Polymer Extrusion Simulation and Die Design:
Grand Challenge and Opportunity

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According to well known experts in this area (Osswald and Gramann, 2001)[1], the complete simulation of the twin-screw extrusion processes should be regarded as one of the '*grand challenge*' problems in polymer processing.

The continues 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, including moving and rotating solid-machinery boundaries and moving free-surface boundaries, 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 accurately represent the complex geometry of extrusion devices and accurate boundary conditions which inherently change along the boundaries and in time.

However, suitable simplifications, based on profound understanding of underlying physical phenomena and utilizing existing empirical results, will provide effective simulation and optimization, which when coupled with critical experimentation, may qualitatively improve design and production speed and product quality, and thus reduce cost of complex polymer extrusion processes and die designs. Computational simulation alone can not replace existing empirical engineering and experience, but it does and will, more-and-more, provide critical results about inner flow and heat transfer phenomena (a critical view inside the "black-box"), which could not have been investigated by any other means. Thus, computational simulation can not and will not compete and displace empirical and experimental engineering, but will complement and enhance it to a new higher level by providing more effective and systematic use of existing experimental results, true what-if-analysis and much faster and less expensive design optimization, and increased quality of the extrusion processes and products.

Polymer extrusion, as one of the most important polymer processing methods, is a very complex and involves the following:

1. Preparation and feeding granular polymer material to the extruder, in some cases including provision of special environmental conditions (oxygen reduction, etc.).
2. Complex mixing, melting, forced flow with moving solid boundaries of extruder screw(s), and heating and cooling of the melt to desired conditions.

[1] T.A. Osswald and P.J. Gramann, *Polymer Processing Simulation Trends*, Society for the Advancement of Material and Process Engineers, Erlangen, Germany, 2001.

3. Constrained flow with heat transfer through the die of a very complex, non-Newtonian polymer melt, which, after exiting through the die lip, continues with moving free boundary flow, where residual stresses in combination with the stretching (pulling) stresses, result in material swelling or/and shrinkage and warpage, which influence the final profile accuracy of the extrudate.

The final extrudate profile dimensions and its consistency and accuracy, depend on: (***a***) overall material properties, (***b***) extruder and die mechanical design, and (***c***) overall process control, including mechanical (kinematics and dynamics), material flow pressure and temperature, and environmental conditions. This is further complicated in polymer processing due to the fact that its critical viscoelastic properties are highly non-linear and dependent on previous stress-strain history and temperature, thus highly dependent on overall velocity and temperature profiles which in turn are dependent on extruder and die dimensions, and process parameters and control. All of this makes it a difficult challenge to produce needed consistency from polymer batch-to-batch, and process control from shift-to-shift.

That is why the polymer extrusion and die design engineering have been, so far, mostly relying on experience, empirical data, and expensive trial-and-error adjustment and tweaking of the die design and process parameters control. However, it is becoming now possible to integrate computational simulation and analysis with existing empirical and experimental experience, and qualitatively raise the polymer extrusion process control and die design to the next level, by substantially increasing the product quality and speed, while reducing the process design and production time, and overall cost.

It is important to repeat again, that computational simulation and empirical extrusion engineering have their exclusive strengths and weaknesses and can not replace each-other, but if properly integrated, will strongly complement each-other, resulting in a *synergistic result* which is much greater than the simple sum of the two constituents.