{C}_0 \cdot \boldsymbol{P}^T(t) \cdot \boldsymbol{\omega}(t) \tag{52}$$

follows with equation (40)

$$\left[\boldsymbol{P}(t)\cdot\boldsymbol{C}_0\cdot\boldsymbol{P}^T(t)\cdot\boldsymbol{\omega}(t)\right]^{\cdot} = -\boldsymbol{P}(t)\cdot\boldsymbol{G}_0\cdot\boldsymbol{P}^T(t)\cdot\boldsymbol{\omega}(t). \tag{53}$$

Equation (53) is a system of three differential equations containing six unknown quantities (three independent components of the rotation tensor $\boldsymbol{P}$ and three components of the angular velocity $\boldsymbol{\omega}$), i. e. the system is indeterminate. It can be solved by taking into account the Poisson equation (21) and the relation

$$\boldsymbol{P}^T(t)\cdot\boldsymbol{\omega}(t) = \boldsymbol{\Omega}(t) \tag{54}$$

between the left ($\boldsymbol{\omega}$) and the right ($\boldsymbol{\Omega}$) angular velocity. It must be distinguished between them because the dot product of two tensors is not commutative:

$$\boldsymbol{S}_l(t) \equiv \dot{\boldsymbol{P}}(t)\cdot\boldsymbol{P}^T(t), \qquad \boldsymbol{S}_r(t) \equiv \boldsymbol{P}^T(t)\cdot\dot{\boldsymbol{P}}(t). \tag{55}$$

In equation (55) $\boldsymbol{S}_l$ and $\boldsymbol{S}_r$ are called the left and the right spin tensor. They are connected with the left and the right angular velocities (see e. g. Zhilin (1996)) as

$$\boldsymbol{S}_l(t) = \boldsymbol{\omega}(t)\times\boldsymbol{E} = \boldsymbol{E}\times\boldsymbol{\omega}(t), \qquad \boldsymbol{S}_r(t) = \boldsymbol{\Omega}(t)\times\boldsymbol{E} = \boldsymbol{E}\times\boldsymbol{\Omega}(t). \tag{56}$$

After introducing the right angular velocity equation (53) takes the form

$$\dot{\boldsymbol{\Omega}} = \boldsymbol{C}_0^{-1}\cdot(\boldsymbol{G}_0\cdot\boldsymbol{\Omega}) - \boldsymbol{C}_0^{-1}\cdot[\boldsymbol{\Omega}\times(\boldsymbol{C}_0\cdot\boldsymbol{\Omega})]\,. \tag{57}$$

The quantities $\boldsymbol{P}$, $\boldsymbol{\omega}$ and $\boldsymbol{\Omega}$ are also time-dependent, which is not explicitly noted. Equations (57) contain only three unknowns, that are the components of the vector $\boldsymbol{\Omega}$. By introducing it the rotation tensor is eliminated. Together with the vectorial equation (57) the Poisson equation for the right angular velocity

$$\dot{\boldsymbol{P}} = \boldsymbol{P}\times\boldsymbol{\Omega} \tag{58}$$

must be solved in order to calculate the components of the rotation tensor in dependence on time. With the equivalent relation of equation (54)

$$\boldsymbol{\omega} = \boldsymbol{P}\cdot\boldsymbol{\Omega} \tag{59}$$

the left angular velocity $\boldsymbol{\omega}$ can be obtained. Because of the non-linearity equations (57) can analytically be solved only for simplified models. In this work a numerical solution procedure is presented. It is significantly easier if, instead of the rotation tensor, the rotation vector $\boldsymbol{\theta}$ is used. It provides another opportunity to quantitatively describe a rotation (see e. g. Menzel et al. (2004)). The equation

$$\dot{\boldsymbol{\theta}} = \boldsymbol{\Omega} + \frac{1}{2}\boldsymbol{\theta}\times\boldsymbol{\Omega} + \frac{1-g}{\theta^2}\boldsymbol{\theta}\times(\boldsymbol{\theta}\times\boldsymbol{\Omega}) \tag{60}$$

with

$$g = \frac{\theta\sin\theta}{2(1-\cos\theta)}, \qquad \theta^2 = \boldsymbol{\theta}\cdot\boldsymbol{\theta}, \qquad \theta = |\boldsymbol{\theta}| = \sqrt{\boldsymbol{\theta}\cdot\boldsymbol{\theta}} \tag{61}$$

is equivalent to the Poisson equation (21) if the rotation vector is used (Zhilin (2000)). Now the system of differential equations that is to be solved takes the form

$$\begin{aligned} \dot{\boldsymbol{\Omega}} &= -\boldsymbol{C}_0^{-1}\cdot(\boldsymbol{G}_0\cdot\boldsymbol{\Omega}) - \boldsymbol{C}_0^{-1}\cdot[\boldsymbol{\Omega}\times(\boldsymbol{C}_0\cdot\boldsymbol{\Omega})]\,, \\ \dot{\boldsymbol{\theta}} &= \boldsymbol{\Omega} + \frac{1}{2}\boldsymbol{\theta}\times\boldsymbol{\Omega} + \frac{1-g}{\theta^2}\boldsymbol{\theta}\times(\boldsymbol{\theta}\times\boldsymbol{\Omega}). \end{aligned} \tag{62}$$

The initial conditions are $\boldsymbol{\Omega}(0) = \boldsymbol{\Omega}_0$ and $\boldsymbol{\theta}(0) = \boldsymbol{0}$. In order that the denominator of the term $\frac{1-g}{\theta^2}$ does not equal zero during the solution procedure of the differential equations, the small number of 0.001 was added. Apart from that, the initial conditions of the components of the rotation vector $\boldsymbol{\theta}$ were also set 0.001. Having solved equations

(62) the rotation vector $\boldsymbol{\theta}$ as a function of time is known. With the following equation the rotation tensor $\boldsymbol{P}$ can be calculated

$$\boldsymbol{P}(\boldsymbol{\theta}) = \frac{1-\cos\theta}{\theta^2}\boldsymbol{\theta}\otimes\boldsymbol{\theta} + \frac{\sin\theta}{\theta}\boldsymbol{\theta}\times\boldsymbol{E} + \cos\theta\,\boldsymbol{E} \tag{63}$$

and with equation (59) the vector of the left angular velocity $\boldsymbol{\omega}(t)$ which is the solution of the equation of motion.

6 Solution of the Equation of Motion

The numerical solution was calculated with the help of the commercial code Mathcad® with the Runge-Kutta method with adaptive increment. It was assumed that the height of the cylindrical particle is 25 times greater than its radius ($H = 25R$). The initial angular velocity was assigned to be

$$\boldsymbol{\Omega}_0 = \begin{pmatrix} 1 \\ 2 \\ 3 \end{pmatrix}. \tag{64}$$

In order to prove the system of differential equations, the results of the numerical solution in the case of a friction-free rotation was compared with the classical solution of the equation of motion. In that case the resistance tensor $\boldsymbol{G}_0$ in the first equation of (62) equals the zero tensor $\boldsymbol{0}$. The results of the, with both methods, calculated left angular velocity are shown in Table 1. The differences between both solutions are very small and result from the solution procedure of the numerical calculation, i. e. from the small difference of the initial conditions.

Table 1. Comparison of the Left Angular Velocity $\boldsymbol{\omega}$ $[s^{-1}]$, Calculated with the Analytical and the Numerical Solution of the Equation of Motion

t $[s]$	$\boldsymbol{\omega}$ (analytical)	$\boldsymbol{\omega}$ (numerical)	t $[s]$	$\boldsymbol{\omega}$ (analytical)	$\boldsymbol{\omega}$ (numerical)
1	$\begin{pmatrix} -0.876 \\ 1.634 \\ 3.250 \end{pmatrix}$	$\begin{pmatrix} -0.876 \\ 1.628 \\ 3.253 \end{pmatrix}$	6	$\begin{pmatrix} -0.918 \\ 2.291 \\ 2.812 \end{pmatrix}$	$\begin{pmatrix} -0.907 \\ 2.304 \\ 2.805 \end{pmatrix}$
2	$\begin{pmatrix} 0.603 \\ 2.660 \\ 2.561 \end{pmatrix}$	$\begin{pmatrix} 0.590 \\ 2.668 \\ 2.556 \end{pmatrix}$	7	$\begin{pmatrix} 0.994 \\ 2.087 \\ 2.942 \end{pmatrix}$	$\begin{pmatrix} 1.001 \\ 2.083 \\ 2.943 \end{pmatrix}$
3	$\begin{pmatrix} -0.167 \\ 1.191 \\ 3.543 \end{pmatrix}$	$\begin{pmatrix} -0.186 \\ 1.202 \\ 3.538 \end{pmatrix}$	8	$\begin{pmatrix} -0.824 \\ 1.558 \\ 3.301 \end{pmatrix}$	$\begin{pmatrix} -0.819 \\ 1.567 \\ 3.297 \end{pmatrix}$
4	$\begin{pmatrix} -0.269 \\ 2.793 \\ 2.476 \end{pmatrix}$	$\begin{pmatrix} -0.265 \\ 2.798 \\ 2.471 \end{pmatrix}$	9	$\begin{pmatrix} 0.516 \\ 2.709 \\ 2.529 \end{pmatrix}$	$\begin{pmatrix} 0.528 \\ 2.710 \\ 2.525 \end{pmatrix}$
5	$\begin{pmatrix} 0.684 \\ 1.397 \\ 3.403 \end{pmatrix}$	$\begin{pmatrix} 0.689 \\ 1.400 \\ 3.401 \end{pmatrix}$	10	$\begin{pmatrix} -0.062 \\ 1.180 \\ 3.550 \end{pmatrix}$	$\begin{pmatrix} -0.042 \\ 1.200 \\ 3.544 \end{pmatrix}$

The actual position of the particle can be illustrated since it can be calculated in the following manner

$$\boldsymbol{m}(t) = \boldsymbol{P}(t)\cdot\boldsymbol{m}_0. \tag{65}$$

In equation (65) $\boldsymbol{m}(t)$ is the unit vector of the longitudinal axis of the particle in the actual and $\boldsymbol{m}_0$ in the initial position, which was chosen to be

$$\boldsymbol{m}_0 = \frac{1}{\sqrt{3}}\begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix}. \tag{66}$$

In both cases, the classical solution and the above presented model of motion, the course of a rotating particle is

similar as is shown in Figure 4 (marked with circles).
If interactions between the particle and the surrounding medium occur, the tensor $\boldsymbol{G}_0 \neq \mathbf{0}$. To give a numerical solution of equations (62) the coefficients ζ and ξ have to be known. In the computations we set $\zeta = \xi = 0.003\, kg/m^2 s$. It can be shown that, if interactions are taken into consideration, the motion of the particle is slowing down. In Figure 4 the line with circular symbols shows the motion if friction is neglected. The consideration of friction results in the line with triangular symbols.

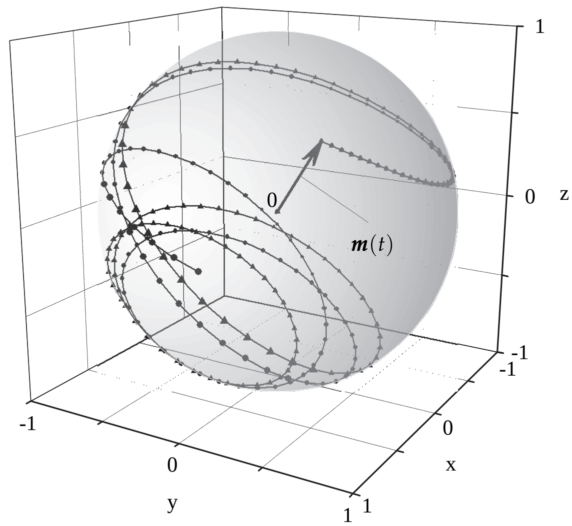

Figure 4. Course of the Rotation of the Particle in the Interval $0\,s \leq t \leq 5\,s$; Circles without Friction; Triangles with Friction

7 Conclusions

In this work a model was developed with which the orientation of a rigid particle, that is suspended in a medium, may be determined. For that the equation of motion of the particle was derived from the balance equation of the angular momentum. The equation of motion was solved numerically on the basis of the Runge-Kutta method. In a first step the obtained angular velocity of the model developed here was, in the case of friction-free motion, compared with the classical solution. It could be shown, that the numerical solution agrees with the analytical one. After that interactions (friction, resistance) between the particle and the surrounding medium were considered. With the assumed values of ζ and ξ the particle rotates with a minor velocity. The rotation of the semi axis of the particle in a time scale of $5s$ was presented graphically.
In order to develop a simulation software with which the orientation of fibers during the filling stage of the injection molding process can be predicted the model must be extended to a multi-particle system. In addition, the friction and the resistance coefficient must be quantified.

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