Abstract

Profile extrusion is a manufacturing process used for continuous plastics profiles with a fixed cross section. The key challenge in the development of profile extrusion dies is to design the transition region between outflow and inflow of the die in such a way, that the material velocity at the outflow is homogeneous. At the current state of the art, die design is experience based and time-consuming running-in experiments need to be performed for each new die. Aim of this work is to develop a new design approach based on numerical shape optimization with the idea of significantly reducing the number of running-in experiments. Based on an existing, in-house flow solver, a shape optimization framework has been established. It contains a geometry kernel, which operates on non-uniform rational B-splines. The framework has been applied to two profile extrusion dies for profiles with rising complexity: a slit profile and a floor skirting. Apart from validating the functionality of the framework, the aim of the test cases was to investigate the influence of the use of the Carreau model on the optimization outcome. From flow simulations, it can be observed that the use of the Carreau model has a definite influence on the resulting flow solution in extrusion die scenarios. However, it is not clear whether this influence extends to the location of the optimal solution.

Key words: plastics profile extrusion dies, shape optimization, NURBS parametrization, homogeneous velocity distribution, Carreau model
1. Introduction

The central component of a profile extrusion line is the extrusion die, whose task is to reshape the plastics melt provided by an extruder into the final product. What makes die design a very challenging task is the strongly nonlinear behavior of plastics melts, namely their shear-thinning and viscoelastic properties. As the viscoelastic effects mainly concern the behavior of the plastics melt behind the extrusion die (e.g. die swell), this work concentrates on the shear-thinning properties. Already the very use of shear-thinning material properties can lead to nonintuitive effects of design changes on the flow field. At the current state of the art, die design relies strongly on the experience-based knowledge of the designer [1]. Simulation tools are often employed to evaluate the initial design before the respective die is manufactured, which can basically be described as a shift of the running-in experiments from the extrusion line onto the computer. Recently, efforts are being made to go one step further and look into automated design methods for extrusion dies based on numerical shape optimization. Two important fields of research within the field of numerical design methods, which allow for some distinction between the different methods, are the definition of the objective function and the representation of the geometry.

Regarding the first point, the homogeneity of the velocity distribution at the die outlet is usually considered to be the primal quality criterion. In all publications known to the authors, this criterion is expressed using a least-squares term. Differences lie in the details. For example, either the average velocity or the flux can be used in the least-squares term, and the evaluation of the term can be done in different ways: it can be aggregated over the nodes, the cells or small segments that the outflow cross section is subdivided into. [1–5] In addition to this primary criterion, some groups examined secondary criteria such as pressure loss or dwell periods [3, 6–9]. An example for an objective function which goes one step further in the manufacturing chain by considering viscoelastic swelling behind the die is presented in [10]. Furthermore, in [11] the optimization of a sheeting die has been performed under multiple operating conditions.

Concerning the geometry representation, there are two fundamentally different approaches [12, 13]. On one hand, there is the possibility to use the same grid for both the calculation of the flow solution and the geometry representation; this is referred to as parameter-free approach. Changes in the geometry present themselves in displacement of individual nodes. Advantages of this approach are the easy model generation and the lack of restrictions on the deformation. However,
there are some unfavorable attributes such as the need for filtering techniques if a smooth surface is to be obtained, the extremely large number of design parameters and the difficulties in making the optimized shape accessible to a CAD-system. The second option for geometry representation is the use of a parameterization. The ways in which parameterization can be applied are manifold, ranging from very simple approaches—such as the variation of flow channel height and length [3–7, 9, 14]—to more elaborate approaches where free-form surfaces are represented using splines [2]. Advantageous about parameterization techniques is the reduction to very few design parameters, which affords more freedom in the choice of the optimization algorithm. Furthermore, the import of the optimized shape into a CAD-system is straightforward. Resulting restrictions to the deformations can be considered an advantage and disadvantage at the same time. If a parameterization is used, the optimization space will be restricted, which sometimes might be a desired effect. Keywords describing such situations are, for example, symmetric deformations or adherence to manufacturing requirements.

The intent of this paper is to present a new design concept for extrusion dies which strongly relies on numerical shape optimization. Furthermore, the presented design method has been applied to two sample extrusion dies, in order to investigate whether the use of a shear-thinning constitutive model, as compared to the purely Newtonian constitutive model, has an influence on the optimal shape for these test cases. Therefore, the remaining part of this article is structured as follows. We state the governing equations of the flow of plastics melt and introduce notation for the shape optimization problem in Section 2. Details about the framework that is used to compute an optimal shape are given in Section 3. The focus is laid on the parameterization and the objective function. In Section 4, we describe a systematic approach to design an initial geometry as an input to the shape optimization framework. The framework is first tested on a simple slit profile and then applied to an industrially-relevant die of a floor skirting profile; the results, particularly regarding the effects of the Carreau model on the optimization, are shown in Section 5. In Section 6, we provide a summary and give a brief outlook on future work.

2. Governing Equations

The flow of plastics melt through an extrusion die can be considered a creeping flow, with a Reynolds number $Re \ll 1$. Creeping flow is characterized by the fact that the advective inertial forces are small compared to viscous forces. This typically occurs, when the velocities are very
low compared to the length scale and the viscosity is very high. Important characteristics of creeping flows are:

- Laminar flow
- Infinite boundary layer (wall effects extend into the entire domain)
- Instantaneity (no time dependence other than time-dependent boundary conditions)

This leads to the stationary Stokes equations as governing equations. With the pressure forces being much higher than gravity for the profile extrusion case, external forces can be neglected. The final governing equation is given in Equation (1).

\[ \nabla \cdot \sigma = 0 \quad \text{on } \Omega, \]
\[ \nabla \cdot u = 0 \quad \text{on } \Omega. \]

Here, \( \sigma \) is the stress tensor and \( u \) is the velocity vector in domain \( \Omega \). For a Newtonian fluid, the viscous stress tensor is assumed to be a linear function of the components of the velocity gradient \( \nabla u \). Furthermore, the material is assumed to be isotropic, i.e., the physical properties are independent of the direction. In particular, this leads to the assumption that the viscosity \( \eta \) can be regarded as a constant for a Newtonian fluid. Considering the rate of strain tensor

\[ \varepsilon(u) = \frac{1}{2}(\nabla u + \nabla u^T), \]

The stress tensor can then be written as

\[ \sigma = -pI + 2\eta \varepsilon(u). \]

What is not accounted for by the Newtonian model is the shear-thinning behavior exhibited by plastics melt, i.e., the viscosity can no longer be considered as constant but depends on the shear rate. A prominent shear-thinning model in the plastics sector is the Carreau model [15, 16]. It uses three parameters to approximate the viscosity curve: \( A \) represents the viscosity at zero shear rate and has the unit \( \text{Pas} \), \( B \) marks the transition point from almost Newtonian to shear-thinning behavior in the viscosity curve and has the unit \( s \), and the dimensionless parameter
defines the slope of the viscosity curve in the shear-thinning region if plotted on a double logarithmic scale. The viscosity and the shear rate are thus related by the following equation:

\[ \eta(\dot{\gamma}) = \frac{A}{(1 + B\dot{\gamma})^C}. \] (4)

Compared to other important shear-thinning models like power law [17], the Carreau model has the advantage that it is valid over a broad range of shear rates, particularly for \( \dot{\gamma} \to 0 \) [15].

A second influence factor on the viscosity is the temperature. However, if the heating is properly designed the temperature in a profile extrusion die can (approximately) be considered as homogeneous when the steady-state is reached. Therefore, it is a good approximation to consider this process to be isothermal. The less complex modeling saves computational time during the costly optimization steps.

Within the shape optimization problem, Equation (1) acts as a constraint in the minimization of the objective function. The objective function \( J \) describes the homogeneity of the outflow velocity distribution and shall be defined in Section 3.2. The complete optimization problem is then:

\[
\begin{align*}
& \text{minimize} \quad J(u, p, \alpha) \\
& \text{subject to} \quad c(u, p; x) = 0 \quad \text{on} \quad \Omega = \Omega(\alpha)
\end{align*}
\] (5)

where \( c \) denotes the state equation, i.e., the Stokes equation (1), \( \alpha \) is the design vector and \( x \) defines the mesh coordinates.

2.1. Flow solver

For the discretization of the Stokes equation, we use P1P1 finite elements, i.e., linear interpolation for the velocity degrees of freedom and also linear interpolation for the pressure. This combination of interpolation functions is known to violate the LBB compatibility condition. Consequently without an appropriate stabilization, the pressure field is likely to present spurious and oscillatory results. The stabilization technique used here is Galerkin/Least-Squares (GLS) stabilization. In the GLS method, the stabilization term consists of an element-by-element weighted least-squares formulation of the original differential equation [18]. The variations in
the viscosity as described by the Carreau model are computed using an element-wise evaluation of the shear rate based on the velocity gradients at the element center.

The flow solver has been tested on a wide range of systems with different architectures, and its scalability has been shown to be satisfactory on up to 4096 processors on a Blue Gene/L system using MPI parallelization [19] allowing for simulations with a large number of unknowns.

3. Modular Shape Optimization Framework

Building on the in Section 2.1 described flow solver, a framework for shape optimization in fluid applications has been developed [20, 21]. This framework, whose structure is depicted in Figure 1, extends the flow solver with two major components: a geometry kernel that updates the computational mesh for given design parameters, and a routine that evaluates the objective function. This information is passed on to an optimization driver that returns an update for the design parameters. The framework is modular in the sense that different optimization methods can be easily added to the driver. Since the major part of the computational costs of the optimization results from the evaluation of the objective function, only the flow solver is executed on parallel processors whereas the optimization algorithm and the shape deformation are done serially. In the following, a more detailed description of the framework is given.

3.1. Mesh update method

The definition of the mapping from the optimization parameters to the computational domain has a substantial influence on the optimization outcome.

The presented framework features a geometry kernel that offers extensive flexibility. The domain boundary is approximated with non-uniform rational B-splines (NURBS). Ever since their first use in the 1970’s, NURBS have grown to become the industry standard for the representation, design and data exchange of geometric information processed by computers. For example, they form the basis of every established CAD-programme—a fact which can be attributed to their flexibility. Both analytical shapes such as circles or conics as well as free-form shapes can be represented exactly using NURBS. Both aspects are important arguments for the use of NURBS in an optimization context. On the one hand, the flow channel geometry can be exported form a CAD system and more importantly, the optimized geometry can be transferred back into the
CAD/CAM system. On the other hand, the optimization process can profit from the flexibility provided by NURBS.

In this case, the optimization parameters correspond to the location and weight of the splines’ control points. To avoid remeshing, the positions of interior nodes are adjusted to boundary deformations according to a mesh-moving scheme. That is, the parameter vector $\alpha$ is mapped first into a (hypersurface) shape $\gamma$ and then into a mesh $x$ that discretizes the domain $\Omega$. The two steps are described below.

**shape update: $\alpha \rightarrow \gamma$**

For 2D-computations, the shape of the boundary is represented by a NURBS-curve, whereas for 3D-computations, a NURBS-surface is needed. The parameterized shape $\gamma$ is governed by a control grid containing $m$ control points, each with a coordinate $P_i$ and a weight $w_i$. Each of the $n_{nb}$ boundary nodes of the finite element mesh has a corresponding local coordinate $\tau_k$ on the spline. Changes in the spline’s shape cause a displacement of the corresponding point. This deformation is transferred to the node on the finite element mesh. The position of a node can be determined using the control point coordinates $P_i$, the weights $w_i$, and the local coordinate $\tau_k$: 

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Figure 1: Structure of the shape optimization framework; at the end of the iteration loop, the optimal design parameters $\alpha^*$ are obtained.
\[ \gamma_k = \sum_{i=1}^{m} P_i w_i N_i(\tau_k) / \sum_{i=1}^{m} w_i N_i(\tau_k) \in \gamma, \quad k = 1, \ldots, n_{nb}. \]  

(6)

A definition of the basis functions \( N_i \) can be found in [22]. How the control points \( P_i \) and the weights \( w_i \) influence the NURBS’ shape is shown in Figure 2.

![Figure 2: NURBS curve with four control points. The increased weight of control point \( P_2 \) gives this control point a stronger influence.](image)

To define a relationship between the design vector \( \alpha \in \mathbb{R}^n \) and the control grid, we introduce

\[
\begin{pmatrix} P_i \\ w_i \end{pmatrix} = a_i + A_i \alpha, \quad i = 1, \ldots, m
\]

(7)

where \( a_i \) defines the initial position and the weight of control point \( i \). This allows to reduce the optimization space dramatically in cases that involve symmetry or control restrictions. Possible control restrictions for the presented application are restrictions which are inherent in the manufacturing processes for extrusion dies. In such cases, two or more control points share the same matrix \( A_i \) so that the number of scalar design parameters \( n \) is less than \( m \).

mesh update: \( \gamma \rightarrow x \)

To adjust the computational mesh to the boundary deformation, the Elastic Mesh Update Method (EMUM) is used [23]. In this method, the computational mesh is regarded as an elastic body reacting with internal displacements \( v \) to the boundary displacements applied to it. For this
purpose, the linear elasticity equation is solved for the mesh:

\[ \nabla \cdot \sigma_{\text{mesh}} = 0, \]  
\[ \sigma_{\text{mesh}}(v) = \lambda (\text{tr} \varepsilon_{\text{mesh}}(v)) \mathbf{I} + 2\mu \varepsilon_{\text{mesh}}(v), \]  
\[ \varepsilon_{\text{mesh}}(v) = \frac{1}{2} (\nabla v + (\nabla v)^T). \]  

In structural mechanics, \( \lambda \) and \( \mu \) are the Lamé-parameters that are needed to constitute the stiffness tensor for isotropic and linear elastic materials. In the context of the elastic mesh update, these parameters are prescribed for each element in order to control its stiffness. This is used especially to increase the stiffness of the smaller elements compared to the larger elements in order to allow larger deformation before the mesh fails. The mesh update equation (8)–(10) is solved with the classical Galerkin finite element method.

3.2. Objective function

Following Szarvasy et al. [24], a correct profile has been obtained when the skeleton line of the cross section matches the designed one, and the thickness distribution is as required. There exist a whole variety of criteria which are known to influence the correctness of the profile, but they are only known in a loose and hard-to-measure sense. These include [15]:

1. homogeneous velocity distribution at the outflow
2. a pressure drop which is as low as possible
3. continuous acceleration of the plastics melt
4. a short dwell period
5. homogeneous die swell.

The relative importance of the homogeneous velocity distribution suggests the use of the velocity magnitude as a basis for the objective function. We propose to subdivide the outflow of the extrusion die into subsections and compute the variance of the local maximal velocity—\( \max(v_{\text{subsection}}) \)—as compared to the average maximal velocity over all sections—\( \bar{v}_{\text{max}} \):

\[ J = \sum_{\text{subsection}} (\max(v_{\text{subsection}}) - \bar{v}_{\text{max}})^2. \]  

9
Choosing the local maximal velocity as opposed to the local average velocity emphasizes local velocity peaks. These peaks might be missed if the same subsection contains a significantly large area of zero velocities due to wall adhesion.

In general, the value of the objective function (11) will depend on the flux. Therefore, if several operating points are to be compared, the values of the objective function have to be scaled according to the different processing speeds. Another important influence factor not only on the value but also on the behavior of the objective function is the number, size and distribution of the subsections, which have been chosen. Since Equation (11) does not contain the area of the subsections, each subsection has the same weight within the objective function. This feature can be used to emphasize certain regions of the outflow as opposed to other regions. The influence of the number of subsections on the behavior of the objective function has been investigated in more detail in [25]. The number of subsections has to be chosen with great care, as a choice inappropriate to the regarded problem can lead to suboptimal designs. The appropriate number of subsections needs to be chosen based on experience and the flow solution of the initial design which gives hints regarding the weaknesses in the design.

3.3. Optimization driver

As indicated in Figure 1, the framework relies on the exchange of state information between two independently executing components—optimization driver and flow solver. The driver contains both gradient-free and gradient-based optimization methods [26, 27]. The current version of the flow solver does not yet provide a gradient of the objective function; a discrete adjoint approach is currently being developed and will be integrated into the framework. Even though an approximation of the gradient using finite differences is affordable for a small number of optimization parameters, we have found gradient-free methods to perform equally well in the numerical examples presented in Section 5.

The optimal design parameters in the examples were obtained using BOBYQA (Bound Optimization BY Quadratic Approximation) [26]. In this derivative-free approach, the objective function $J$ is approximated by a quadratic function $Q$ that is required to equal the original function at a given number of interpolation points. The remaining degrees of freedom are specified by minimizing the Frobenius norm of the change in the second derivative of consecutive iterates:

$$Q_{k+1}(x_j) = J(x_j), \quad j = 1, \ldots, m \quad \text{and} \quad \|\nabla^2 Q_{k+1} - \nabla^2 Q_k\|_F \rightarrow \min. \quad (12)$$
The quadratic model is improved by updating the set of interpolation points and, depending on the improvement, the trust region radius (where the trust region radius defines the area around the current iterate from which the points utilized for the quadratic approximation are chosen). Furthermore, box constraints can be imposed on the optimization parameters, which offers a way to include simple geometric constraints.

4. Model Generation

In order to be able to perform a shape optimization, first, an initial geometry has to be determined. An efficient optimization procedure relies on a simple and fast determination of an initial geometry which is already close to an optimum. Subsequently, a FE-model of the flow channel in connection with an appropriate parameterization needs to be generated (cf. Figure 3).

![Figure 3: Steps in the model generation process.](image)

4.1. Simplified Layout of the Initial Geometry

Applying the shape optimization framework as described in Section 3 to a conventional initial design from a die designer can lead to a significant reduction of the number of running-in experiments and the associated costs. However, the use of numerical shape optimization contains an additional simplification potential within the design process. The requirements for an initial geometry intended for shape optimization are different from the requirements for an initial geometry for running-in experiments. In the latter case, the initial geometry has to be as close as possible to the expected optimum, as each additional running-in experiment is much more costly than a refined design within the CAD-model. This is not true for the initial geometry for shape optimization, where a reduced amount of user input is desirable. Essentially, there is a trade-off between the number of required optimization steps and the effort to provide a suitable initial
geometry; the closer the initial geometry resembles an optimum, the fewer steps are needed to obtain the optimal design. On the other hand, if some basic requirements are met, the framework might still be able to find an optimum even with a crude initial design. Basic requirements include, e.g., a suitable pre-distribution of the plastics melt, sufficient acceleration of the material, and avoiding stagnation regions in the die.

In this work, we propose a systematic way of deriving an initial geometry from the profile geometry that serves as an input to the optimization framework. This geometry fulfills the above mentioned basic requirements, yet its design is straightforward, thus, exploiting the full potential of applying numerical shape optimization to die design. The central concept is to install an intermediate level which is placed at one third of the flow channel length. Shape and dimension of the intermediate level are derived from the profile cross section in two steps. First, an abstract representation of the profile cross section is generated by identifying its basic building blocks. The building blocks considered here are: segments, corners, T-junctions, and end pieces [28]. Curved or slanted building blocks can be approximated by a combination of straight segments with 0°, 45°, or 90° angles inbetween. Other basic identification factors are length l and height h of the building blocks as defined on an example of the abstraction process given in Figure 4.

![Figure 4: Abstraction of the cross section of a floor skirting profile. The leftmost building block is a segment with length $l_1$ and height $h_1$.](image)

Second, the abstracted cross section is scaled up to obtain the final dimensions of the intermediate level. The main purpose of the scaling is to fulfill the requirement of sufficient compression. Looking at segments, for example, due to manufacturing restrictions and to the higher dependency of the flow resistance it is reasonable to achieve steady acceleration of the material mainly over scaling the height. Therefore, a suitable scaling factor for the height is 300 %, whereas the length should only be scaled by 10 %. These scaling factors are derived from empirical rules, which are state-of-the-art in industrial die design as there exist no analytically solvable
formulae for profile extrusion flow channels [15]. In most cases, a profile consists of more than one building block. This means that the flow through one section is no longer independent, but influenced by the other sections. As a result of this interaction, the additional requirement of material pre-distribution needs to be accounted for. Therefore, the scaling factor needs to be adjusted according to the estimated flow resistance in each building block. If, for example, a profile is built up of several sections of different height, sections with relatively small height at the outflow need to be made comparatively higher at the intermediate level. This ensures an approximate balancing of the flow resistance among the sections. The original scaling factor of 300 % is multiplied by \((\frac{h_{\text{avg}}}{h_{\text{out}}})^3\), where \(h_{\text{avg}}\) denotes the average segment height at the outflow.

The power of three is used as the formula to approximate the pressure drop in simple profiles [15] contains the height in just the same way.

The three-dimensional flow channel geometry is then generated between the three known cross sections (inflow, intermediate level and outflow) using a linear morphing algorithm. The corresponding edges in the cross sections can be connected with lines in a CAD-programme and, thus, the surface area can be created with a morphing tool. The resulting flow channel for the profile in Figure 4 is shown in Figure 5. It is already constructed of NURBS surfaces. However, in general a reparameterization of these surfaces will be necessary to establish a parameterization as described in the next section.

![Figure 5: Initial geometry created by the morphing algorithm.](image)
4.2. Parameterization

Starting from this initial geometry, the optimization framework is used to optimize the part of the flow channel between the intermediate level and the outflow. This requires two steps which at first are independent from each other. One is the generation of an FE-mesh, which is accomplished in the standard fashion, and the other is the representation of the shape by NURBS parametrization. This second task utilizes the NURBS representations already present in the CAD-model. The NURBS surfaces are reparameterized in order to obtain a number and distribution of control points which is particularly suitable for the desired deformation. The final NURBS representation of the deformable surfaces is exported from the CAD-programme and made available to the shape optimization framework. As this representation will remain intact throughout the entire optimization process (only the coordinates of the control points are adapted), it can later easily be used to transfer the optimal geometry back into the CAD-programme. As the final preprocessing step, the boundary nodes of the FE-mesh need to be connected to specific parameter values on the NURBS surface. This connection is performed via a fitting algorithm based on a damped steepest decent method.

5. Numerical Examples

We present two examples, where the introduced die design method has been applied to products of varying complexity. The first example is a slit profile and solely used as a test case for the method and the implementation. With the floor skirting profile as a second example, the applicability to more complex profiles is demonstrated.

5.1. Slit Profile

The chosen slit profile has a width of 100 mm and a height of 1.5 mm. In accordance with the scaling presented in Section 4, the corresponding intermediate level has a width of 110 mm and a height of 4.5 mm. The overall length of the extrusion die is 100 mm and the intermediate level is located at one third of its total length. The connection between the inflow, the intermediate level and the outflow has been constructed using a linear morphing algorithm.

Regarding the parameterization, one half of the upper part of the extrusion die has been modeled. It is represented using a NURBS surface with 16 equally-distributed control points. The chosen deformation allows for movement of the two control points indicated in Figure 6.
Both control points are controlled by the same parameter $\alpha$ and are only allowed to move in the direction normal to the surface.

From a theoretical point of view, this particular extrusion die, as constructed using the design method, is already optimal regarding the velocity distribution along the skeleton line. This is due to its symmetry in all directions. Therefore, to start out the optimization, the finite element mesh is deformed away from its optimal position at $\alpha = 0$ to $\alpha = 1$, resulting in a deviation of 1 mm of the two free control points away from their original position. The aim of this test is to see how well the optimization algorithm can find back to the actual optimum of $\alpha = 0$.

Using BOBYQA on a finite element mesh with 2,194,731 elements, the optimal $\alpha$ obtained is $-4.18 \times 10^{-2}$, which is in good agreement with the expected value. The number of function evaluations necessary was 10 when the number of interpolation points was 3. In this case, the objective function (11) has been reduced by 99.05 %. Since the Newtonian constitutive model was used in this case, the optimal value of $\alpha$ (but not of the objective function) is independent of the flow rate. In this case, the objective function has been computed on six subsections (cf. Figure 7). The four middle sections are all of the same size whereas the two end sections have only one half of this size. The purpose of the smaller size of the end sections was to reduce the influence of the wall adhesion effect on the objective function. Figure 7 also compares the average velocity in each subsection for the initial and the optimal geometry.
Figure 7: Velocity distribution at the outflow of the slit geometry. In (b), the average velocity of each subsection is compared for the initial and the optimal geometry.
5.2. Floor Skirting

A more complex extrusion die is depicted in Figure 9. It is designed to manufacture a floor skirting. The channel thickness is 2 mm in all parts of the profile, including the bridge. The profile’s width is 22 mm and the flow channel length is 135 mm. Since the thickness of the entire outflow geometry is uniform, the critical spot as far as the velocity distribution is concerned is the T-junction. Here, the distance to the wall is farther for the material, i.e., the wall adhesion effect is reduced and the velocity increases. At the same time, the velocity in the bridge is severely reduced due to the size of the wall surface. The velocity distribution at the outflow is qualitatively shown in Figure 8 and plotted over subsections in Figure 9. For this particular figure, the volume flow was chosen to be 30.65 cm³/s. The utilized finite element mesh has 688,713 elements.

The subdivisions of the outflow cross section have been chosen in such a way, that the critical spot at the center of the profile is emphasized. In the areas where little changes in velocity are expected over a wide range of the profile, the subsections are chosen larger than in the adjacencies of the bridge. Overall, 9 subregions were created with an area between 4.72 mm² and 46.37 mm² as depicted in Figure 9.

In order to homogenize the outflow velocity, a parameterization has been chosen, which makes the top of the bridge, as well as the surface opposite of the bridge, deformable (cf. Figures 8 and 11). The top of the bridge is chosen, as the initial velocity profile at the outlet shows
a significantly lower velocity in the bridge (cf. Figure 8 and subsections 3, 4, and 5 in Figure 9). By enlarging this area the flow resistance should be reduced and, hence, the flow is accelerated in this section. The surface opposing the bridge is chosen, because it is one industrially applied option to include a dent at this position to raise the flow resistance. The deformation is based on two optimization parameters, one controlling the deformation of the upper surface \( (\alpha_1) \) and one for the lower surface \( (\alpha_2) \). All control points are displaced in the direction normal to the flow direction. The aim is to reduce the flow resistance within the bridge by making it wider and at the same time increase the flow resistance in the bottom part of the die by increasing the amount of wall surface. Deformations induced on the upper surface, i.e., with the design parameter \( \alpha_1 \), almost exclusively affect the velocity in the bridge, which is why its influence on the objective function will be very limited. Even large deformations are expected to have only little effect. Particularly, the optimum with respect to velocity distribution if only \( \alpha_1 \) were to be considered will probably be situated far from the feasible range. This has several reasons: in the setting of the optimization framework, it is the finite element mesh which will become invalid for large deformations; in reality issues like dead water areas and manufacturing restrictions become relevant. Therefore, the design parameter \( \alpha_1 \) is only beneficial in conjunction with other deformations; in this case, the deformation of the lower surface, controlled via \( \alpha_2 \). As the latter deformation occurs in the middle of the main flow channel, it will not only affect the bridge, but also lead to a redistribution of the material between the two sides of the die, affecting the flow in a much larger region. Consequently, the objective function is expected to react much more sensitively to \( \alpha_2 \) than to \( \alpha_1 \).

In order to obtain an overview of the problem, the objective function presented in Section 3.2 is evaluated at selected points in the feasible region of the deformation for both a Newtonian constitutive model and with the Carreau model. The parameter \( \alpha_1 \) is varied between 0 and 2.3 with a step size of 0.25 and \( \alpha_2 \) is varied between 0 and 5.3 with a step size of 0.5. For both scenarios, the optimal value lies at the boundary of the optimization space as far as \( \alpha_1 \) is concerned, but within the optimization space for \( \alpha_2 \). It can be observed that the characteristics are alike for both constitutive models, particularly the location of the optimum which is \( \alpha_{\text{opt}} = (2.3, 5.0) \). Only the absolute values and the slope differ (cf. Figure 10).

In addition to the function evaluations, optimizations were performed with BOBYQA. All optimizations were based on the same parameters for BOBYQA, namely 5 interpolation points
Figure 9: Outflow subsections for the floor skirting die. The nine sections have different sizes; relatively smaller sections help to better capture the critical spot at the T-junction. As material model, the Carreau model with measured values for acrylonitrile butadiene styrene (ABS) has been used.
to approximate the objective functions, an initial trust region radius of 2 and a final trust region radius of 0.01. Regarding CPU time, one function evaluation requires about 5 minutes in the Newtonian case and about 10 minutes in the case of the Carreau model on 32 Intel Xeon E5450 3.0 GHz processors for the flow solution plus one additional processor of the same type for the optimizer. The optimization results support the observations of the function evaluations. Using a Newtonian constitutive model (with viscosity $\eta = 6589 \ P_{as}$) an optimum of $\alpha_{opt} = (2.041, 5.004)$ is determined. The resulting shape is shown in Figure 11 and the velocity distribution is indicated in Figure 9. The objective function is reduced by 37.0 % and 25 function evaluations are needed to obtain this result. When the Carreau model is included into the simulation, the number of function evaluations until an optimum is reached increases significantly. The optimal $\alpha$ obtained for $A = 6589 \ P_{as}$, $B = 0.138 \ s$ and $C = 0.725$, which are material parameters for acrylonitrile butadiene styrene (ABS) determined at the IKV with a high-pressure capillary rheometer, is $\alpha_{opt} = (2.387, 4.857)$. As compared to the starting point $\alpha = (0.0, 0.0)$, the objective function is reduced by 47.7 % after 58 function evaluation steps.

With $A = 6523 \ P_{as}$, $B = 0.0187 \ s$ and $C = 0.9079$, the material parameters for polyvinyl chloride (PVC) again determined with a high-pressure capillary rheometer, the optimal value for $\alpha$ is computed to $\alpha_{opt} = (2.335, 4.569)$ after 35 function evaluations, a value lower than in the case of ABS. As the parameter $B$ is 10 times lower in the case of PVC than for ABS, the range of shear rates in which PVC behaves like a Newtonian fluid is much larger. Apparently, this reduced
amount of non-linearity affects the costs for the optimization noticeably. Taking into account numerical errors in the simulation and uncertainties introduced by the optimization procedure (e.g. influence of the subsection distribution on the objective function, influences due to the iterative nature of the algorithm, such as the stop criterion) the optimal value $\alpha_{\text{opt}}$ is considered to be not significantly dependent on the use of the Carreau model to represent shear-thinning, even for this more complex case compared to the slit considered in Section 5.1. Minding of the increase in the number of function evaluations, the use of the Carreau model cannot be recommended for this case. Figure 11 illustrates the final shape of the deformable domains corresponding to $\alpha = (2.041, 5.004)$, the optimal value in the Newtonian case. Although a significant reduction of the objective function is achieved, the material distribution at the outflow is still not homogeneous enough for the die to be utilized in production. The parametrized region needs to be larger and more complex deformations need to be considered in order to increase the latitude of the optimization framework.

6. Conclusion and Outlook

A new design concept for profile extrusion dies, based on numerical shape optimization, has been introduced and its applicability to industrially-relevant extruded plastic profiles has been discussed. The design concept consists of two steps:
- systematic design of the initial geometry
- numerical shape optimization of the flow channel.

The initial shape is built up from an intermediate level, responsible for the pre-distribution and sufficient acceleration of the material. The quality of this initial die is then improved utilizing a numerical shape optimization algorithm. Key ingredients of the algorithm are the geometry parameterization with NURBS, where the control point positions serve as design variables, and the objective function which is based on a least-squares formulation of maximal and average velocities computed over subsections of the outflow.

Two test cases were presented to illustrate the capabilities of the developed method. The first test case was based on a simple slit geometry combined with a Newtonian constitutive model. It was used to verify the principal functionality of the shape optimization approach. After the initially optimal slit geometry had been deformed, the optimization framework successfully returned to the initial design as the optimal solution. As a second case with a more complex geometry, a floor skirting die has been investigated. The applied deformation resulted in a significant, but not yet sufficient, reduction of the objective function. More complicated deformations will need to be considered in the future offering more design flexibility. In addition, the influence of the applied material model was investigated. The results indicated that for this test case, the consideration of shear-thinning effects does not have a significant impact on the characteristics of the objective function.

In future work, the subject of good parameterizability needs to be addressed as an additional requirement for the initial geometry. This means that the initial geometry needs to be established in such a way, that the number of control points needed to represent this geometry is as small as possible. Particularly, one needs to adjust the local control point density to the desired deformation. Prerequisite for establishing numerical shape optimization techniques as a means of die design in industrial practice is the quantitative assessment of the possible cost and time savings. It is therefore planned to directly compare these figures for the conventional design of a die, and for the proposed approach which relies on the shape optimization framework. To this end, an industrially-relevant profile geometry will be chosen and a suitable die will be designed by an industrial partner monitoring in detail associated time and costs of, for example, the construction and the number of running-in experiments. At the same time, the optimal die shape will be computed by applying the shape optimization framework, and the quality of the resulting die will be
tested in practice on an extrusion line.

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