

Zeitschrift Kunststofftechnik Journal of Plastics Technology

archivierte, peer-rezensierte Internetzeitschrift des Wissenschaftlichen Arbeitskreises Kunststofftechnik (WAK)
archival, peer-reviewed online Journal of the Scientific Alliance of Polymer Technology
www.kunststofftech.com; www.plasticseng.com

eingereicht/handed in: 22.01.2009
angenommen/accepted: 25.08.2009

**Prof. Marek Behr¹, Ph.D., Prof. Dr.-Ing. Dr.-Ing. E. h. Walter Michaeli²,
Dipl.-Ing. Stefanie Elgeti¹, Dipl.-Ing. Mike Nicolai¹, Dipl.-Math. Markus Probst¹,
Dr.-Ing. Björn Fink², Dipl.-Ing. Christian Windeck²**

¹: **Chair for Computational Analysis of Technical Systems (CATS), RWTH Aachen,**

²: **Institute of Plastics Processing (IKV), RWTH Aachen**

Towards Shape Optimization of Extrusion Dies Using Finite Elements

The final shape of profile extrusion dies is determined in an empirical process; a die designer iteratively modifies the shape until the quality restrictions of the extrudate are satisfied. Fluid flow simulations can aid in quickly judging different designs but cannot eliminate the empirical nature of the process. This can be changed by a framework that couples fluid flow simulations with a mathematical optimization algorithm. Without further user interaction, the framework computes the die's optimal shape. The functionality of the framework is demonstrated at the shape of 2D models, these are optimized aiming at a homogeneous velocity distribution at the outlet.

Auf dem Weg zur Fließkanaloptimierung von Extrusionswerkzeugen mit Finiten Elementen

Die finale Fließkanalgeometrie eines Profilextrusionswerkzeugs wird in einem empirischen Prozess bestimmt, in dem der Konstrukteur iterativ Änderungen an der Form vornimmt. Strömungssimulationen können dabei helfen, unterschiedliche Varianten zu beurteilen. Dies ändert aber nichts am empirischen Charakter der Auslegung. Durch die Kopplung von Strömungssimulationen mit mathematischen Optimierungsalgorithmen soll daher ein höherer Automatisierungsgrad erreicht werden. Die Funktionalität der Software wird anhand von 2D-Modellen demonstriert, deren Form hinsichtlich einer Gleichverteilung der Geschwindigkeit am Austritt optimiert wird.

Towards Shape Optimization of Extrusion Dies Using Finite Elements

M. Behr, Prof. W. Michaeli, S. Elgeti, M. Nicolai, M. Probst, B. Fink, C. Windeck

An important aspect in the construction of extrusion dies is the design of the transition region between inlet and outlet of the die. The path to the final shape is many times an iterative and empirical process; a die designer makes decisions about shape modifications. Fluid flow simulations can aid in quickly judging different designs but cannot eliminate the empirical nature of the process. To increase the amount of automation, we propose a framework that couples fluid flow simulations with a mathematical optimization algorithm. The initial design is parameterized by spline curves and design goals are formulated in an objective function. Without further user interaction, the framework computes the die's optimal shape. To demonstrate the functionality of the framework, the shape of 2D models of an infinite slit and a double-slit are optimized aiming at a homogeneous velocity distribution of the plastics melt at the outlet. In both cases, the objective function that measures deviations from a homogeneous distribution is reduced significantly.

1 INTRODUCTION

The rheological design and manufacturing of profile extrusion dies is considered to be one of the most difficult and therefore cost-intensive aspects in extrusion technology with regard to exact and profitable profile shapes [1]. The problem faced by the die designer is the transformation of the originally circular-shaped plastics melt into its desired shape. Only the cross-sections at the inlet and the outlet are fixed (*Figure 1*), whereas the transition region can be altered nearly arbitrarily. For simple geometries such as slits, annular slits etc., there exist analytical solutions for the flow equations [1]. The variety of profile shapes, however, makes it usually impossible to calculate an exact analytical solution.

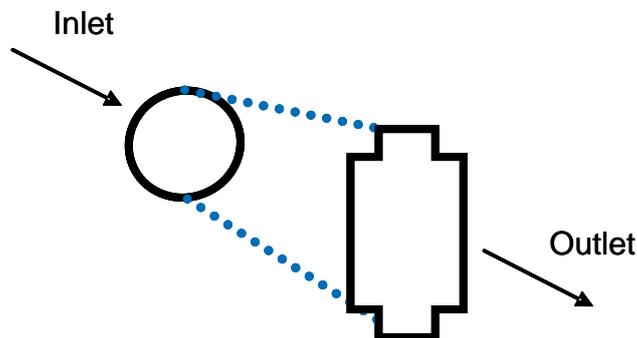


Figure 1: Illustration of the problem

Since it is not possible to calculate the flow channel geometry meeting the requested quality criteria directly, profile extrusion dies are manufactured in an iterative manner. Usually, the die designer designs the flow channels by adding or removing material to the die based upon experience and data obtained from running-in trials. For more complex geometries, up to 15 iterations may be necessary. This kind of die optimization is time-consuming and expensive as large quantities of material are needed and machinery is occupied for a certain amount of time during running-in trials. One option to improve the design process of profile dies is to establish computational fluid dynamics (CFD) based models and to transfer the iterative design process from machinery to computers. As weaknesses can be corrected before the real die is manufactured, the iterative process is simplified. Still, the experience of the die designer remains necessary to decide how the flow channel geometry has to be corrected between the separate simulations to improve the agreement with the quality criteria.

One goal of the cluster of excellence “Integrative Production Technologies for High-Wage Countries” at the RWTH Aachen University is to individualise mass-production. A topic covered in this context is the shortening of the design process for extrusion dies, making the large-scale process extrusion also applicable to smaller scales.

In order to reach this goal, the Chair for Computational Analysis of Technical Systems (CATS) and the Institute for Plastics Processing (IKV) collaborate on improving those production processes. In the past, several research projects at IKV dealt with automated profile die optimization [2, 3], but an important advancement will be the direct integration of a shape optimization tool into XNS, the in-house CFD program developed at CATS. Starting from an initial shape, the program automatically finds the flow channel shape with the optimal fit to the restrictions imposed by the designer. This process does not require any further user interaction. Similar attempts are reported by Sun and Gupta [4], who coupled a 3D flow simulation of a flat die with a BFGS algorithm in order to optimize certain geometrical parameters of the die. Also concerned with optimization of flat dies are Na and Lee in [5]. The parameterization used in

these works is strongly related to the category of the presented die (slit) and lacks extensibility to more complicated profiles. In [6], Debbaut concentrates on die swell and uses optimization techniques to find the outflow geometry, which will lead to a specified product geometry.

This paper will introduce the planned changes in the flow solver and show some numerical test cases in two dimensions that were computed during initial development. Chapter 2 sketches the optimization framework surrounding the flow solver and the underlying methodology, whereas Chapter 3 gives further insight into the geometry kernel needed for handling of the shape deformations. In Chapter 4, objective functions suitable for the extrusion process are presented, leading to the first numerical test cases computed with the new framework in Chapter 5. Chapter 6 is dedicated to conclusions and the next steps.

2 OPTIMIZATION FRAMEWORK

In production technology and other fields of engineering, the term optimization is commonly used to express the fact that a method in question is capable of increasing the efficiency of a process. If computer simulations are involved, this could mean that several scenarios with different production parameters are evaluated, and the "optimal" configuration is then chosen. The limitations of such an approach are obvious: The optimum will depend on the (finitely many) preselected scenarios, and the engineer has to set up all simulations individually.

In contrast, the proposed shape optimization framework automatically selects promising parameter values in an iterative process that does not require user interaction. The parameters can be varied continuously over a wide range. After the user specifies the goal of the optimization and formulates it in a mathematical objective function, the algorithm will start to modify the initial parameters until no further improvement is possible. The objective function to be minimized J can be a weighted combination of several criteria J_i the user wants to be accounted for in the optimization process:

$$J = \sum_i w_i \cdot J_i$$

The shape optimization framework has a modular structure with three main components as shown in *Figure 2*. Thus, high flexibility is accomplished by allowing to substitute single components if desired.

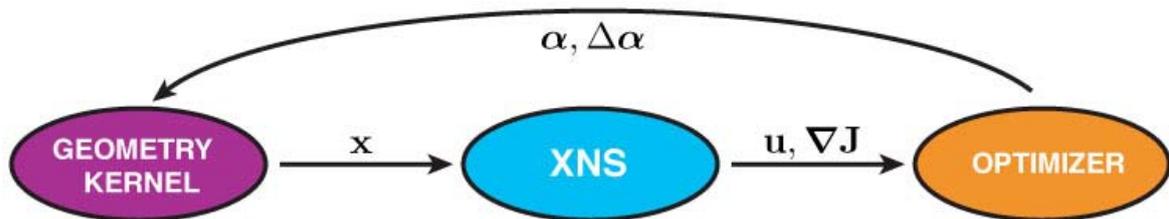


Figure 2: Optimization framework

At the core of the framework is an in-house, highly parallel finite element (FE) solver, which computes the flow field in the extrusion die for a given shape. To account for specific flow characteristics of polymers, the Carreau material model [7], as well as a model for fluids of the Oldroyd family, are implemented in the flow solver [8]. The Carreau model, as shown in (Eq. 1), has recently been added and its implementation was validated against an analytical test case and experiments [9]. This equation connects the relation between the viscosity η and the shear rate $\dot{\gamma}$ with the Carreau parameters A, B and C.

$$\eta(\dot{\gamma}) = \frac{A}{(1 + B \cdot \dot{\gamma})^C} \quad (\text{Eq. 1})$$

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 [10] allowing for simulations with a large number of unknowns.

Automatic optimization depends on an efficient way of generating a new computational mesh in each step, while keeping the number of parameters subject to optimization as small as possible. This procedure is contained in a geometry kernel that forms the second component of the framework. Node movement could for example be prescribed by an explicit mathematical function that depends on a few parameters; however, this approach is typically too restrictive. Instead, the surfaces are parameterized by Nonuniform Rational B-Splines (NURBS), which then determine how interior nodes adjust. This technique is described in detail in Chapter 3.

The third component is an optimizer that gradually minimizes the chosen objective function over the parameter space. For a given parameter vector, the optimizer computes an update that is returned to the geometry kernel, and thus, determines the shape in the next iteration. Currently, the initial shape given to the optimizer is a NURBS model fitted to the original shape of the die that is to be optimized. At a later stage, the optimization framework might also simplify the construction process; it could be sufficient for the design engineer to draw in a CAD software package a rough sketch of the die's shape. The NURBS model

of this sketch could be used as an input to the optimizer that automatically adds more detailed features if necessary. To update the optimization parameters, the proposed framework exploits information about the gradient of the objective function. The gradient can be obtained either with a finite difference approach or, more efficiently, by computing analytic gradients from the solution of sensitivity or adjoint equations [11]. A commonly used, gradient-based optimization method is the so-called Quasi-Newton method [12] in which the first-order Taylor series of the gradient is used to compute the parameter update. The gradient has to vanish at a minimizer of the objective function, which means that

$$\nabla J(\alpha_0 + \Delta\alpha) = \nabla J(\alpha_0) + H\Delta\alpha \quad (\text{Eq. 2})$$

where H denotes the Hessian of the objective function. In Quasi-Newton methods, the Hessian is approximated rather than computed exactly. Taking the identity matrix as approximation in the first step, the parameter update $\Delta\alpha_k$ at step k is computed from (Eq. 2) solving

$$H_k \Delta\alpha_k = -c_k \nabla J(\alpha_k). \quad (\text{Eq. 3})$$

The scalar c_k is obtained in an (inexact) line search process, and the new parameter vector is given by $\alpha_{k+1} = \alpha_k + \Delta\alpha_k$. Figure 3 illustrates the general idea behind a gradient-based optimization algorithm with line search. There are several possible choices to update the approximate Hessian H_k . A popular one is BFGS update (named after its inventors Broyden, Fletcher, Goldfarb and Shanno) that uses the value of the gradient at the new parameter vector α_{k+1} . Setting

$$\begin{aligned} g_k &:= \nabla J(\alpha_{k+1}) - \nabla J(\alpha_k) \\ h_k &:= H_k \Delta\alpha_k \end{aligned} \quad (\text{Eq. 4})$$

the BFGS update is given by

$$H_{k+1} = H_k + \frac{g_k g_k^T}{g_k^T \Delta\alpha_k} - \frac{h_k h_k^T}{\Delta\alpha_k^T h_k} \quad (\text{Eq. 5})$$

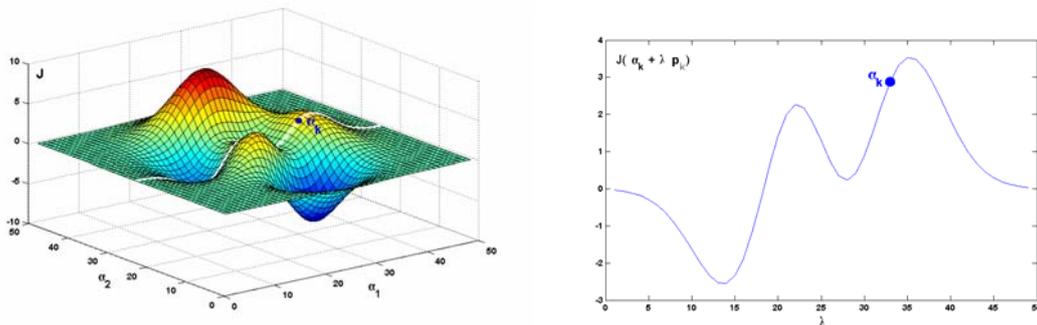


Figure 3: Quasi-Newton line search (left: search direction, right: step size)

It should be noted that the Quasi-Newton method only guarantees to find local minima of the objective function. However, global optimization algorithms are not guaranteed to converge at all. Furthermore, due to the high computational expense for evaluating the objective function, these methods are not suitable for the presented applications.

3. GEOMETRY KERNEL

The optimization process is an iterative process. Each step computes a new geometry and therefore a new mesh is required for the next simulation. In order to keep the optimization procedure independent of other programs (e.g., CAD-software or grid generators), it is convenient and very efficient to deform one initially generated mesh adjusting it to the new geometry. Doing this on an individual node basis however, would result in an unmanageable number of parameters for 3D grids. Parameterization of the geometry will decrease the number of optimization parameters significantly.

In this work, a parameterization with NURBS curves, respectively NURBS surfaces for 3D, has been chosen. NURBS are an important component of CAD/CAM-systems and part of numerous industry standards (e.g. IGES, STEP), guaranteeing the compatibility between shape optimization with the proposed framework and the conventional design process. A major benefit of NURBS is their capability to represent a diversity of shapes, reaching from analytical shapes such as conics and quadratic surfaces to free-form entities most likely found in industrial applications. The shape of a NURBS is controlled through the number and position of its control points, the weights associated with this control point and the scope of the B-spline basis functions between the control points.

A NURBS-curve of degree K is defined as

$$\mathbf{C}(\tau) = \frac{\sum_{i=0}^n N_{i,K}(\tau) \beta_i \mathbf{P}_i}{\sum_{i=0}^n N_{i,K}(\tau) \beta_i} \quad 0 \leq \tau \leq 1 \quad (\text{Eq. 6})$$

where \mathbf{P}_i are the positions of the control points, β_i the weight of each control point and $N_{i,K}(u)$ are the K -th degree B-spline basis functions.

Once the edge of the shape is parameterized through NURBS, it can be modified based on the coordinates and weight of the active control points. For this purpose, each control point is related to the design vector α through a control matrix \mathbf{A}_k in the following way:

$$\begin{pmatrix} \mathbf{P}_k \\ \beta_k \end{pmatrix} = \mathbf{a}_{0k} + \mathbf{A}_k \alpha. \quad (\text{Eq. 7})$$

\mathbf{a}_{0k} is the original state of the control point.

This general formulation, connecting the actual optimization parameter α to the shape, is highly flexible. For example, control points may very easily be made inactive by setting the respective \mathbf{A}_k to zero. Control points that should move symmetrically or antisymmetrically will be controlled by the same control matrix (with different signs in the latter case). In addition, this formulation guarantees differentiability.

4 OBJECTIVE FUNCTIONS

Common objectives in the design of extrusion dies are a uniform velocity distribution at the outflow, a pressure drop which is as low as possible, continuous acceleration of the plastics melt, a short dwell period, and many more.

This description of the objectives needs to be transferred into a mathematical formulation, constituting the so-called objective function (cf. Chapter 0). *Figure 4* exemplifies the following concepts by means of an L-profile. The objective functions that were chosen in this project reflect the uniform velocity distribution in two variants (J_1) and the pressure drop (J_2) as the two main criteria for the extrusion process (cf. [1]). The most useful expression for J_1 still needs to be established in the course of the project. In the first option for J_1 , the variance of

the average velocity in subsections of the outflow is minimized. The advantage is that the results can be easily compared to experiments. The second version of J_1 computes the integral over the absolute value of the gradient perpendicular to the flow direction of the outflow velocity. It is important to note that the nodes on the edges (depicted in pink) need to be excluded from the computation as the no-slip condition at the wall (wall adhesion of the polymer) leads to a locally very steep gradient. This physical phenomenon cannot and should not be circumvented. As far as the velocity distribution is concerned, a value of zero for any of the two versions of J_1 indicates a global optimum, which points to a completely uniform velocity distribution. J_2 is simply the difference between the pressure integrated over the inflow and the outflow domains. This objective function is intended to give a second criterion that will help identify the optimal shape as the first criterion may be satisfied by a variety of possible shapes. If there are two shapes, which satisfy the velocity distribution criterion equally well, the one with the pressure drop lower relative to the other should be the better choice. However, the pressure drop must not decrease below the minimum operating pressure, necessary to keep the process stable. If at all necessary, this could be handled using a penalty approach. The objective functions J_1 and J_2 , and more if necessary, are combined in a weighted sum. The weights are used to emphasize the relative importance of the homogeneous velocity distribution over the pressure drop criterion.

$$J = \sum_i w_i J_i \quad (\text{Eq. 8})$$

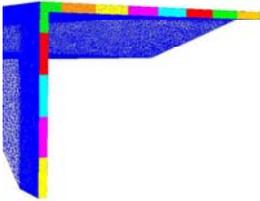
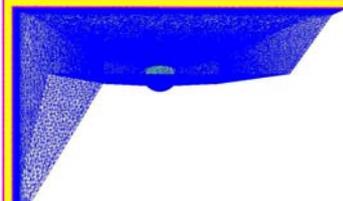
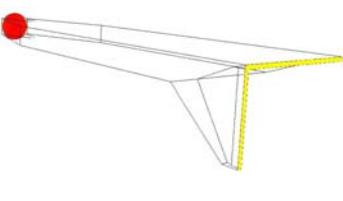
J_1		J_2
$\sum_{\text{region}} (\bar{v}_{\text{region}} - \bar{v}_{\text{total}})^2$	$\int_{\Gamma} \nabla v d\Gamma$	$\int_{\text{in}} p d\Gamma - \int_{\text{out}} p d\Gamma$
		

Figure 4: Objective functions

5 NUMERICAL TEST CASES

The two test cases that will be presented in this paper were designed as a validation of the interaction between all components of the framework, namely the flow solver including its material models, the optimizer and the geometry kernel. Furthermore, they give some further insight into the applicability of the chosen objective functions for the optimisation. All test cases were computed on a single 2.30 GHz PowerPC G5 processor and took between just about 10 and 47 minutes. The rheological data used to describe the shear-thinning fluid is obtained at a capillary rheometer for an acrylonitrile butadiene styrene (ABS), type Novodur P2HE (Lanxess AG, Leverkusen). The Carreau parameters for the shear-thinning fluid are $A=8109$ Pas, $B=0.1148$ s and $C=0.737$, the constant viscosity of the Newtonian fluid is chosen matching parameter A.

5.1 Infinite Slit

The first test case that has been computed with the developed framework is the two-dimensional model of a slit. The scenario is sketched in *Figure 5*. Due to symmetry, only the bottom half of the slit has been modelled. At the inflow (flow rate $1333 \text{ mm}^2/\text{s}$), a parabolic velocity profile is assumed. At the outflow, the flow direction is restricted to the direction normal to the boundary. In between, wall adhesion is assumed. The computations were performed on a triangular finite element mesh with 1325 nodes and 2433 elements, *Figure 5*. The height at the inflow is 2 mm, the height at the outflow is 3 mm and the length in between is 17.25 mm. This resolution proved to be sufficient in a mesh refinement study, as a finer mesh with 5060 nodes and 9721 elements only changed the initial value of the objective function by 0.15 %. The outer part of the geometry (blue in *Figure 5*) has been approximated with a NURBS with seven control points, three of which are unconstrained. *Figure 6* compares the results for a Newtonian fluid and a shear-thinning fluid. The objective function, in this case, resembled the first version of J_1 from Chapter 4. The outflow has been subdivided into six equal pieces, and the variance of the average velocity of each section versus the overall average velocity was minimized. The objective function could be significantly reduced for both the Newtonian and the shear-thinning fluid. The exact values are provided in Table 1.

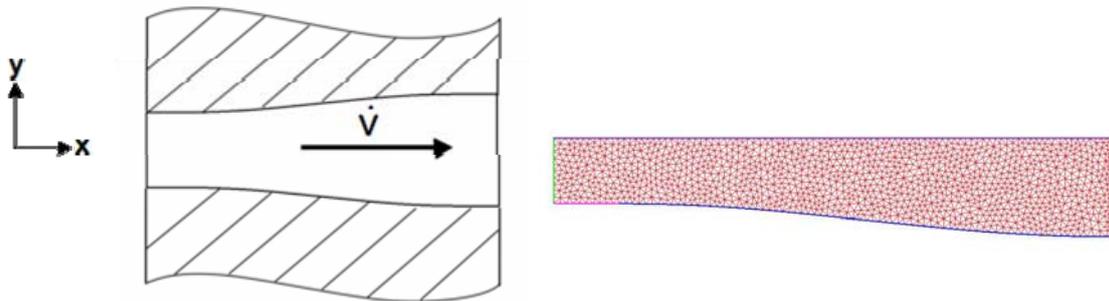


Figure 5: Geometry and mesh for test case 1

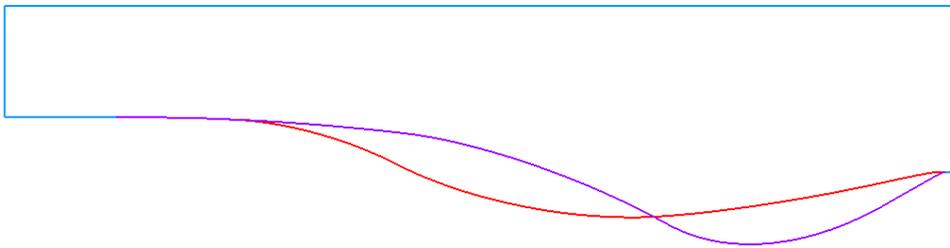


Figure 6: Results with Carreau (red) and Newtonian (purple) material model

	Objective function		
	Initial value	Final value	Reduction [%]
Newtonian fluid	5735.26	4016.47	29.96
Shear-thinning fluid	3354.79	1635.90	51.24

Table 1: Values of the objective function for test case 1 (J_{1a})

In a second run, the objective function was modified and now resembled the second version of J_1 . Confer Figure 7 and Table 2 for the results. Even though the deformation was larger, the overall reduction of the objective function was lower than for the first case.

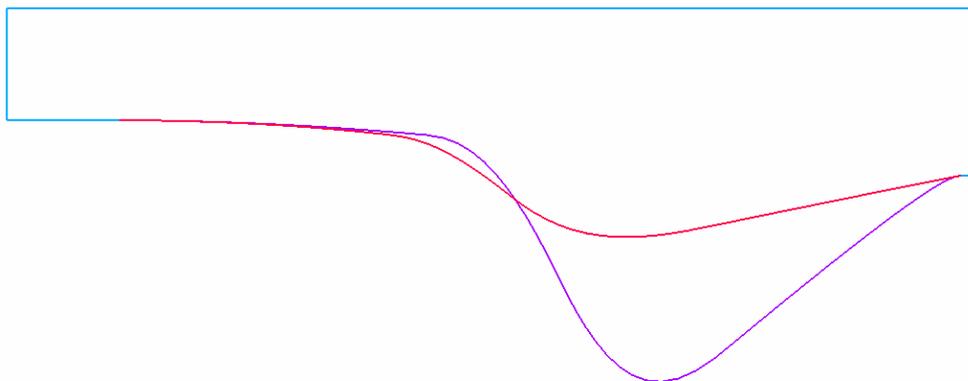


Figure 7: Results with Carreau (red) and Newtonian (purple) material model (J_{1b})

	Objective function		
	Initial value	Final value	Reduction [%]
Newtonian fluid	670.00	611.15	8.78
Shear-thinning fluid	569.60	517.57	9.13

Table 2: Values of the objective function for test case 1 (J_{1b})

In both cases, there needed to be a way to penalize the deformation, preventing the formation of stagnation zones. Instead of implementing an objective function penalizing stagnation zones directly, an effective way to handle this proved to be the inclusion of the quality of the deformed mesh into the objective function, since this value is always computed during the simulation. As all meshes are derivations of one original mesh, a strong deformation of the initial shape will stretch the individual elements of the mesh, leading to a mesh of lower quality. How much emphasis is put on this second aspect is up to the user and will have an influence on the final result, limiting the possible reduction of the objective function. In the future, the inclusion of other penalization terms is planned.

5.2 Double slit

The second test case aims at representing the redistribution of material that will be very important for three-dimensional cases. The geometry is sketched in Figure 8. The velocity profile at the inflow is again assumed to be parabolic. Wall adhesion is assumed throughout the entire profile. The outflow condition again restricts the flow to the direction normal to the boundary. The objective is to match the average velocity of both subdivisions of the outflow (J_1). In the original scenario, the average fluid velocity at the outflow is much higher in the

bottom part, Figure 9 (left). Part of the interior wall (blue in Figure 8) has been approximated with a NURBS of degree 3 with 11 control points.

The material parameters are assumed as in test case 1, the flow rate is $20.8 \text{ mm}^2/\text{s}$. The geometric dimensions are: inflow height 5 mm, height of 2 mm at the top outflow section and of 4 mm at the bottom section. The whole die is 16 mm long. Similar to section 5.1, there is one simulation with a Newtonian material model and one with the Carreau model.

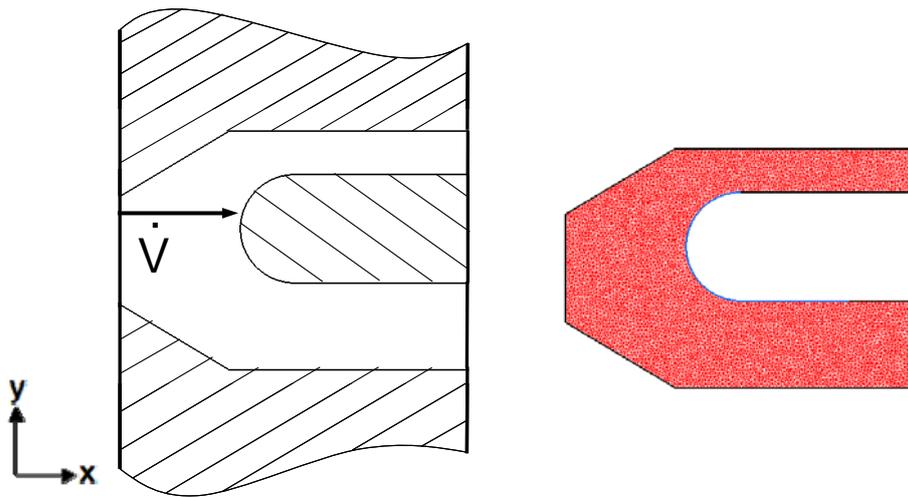


Figure 8: Depiction of test case 2

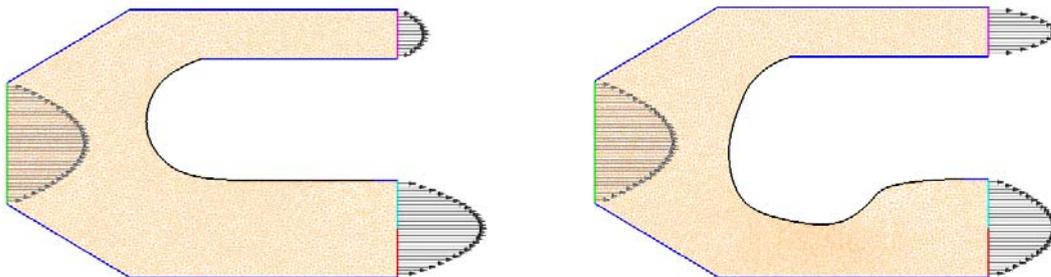


Figure 9: Velocity profile before and after the optimization (Newtonian case)

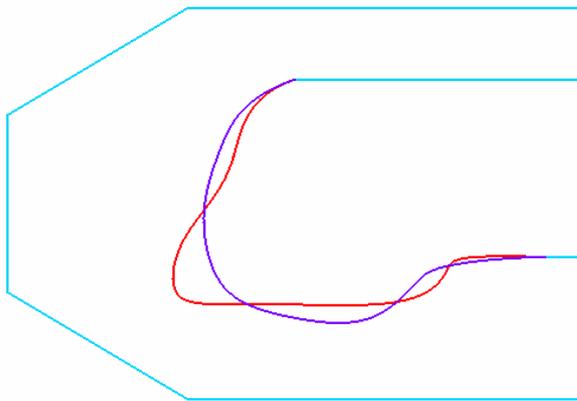


Figure 10: Double slit results with Carreau (red) and Newtonian (purple) material model

	Objective function		
	Initial value	Final value	Reduction [%]
Newtonian fluid	26.46	$0.23 \cdot 10^{-4}$	99.99
Shear-thinning fluid	30.35	$0.22 \cdot 10^{-3}$	99.99

Table 3: Values of the objective function for the double slit

Notice that the results for both cases are almost ideal. An objective function of nearly zero signifies just about equality of the average velocities on both arms. This can also be confirmed visually in the right part of Figure 9.

6 CONCLUSIONS

The previously described methodology provides a fast, efficient way to automatically design extrusion dies. The experience and knowledge of the extrusion die designer enter entirely into the initial stage of the optimization process where desired characteristics, such as a homogeneous material distribution at the outflow, are specified as optimization goals. Leaving the following design optimization to mathematical algorithms opens up the chance of identifying non-intuitive geometries that would not be found in a manual parameter optimization process. Due to the modular structure of the framework, additional optimization algorithms and geometry modification tools can be added provided that suitable interfaces are established.

The next steps will be the explicit calculation of the gradients as well as the extension of the geometry kernel to three dimensions.

Acknowledgement

The depicted research was funded by the Deutsche Forschungsgemeinschaft (DFG) as part of the program Cluster of Excellence "Integrative Production Technology for High-wage Countries" at RWTH Aachen University. We are very grateful for the support of the project.

Our thanks also go to DAAD D/06/28176.

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Stichworte:

Profilextrusion, automatische Optimierung, Fließkanal, Zielfunktional

Keywords:

Profile extrusion, automated optimisation, flow channel geometry, objective function

Autor/author:

Dipl.-Ing. Stefanie Elgeti
 Dipl.-Ing. Mike Nicolai
 Dipl.-Math. Markus Probst
 Prof. Marek Behr, Ph.D.
 RWTH Aachen
 Lehrstuhl für computergestützte Analyse technischer
 Systeme
 Schinkelstr. 2
 52062 Aachen

E-Mail-Adresse: elgeti@cats.rwth-aachen.de
 Webseite: www.cats.rwth-aachen.de
 Tel.: +49(0)241/80-99922
 Fax: +49(0)241/80-99910

Dr.-Ing. Björn Fink
 Dipl.-Ing. Christian Windeck
 Prof. Dr.-Ing. Dr.-Ing. E.h. Walter Michaeli
 RWTH Aachen
 Institut für Kunststoffverarbeitung
 Pontstr. 49
 52062 Aachen

E-Mail-Adresse: windeck@ikv.rwth-aachen.de
 Webseite: www.ikv.rwth-aachen.de
 Tel.: +49(0)241/80-27271
 Fax: +49(0)241/80-22316

Herausgeber/Editor:

Europa/Europe
 Prof. Dr.-Ing. Dr. h.c. Gottfried W. Ehrenstein, verantwortlich
 Lehrstuhl für Kunststofftechnik
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 Deutschland
 Phone: +49/(0)9131/85 - 29703
 Fax.: +49/(0)9131/85 - 29709
 E-Mail-Adresse: ehrenstein@lkt.uni-erlangen.de

Amerika/The Americas
 Prof. Prof. h.c Dr. Tim A. Osswald,
 responsible
 Polymer Engineering Center,
 Director
 University of Wisconsin-Madison
 1513 University Avenue
 Madison, WI 53706
 USA
 Phone: +1/608 263 9538
 Fax.: +1/608 265 2316
 E-Mail-Adresse:
osswald@enr.wisc.edu

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 Fax: 089/99 830 - 156
 E-mail-Adresse: harth@hanser.de

Beirat/Editorial Board:

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