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Rheology of Additive Manufacturing Processes for Medical Silicone

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Micro Abstract
The objective of this project is to simulate the 3D-printing of medical grade silicone to support patient specific implant development. This requires the formulation of a thermodynamically consistent finite strain curing model, whereby a multiphysics approach for the mechanical, thermal and chemical fields is necessary. Due to the complexities of the manufacturing process, the Optimal Transportation Meshfree method is used to obtain a numerical solution.

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Introduction

In the health care industry the treatment of neuronal hearing loss with cochlea implants is a well established medical intervention. Since only standard implant sizes are available, a patient specific additive manufacturing process to improve their functionality is desirable.
Therefore, a prototype 3D-printer device was built by the Excellence Cluster Hearing4all of the Hanover Medical School (MHH) [3], using Room Temperature Vulcanisation (RTV) medical grade silicone. The material behaviour can be characterised as viscoelastic and process dependent. Due to the curing phenomena, which is an exothermal chemical reaction leading to the crosslinking of polymer chains, the material transforms from a viscoelastic fluid into a viscoelastic solid. The additive manufacturing is then performed by an extrusion of the fluid like material. To obtain higher geometrical precision, heat curing is induced by an infrared laser. The heating accelerates the curing and in turn the solidification and this reduces material spreading.
The influence of processing parameters such as extrusion rate and translation velocity can be estimated based on operator experience. However, the material behaviour during the printing process is not yet fully understood. Therefore, the objective is to simulate the 3D-printing of medical grade silicone in support of patient specific implant development. This includes, besides the modelling of the printing simulation, a thermodynamically consistent formulation of a large strain curing model.

1 Large strain curing model

From the numerical point of view a multiphysics approach for the mechanical, thermal and chemical fields is necessary. This includes the formulation of a thermodynamically consistent curing model. Due to observed material spreading up to 30 percent [3] for the sample medical silicone, a finite strain curing model has to be applied. The used model is based on Lion's idea [2] of decomposing the deformation gradient, cf. equation (1), into a mechanical, chemical and thermal part,

$$\mathbf{F} = \mathbf{F}_M \mathbf{F}_C \mathbf{F}_\Theta, \tag{1}$$

respectively. This includes the modelling of thermal expansion and volume shrinkage with an isotropic approach for the chemical

$$\mathbf{F}_C \quad = \quad g(\dots)^{1/3}\mathbf{1} \quad g(\dots) = g(\alpha) = 1 + \beta_c \alpha \quad \beta_c \leq 0 \tag{2}$$

and the thermal deformation gradient

$$\mathbf{F}_\Theta \quad = \quad \varphi(\dots)^{1/3}\mathbf{1} \quad \varphi(\dots) = \varphi(\alpha) = 1 + \beta_\Theta \alpha \quad \beta_\Theta \geq 0. \tag{3}$$

1.1 Mechanical part

The viscous mechanical material behaviour is modelled with a generalised Maxwell-model (e.g [4]) as depicted in Figure 1. This model consists of an equilibrium spring with shear modulus μ_∞

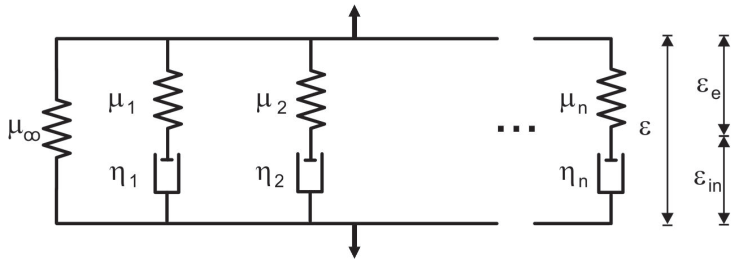

Figure 1. Generalised Maxwell-model to capture viscoelastic behaviour

and n Maxwell-elements with one spring and dashpot each. Due to the pure elastic behaviour of the springs and the inelastic behaviour of the dashpots, the total strain ε is decomposed into an elastic ε_e and an inelastic part ε_{in}. Computationally an evolution equation for the inelastic strain of each Maxwell-element has to be formulated and solved.

1.2 Process dependencies

During the printing process material curing occurs and the shear moduli, as well as the viscosities, are evolving. Thus, they need to be formulated as process dependent variables. The basis of the process dependent formulation is the introduction of the so-called degree of cure α. It represents the fraction of crosslinked polymer chains and is defined in the range $[0, 1]$. The evolution of the degree of cure is dependent on the specific reaction kinetics. Commonly, an Arrhenius-type evolution equation of the form

$$\dot{\alpha}(\Theta) = [A_1(\Theta) + A_2(\Theta)\alpha^m](1 - \alpha)^n, \tag{4}$$

where

$$A_1(\Theta) = A_{c1} e^{-\frac{B_1}{\Theta}} \quad A_2(\Theta) = A_{c2} e^{-\frac{B_2}{\Theta}} \tag{5}$$

is used to describe the kinetics. It is a function depending on the temperature Θ and four parameters which have to be determined experimentally. The introduced shear moduli and viscosities are then functions of the temperature and the degree of cure.

2 Numerical approximation scheme

Due to the geometrical complexities of the printing process, the Optimal Transportation Meshfree (OTM) method [1] is used to obtain a numerical solution. Similar to the Finite Element Method (FEM), the OTM method is an approximation on the continuum scale based on the weak form of the governing partial differential equation. In the present case, the equation of linear momentum

and the energy equation are solved.
Similar to the FEM, the OTM approximation scheme consists of nodal and integration points, the so-called material points. However, there are no fixed elements containing a specific nodal connectivity. All nodes inside a predefined support domain are associated with the specific material point and all surrounding material points form the influence domain of a node. In Figure 2 the two different kind of points with their domain are illustrated, nodal points in white and material points in red. The support and influence domain of the points are dynamically updated, such that two approaching bodies can simply merge and large deformations can be computed without requiring re-meshing.

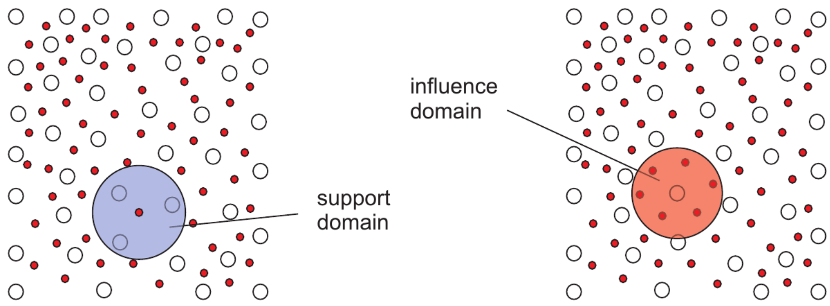

Figure 2. Support domain of nodal points and influence domain of material points

3 Results

As a first step, the resulting thermo-chemo-mechanical coupled equations are implemented into the in-house OTM-code and verification examples exhibiting chemical shrinkage and thermal expansion are successfully performed. As an example, the verification of chemical shrinkage is presented. In Figure 3 the geometry of the quasi two-dimensional verification example with dimensions $20 \times 5 \times 0.5$ [mm] is depicted. On the bottom and the top the displacements are

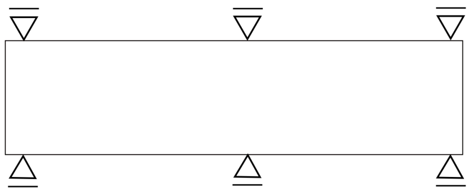

Figure 3. Dimensions and boundary conditions of the verification example

constrained in x- and y-direction and all displacements in z-direction are inactive with no applied external loads. In Figure 4 the deformed shape of the initial body is depicted. On both sides a contraction is observable which indicates a volume shrinkage, thus chemical shrinkage takes place.

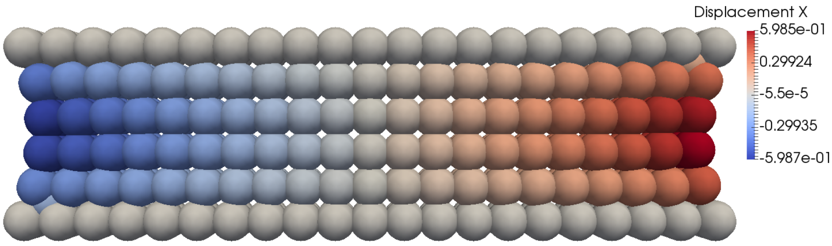

Figure 4. Displacement field of verification example which indicates a chemical shrinkage

As a next step the material extrusion is modelled within the OTM method. In Figure 5 the displacement field of a preliminary 3D printing simulation is depicted. It can be seen that printed material remains on the printing plate and the extrusion cylinder continues its movement and extrusion in a linear fashion. With the developed code it is now possible to simulate the first phase of the printing process.

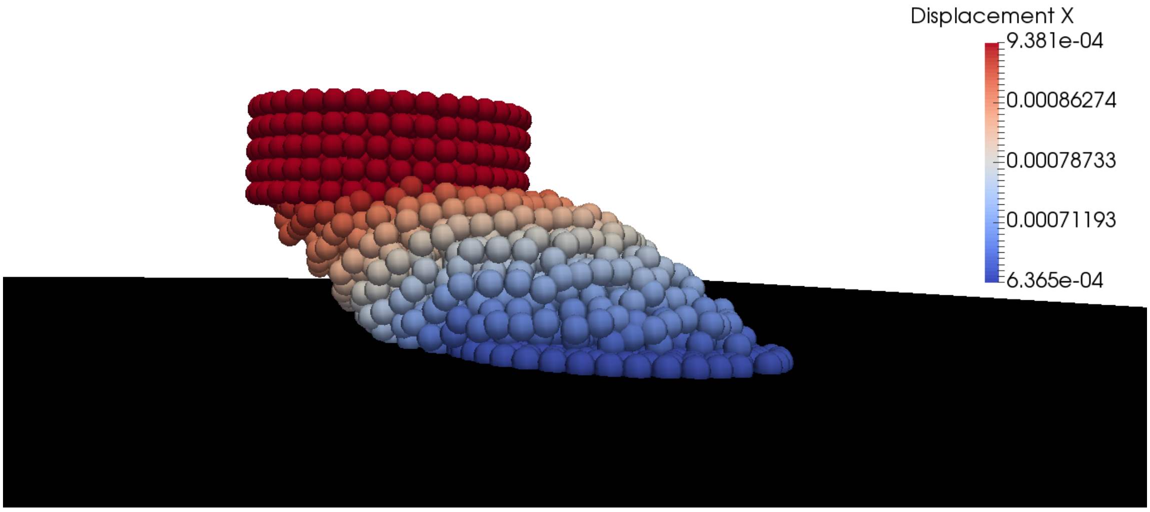

Figure 5. Displacement field in translation direction of 3D printing simulation

Conclusions

The Lion model appears to be a sound basis for a thermodynamically consistent formulation of a large strain curing model, where the mechanical part is modelled by a generalized Maxwell model. It includes all necessary aspects of curing as chemical shrinkage and thermal expansion and possesses 'enough freedom' for the upcoming material fit and modelling of the process dependent variables.
Furthermore, the OTM method seems to be a promising approach for 3D printing simulations, where the preliminary development has been successfully completed.

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