EXTRUSION SIMULATION AND EXPERIMENTAL VALIDATION TO OPTIMIZE PRECISION DIE DESIGN

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Abstract

A CFD-simulation is performed for an existing die and compared with the actual polymer flow and dimensions of the extrudate. Experimental validation of the simulation is used to improve new die design by integrating flow simulation through the 3-D die geometry and the free-surface flow with swelling after the die. Modified die-land-and-lip profile is optimized using the so-called "inverse extrusion" simulation with an objective to improve accuracy of extrudate dimensions.

Introduction

A twin-screw extrusion line has been commissioned recently at Fermi National Accelerator Laboratory (FNAL) in collaboration with Northern Illinois Center for Accelerator and Detector Development (NICADD), to perform R&D, prototyping, and economical production of extruded plastic scintillators for large-scale accelerator detectors. For example, MINOS (Main Injector Neutrino Oscillation Search), a long-baseline neutrino-oscillation experiment, requires several hundred tons of finished plastic scintillators [1]. At about $40 per kilogram cost of cast plastic scintillator, a large-scale detector will not be affordable. However, using extruded plastic scintillators the cost is estimated at about $10/kg, and with further developments, it is expected to go down to $5/kg. The extrusion line consists of a Berstorff 40-mm diameter, 1.36 m long, twin-screw extruder (ZE 40A UTS; 200 HP), two K-Tron automated feeders (for polymer pellets and fluorescent dopants) and Conair downstream equipment (40 cm square, 5.2 m long vacuum and 6.4 m long spray cooling-tanks, belt-puller and saw). A Novatec compressed-nitrogen drier is utilized to purge and dry the polymer pellets before extrusion, in order to improve optical properties of the extrudate.

In a collaborative project with NICADD/FNAL the Department of Mechanical Engineering at Northern Illinois University is developing more effective die design utilizing CFD simulation of extrusion flow and heat transfer processes. The objective is to achieve ultimate precision and quality of different, hollow-extrudate final profiles. Due to inherited sensitivity of final-product quality and precision on multiple controlling parameters of rather complex extrusion processes, the optimal extrusion die design is the first step, to be complemented by an optimal design of vacuum-calibrator sizing-and-cooling tools, as well as investigation and optimization of the extrusion process control for an ultimate quality and precision of the final product. Initial experiments at FNAL with two existing dies are used to validate CFD simulations and to provide critical data, not accounted for by the simulation, for more accurate die design. It has been realized that limitations and benefits of simulation and experimentation cannot replace each-other, but they may complement each-other synergistically. Furthermore, it has been realized that full comprehension of all extrusion processes and polymer melt properties is very important for effective die and calibrator design, and critical for extrusion process set-up and control, to achieve ultimate goal, high quality and precision of final extrudate profiles for plastic scintillators.

Plastic Scintillator Properties

A commercial grade, general-purpose polystyrene, Styron 663, made by Dow Chemical Co, was used as the base material. Its price range is about $1.50 per kg of pellets. The plastic scintillator is made by adding pre-mixed dopants, 1% PPO and 0.03% POPOP, available from Curtiss laboratories (Bensalem, PA, at about $200/kg), into Styron 663 pellets. The measured melt viscosity of Styron 663 with and without dopants, as function of shear rate and temperature are presented on Fig. 1. The viscosity data are curve fitted using the least-square method with the Carreau-Yasuda model, see Eq. (1), and the corresponding coefficients with other relevant thermo-mechanical properties are given in Table 1.

$$\eta = \eta_\infty + (\eta_0 - \eta_\infty)\left[1 + (\lambda\dot{\gamma})^a\right]^{\frac{n-1}{a}} \qquad (1)$$

The polystyrene melt is known as moderately viscoelastic material, however its viscoelastic properties were not available and neglected in our simulation at this time. In addition, viscosity is not only function of temperature and shear rate as measured under isometric flow conditions in a laboratory [2], but also depends on previous shearing and thermo-mechanical degradation in general, which in turn depends on velocity gradients, pressure, and temperature in extrusion barrel and other components, including die. Also, scintillator optical properties are influenced by thermo-mechanical polymer degradation, as well as residual stresses due to finite

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cooling and solidification rates including pulling drawdown during extrusion. These drawbacks could be minimized by better design and control of extrusion components and processes.

Extrusion Die Design and CFD Simulation

According to polymer extrusion experts [3], the complete simulation of the twin-screw extrusion processes should be regarded as one of the '*grand challenge*' problems in polymer processing. However, the continuous and fast development of powerful computing hardware and proficient numerical techniques are now making it possible to simulate, analyze and optimize three-dimensional extrusion processes with complex geometries, as well as non-linear and viscoelastic polymer behavior. However, this is a grand challenge and is not going to be an easy task, but newly developing computing tools have a tremendous potential to uncover important inside details of the extrusion processes, like velocity, pressure and temperature fields in the region of interest, which is not possible to be done experimentally. The main challenge is and will be to completely and accurately represent the polymer material behavior, a very complex viscoelastic melt, which properties are changing from batch-to-batch and are dependent and changing with process parameters, like shearing flow rate and temperature. Another challenge is to properly represent the complex geometry of extrusion devices and accurate boundary conditions which inherently change along the boundaries and in time.

The desired extrudate final-profile is 10 mm × 20 mm rectangular cross section with 1.1 mm diameter circular hole at its center, to accommodate wavelength-shifting optical fiber, which has much higher light attenuation length than the Scintillator bulk. A suitable die is designed and fabricated to provide a streamlined flow and desired extrudate profile, see Fig. 2. In order to simplify fabrication and handling, the die consists of 5 plates, each having its own specific function. After polymer melt exits the extruder barrel and flows through screened breaker plate, it is metered by a melt gear-pump before entering the die. The first die plate, Melt-Pump Adapter, connects the 55 mm diameter output of melt gear-pump to the Spider Adapter plate which in turn connects to the Spider plate with three spiders. The spiders are used to hold a hollow pin to shape the extrudate center hole. A connected hole is made in one of the spiders, from pressurized Nitrogen line to the hollow pin, to maintain gas pressure and thus shape of the hole in the extrudate. Then, the polymer flows through Pre-Land plate (with a centering Bushing), changing its shape from circular to a curved, rectangular-like cross-section of the last, Die Land plate with the uniform cross section, allowing the polymer melt to 'relax' before exiting the die. The center pin is fixed to the spider structure and its exit cross section is an elliptical-like so as to obtain a circular hole in the final extrudate after free flow swelling and relaxation. At the same time the polymer melt exiting the curved, rectangular-like die land cross-section is expected to reshape into desired rectangular profile downstream. The *'art of die design'* is to predict 'properly irregular' die shape (with minimum number of trials) which will allow melt flow to reshape and solidify into desired (regular) extrudate profile. Powerful computational simulations, when properly utilized, will improve and speedup die design, resulting in over-all cost reduction.

The objective of this CFD simulation is to determine the optimum die shape including the die land and pin profiles to obtain the desired dimensions of the extrudate profile. A commercial, CFD finite-element code Polyflow® [4] is used to simulate the three-dimensional (3-D) die flow and heat transfer as well as the free surface flow 25 mm downstream from the die exit, see the corresponding computational simulation domain in Fig. 2. The computational domain resembles the real 3-D die geometry and a free surface flow after the die, where velocity redistribution (equalization) and stress relaxation take place in a short distance downstream from the die exit. Even though the extrudate profile and the die-lip are quadri-symmetrical, due to complex spider-and-transition die structure, it was necessary to simulate half of the real flow domain. The domain is further divided into several sub-domains to facilitate application of related boundary conditions, see Fig. 2, i.e.:

> Inlet (1): fully developed inlet velocity corresponding to actual mass flow rate of 50 kg/hr and uniform inlet temperature (473 K or 200 °C); walls (2): no slip at the die walls ($V_n = V_s = 0$; normal and streamline velocities, respectively), and uniform die wall temperature 473 K; symmetry planes (3): shear stress $F_s = 0$, $V_n = 0$, normal heat flux $q_n=0$; free surface (4): zero pressure and traction/shear at boundary ($F_n = 0$, $F_s = 0$, and $V_n = 0$), and convection heat transfer from the free surface to surrounding room-temperature air; outlet (5): normal stress $F_n = 0$ or specified; all domains: viscous dissipation was neglected for our flow conditions (after verification)

Due to the complex 3-D geometry of the die and the nonlinear relationship between polymer viscosity and shear rate, an elaborate finite element mesh was developed to facilitate numerical stability of the solution, see Fig. 3. It consists of 30,872 elements with structured hexahedral mesh in the die land and free surface, and unstructured tetrahedral mesh in the remaining portion. Simulations are run on a Windows 2.52-GHz-processor PC with 1-GB RAM. On this platform, 19 hours and 36 minutes of CPU time was required to obtain full, non-isothermal inverse simulation results (new die-land profile). However parametric analysis may be and was performed much more efficiently by simulating flow in the die-land and/or pre-land regions only, neglecting inertia term, and with a quarter of the real flow domain due to quadri-symmetry in that region.

Simulation and Actual Test Results

Extrusion simulations were run for the existing die geometry and actual extrusion process parameters. The extrudate profile obtained with simulation is similar to the shape obtained during actual extrusion, compare Fig. 4 (existing-die extrudate simulation profile) with Fig. 5. Midsection sample sagging is due to non-uniform cooling in the calibrator and drawdown downstream which was outside simulation domain. About 5% deviations in width and height may be justified with simulation limitations as well as with effects of cooling and drawdown pulling during actual extrusion. It is also known that die swell ratio becomes smaller as the melting temperature and melting residence time are increased [5]. The powerful 'inverse extrusion' feature of the CFD application software [4] was used to obtain a modified die-land and center-pin profiles to produce a rectangular extrudate with a circular hole at its centre, see Fig. 4. The target product dimensions were given 5% larger (2.1 cm × 1.05 cm) to compensate for the drawdown and cooling effects in the calibrator and further downstream. The program takes into effect the die swell due to velocity relaxation of the melt in the free-surface region as it exits the die, and computes the required die-land and center-pin profiles to obtain the desired extrudate dimensions after the melt exits the free surface region.

Typical results of velocity and pressure distributions are given in Fig. 6. From careful inspection of velocity distribution and the fact that pressure decreases steadily downstream, it is evident that there are no re-circulating regions within the die and that the die is well streamlined. The maximum velocity of the polymer is approximately 14.1 cm/s and the average velocity at the outlet is 6.1 cm/s. The shear rate ranges from zero to 300 sec^{-1}, being the highest at the center-pin wall. Around the die-land walls the shear rate varies in the range from 70 to 150 sec^{-1}. The outer surface of the polymer is cooled from 473 K to 465 K when it comes out of the free surface flow region, 2.54 cm from the die exit.

Conclusion

Simulation results, including 3-D existing die geometry, measured polymer melt viscosity and actual extrusion boundary conditions, were calculated and compared with extrudate profile obtained during actual extrusion. Discrepancies between computational simulation and extrudate dimensions under the well-controlled extrusion process were within 5% and on occasion 10%. It was hard to maintain consistency of final extrudate product, due to some issues in achieving consistent stock feeding and optimum vacuum-calibrator sizing and cooling. However, the existing die simulation profile-form-shape was in qualitative agreement with actual extrusion sample profile.

New, improved die-land profile was designed using so-called inverse extrusion simulation. It is evident that further improvements are possible by including polymer melt viscoelastic properties when available, and improvement of vacuum-calibrator design is critical, since precise hollow-profile dimensions are finalized during cooling and solidification in the vacuum-calibrator and further cooling downstream. Observed inconsistencies in the final extrudate profile indicate the importance of better process optimization and control.

Considering the experience and initial progress in using powerful simulation software and well-equipped and instrumented extrusion line in FNAL, as well as specific issues identified for further investigation and improvements, it is expected to achieve consistent quality and dimensions of the extrudate profile within 1% in the future. Regardless of rather simple final profile, this is still going to be a challenge, due to inherited difficulties in balancing localized cooling of rather thick extrudate profile with internal hole and corners related asymmetry.

References

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Key Words

CFD simulation, inverse extrusion, hollow-profile extrusion, die design

TABLE 1: Doped Styron 663 thermo-mechanical and viscosity properties

Property	Value	*Carreau-Yasuda* coefficients, Eq.(1), at 473K	
Density ρ *[Kg/m^3]*	1040	η_0 *[Pa-s]*	13,400
Specific heat C_p *[J/Kg-K]*	1200	η_∞ *[Pa-s]*	0
Thermal conductivity *K [W/m-K]*	0.1231	n	0.351
Thermal volumetric coefficient β *[m/m-K]*	6.60e-5	λ	0.527
		a	0.845

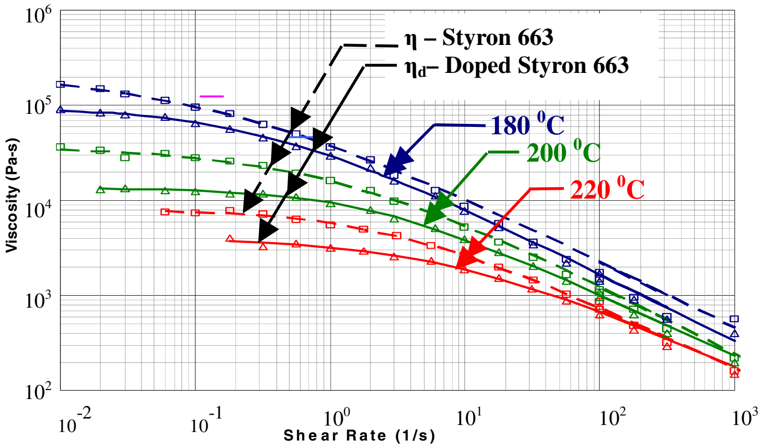


Fig. 1: Styron viscosity data, with and without Scintillator dopants

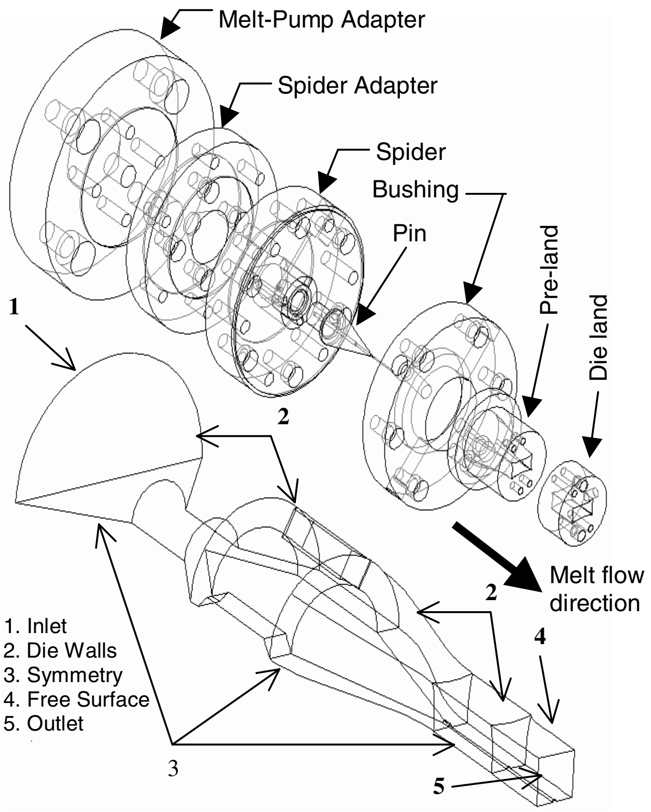


Fig. 2: Exploded view of extrusion die and computational and boundary domains

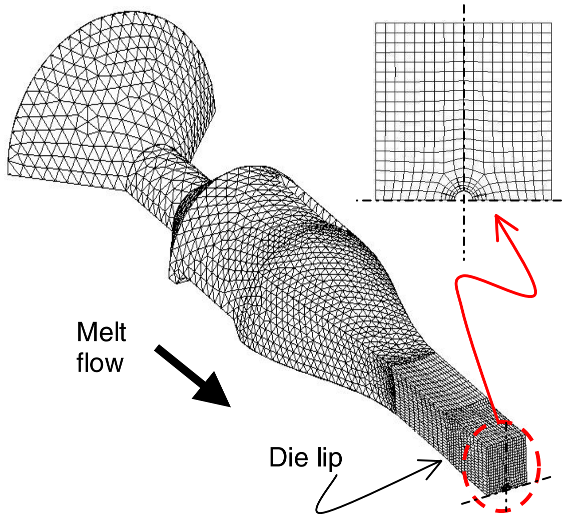


Fig. 3: Finite element 3-D domain and half of extrudate profile mesh

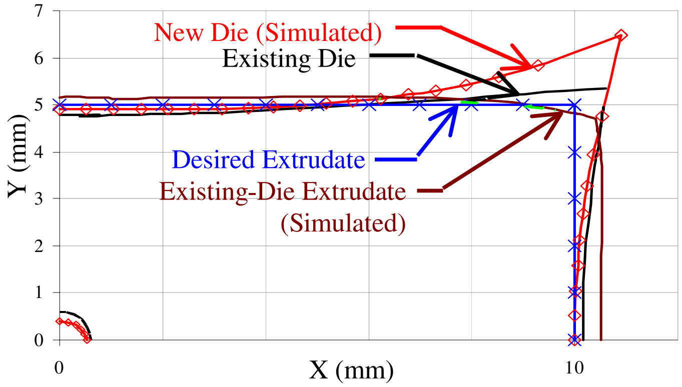
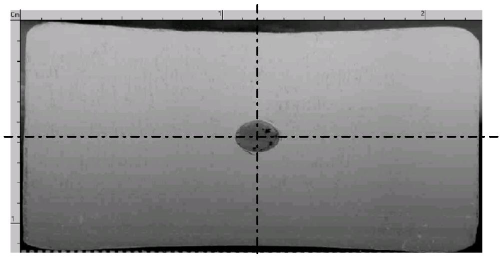


Fig 4: Existing die, corresponding simulation and new improved-die profiles



$V_{take\text{-}up} = 6.02$ cm/s, $P_{Vacuum} = 2.5\ H_2O$, and $P_{N2} = 7.9\ H_2O$

Fig. 5: Typical extrudate sample profile

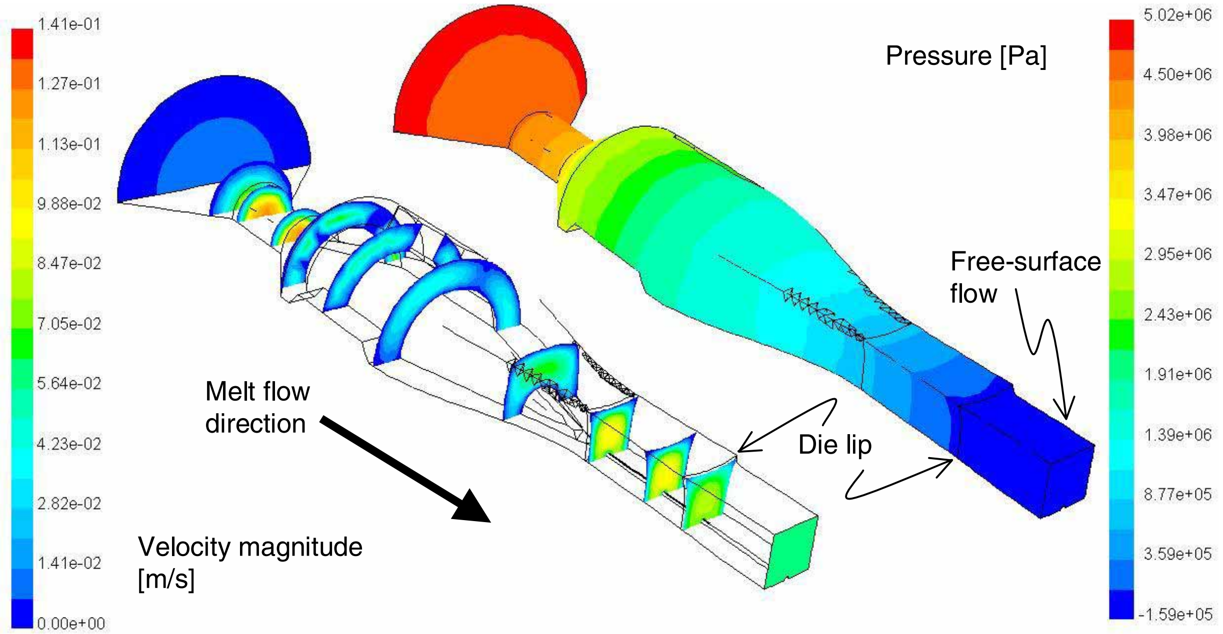


Fig. 6: Contours of velocity field at different cross-sections and pressure distribution simulation results