# Polymer Processing Simulations Trends

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## 1 Introduction

In most polymer processes the quality of the final part is greatly dependent on the melting, flow and mixing of the polymer. The optimization of the equipment and manufacturing process, as done today, is time consuming and expensive. Quantifying flow and heat transfer is an even more intimidating task. Furthermore, reproducing the properties of a particular blend from batch to batch, or part performance from shift to shift, can be extremely difficult. Obviously these barriers make numerical simulation of polymer processes a viable alternative when optimizing and analyzing the process.

Traditionally, when simulating polymer processes the main concern of the engineer has been to accurately represent the material behavior using complex models. Although many problems still exist regarding polymer material models, today one can easily deal with the shear thinning behavior, temperature dependence and to some degree the viscoelasticity of polymers. In fact, to date a large number of processes have been realistically simulated in polymer processing ranging from mold filling with fiber orientation, shrinkage and warpage to extrusion with viscoelastic effects. However, only a few fully three-dimensional models of realistic processes have been solved. Simulating a fully three-dimensional process involves intensive labor trying to accurately represent the geometry of the device and also requires large amounts of computation and data storage. Obviously, computational demands have been dampened by the enormous increase in computational power available to the engineer at the desktop. The labor intensity and requirements of computer performance are multiplied by the added complexity of moving boundaries. There are two types of moving boundaries that are very common in polymer processing: *moving free boundaries* and *moving solid boundaries*. Moving free boundary problems are encountered in mold filling, extrudate swell, coating problems, inside the extruder at the screw, to name a few. Solid moving boundaries are those where the actual cavity that contains the polymer changes in shape during the process, i.e. the rotating mixing heads in an internal batch mixer or the screw and mixing elements in a single screw extruder. An assumption that the device is completely filled with melt is taken, which may not always be realistic The most complex process that involves solid moving boundaries is the intermeshing twin screw extruder. Here, the domain of interest, i.e. the polymer, is constantly changing shape as the screws, mixing heads and kneading blocks rotate. The self-wiping arrangement of these systems adds to the complexity of the problem, since it involves very small gaps, which introduce numerical complications. One should regard the complete simulation of the twin screw extrusion processes including melting, melt conveying, mixing, die flow to the prediction of final morphology, including coalescence and a partially filled system, should be regarded as one of the grand challenge problems in polymer processing.

The advent of more powerful computers and efficient numerical techniques are now beginning to make it possible to simulate three-dimensional problems of complex geometry with non-linear material behavior.

This paper presents a general overview of the state-of-the art techniques used for the modeling and simulation of polymer processes. A brief background on numerical techniques and basic modeling in polymer processing is presented. A discussion on two-dimensional models that are used to simulate three-dimensional flows is followed by recent advancements in full three-dimensional models.

## 2. Rheology

Most polymer processes are dominated by the shear strain rate. Consequently, the viscosity used to characterize the fluid is based on shear deformation measurement devices. The rheological models that are used for these type of flows are usually termed *Generalized Newtonian Fluids (GNF)*. In a GNF model the stress in a fluid is dependent on the second invariant of the stain rate tensor, which is approximated by the shear rate in most shear dominated flows. The temperature dependence of GNF fluids is generally included in the coefficients of the viscosity mode. The shear viscosity of a typical polymer melt is shown in Fig. 1. Various models are currently being used to represent the temperature and strain rate dependence of the viscosity.

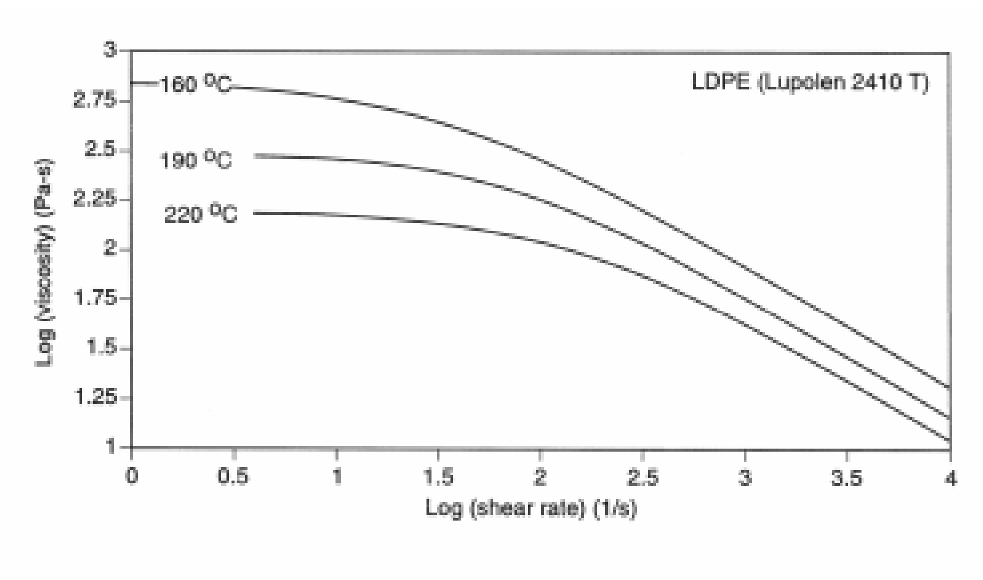


*Figure 1. Shear viscosity curve for LDPE*

The power law model is a simple model that accurately represents the shear thinning region in the viscosity curve, but neglects the Newtonian plateau at small and large strain rates. The major disadvantage of this model is that the viscosity goes to infinity at low stain rates and zero at high strain rates. The infinite viscosity leads to erroneous results in problems where there is a region of zero shear rate, such as in the center of a tube. However, this problem can be overcome by using a truncated model where a constant viscosity is assumed in the strain rate region of Newtonian behavior.

A model that fits the complete range of strain rate is one developed by Bird and Carreau [1]. The Bird-Carreau model accurately models the Newtonian plateau observed at low and sometimes high strain rates, and the shear thinning region in-between.

The Bingham model represents the rheological behavior of materials that exhibit a “no flow” region below certain yield stresses, such as polymer emulsions, slurries and some food products such as ketchup. Above a yield stress the material flows like a Newtonian liquid.

The tendency of polymer molecules to “curl-up” while they are being stretched in shear flows results in normal stresses in the fluid that greatly affect the flow field in certain cases. Additionally, most polymer melts exhibit an elastic as well as a viscous response to strain. This puts them under the category of viscoelastic materials. There are no precise models that accurately represent this behavior in polymers. However, various combinations of elastic and viscous elements have been used to approximate the material behavior of polymer melts[1]. Some models are combinations of spring and dashpots to represent the elastic and viscous responses, respectively. The most common ones being the Maxwell model for a polymer melt and Kelvin or Voight model for a solid. One model that represents shear thinning behavior, normal stresses in shear flow and elastic behavior of certain polymer melts is the K-BKZ model [2-3].

Elongational of “shear-free” flows are the least studied types of flows that occur in polymer processing. A major reason for this is that they are not as common as shear flows that dominate extrusion and injection molding. However, in certain polymer processes, such as fiber spinning, blow molding, thermoforming, foaming and compression molding, under specific processing conditions, the major mode of deformation is elongational. Moreover, the elongational viscosity that is needed for simulation is difficult to measure and thus requires expensive equipment.

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[1] For a more detailed presentation concerning rheological models the reader is referred to Bird, R.B., R.C. Armstrong and O. Hassager, Dynamics of Polymeric Liquids, Vol. 1, Wiley, New York (1987). In addition, Bird and Wiest give a complete review paper on models available to model viscoelastic behavior of polymer melts in Bird, R.B., and J.M. Wiest, "Constitutive Equations for Polymeric Liquids,*" Annu. Rev. Fluid Mech., 27,* 169-93, 1995.

## 3. Modeling

In order to be able to predict and model complex polymer flows, one must first have a basic understanding of the mathematics that govern the flow. Regardless of the complexity of the flow, it must satisfy certain physical laws. These laws can be expressed in mathematical terms as the conservation of mass, the conservation of momentum, and the conservation of energy. In addition to these three conservation equations, there may also be one or more constitutive equations that describe material properties, i.e. shear thinning behavior. Since these equations may also be coupled together, i.e. temperature dependent viscosity, the solution can become even more complex. The goal of the modeler is to take a physical problem, apply these mathematical equations and solve them to predict the flow phenomena. Although analytical solutions to the conservation equations for some simple two-dimensional shapes are available, when more complex two-dimensional problems or three-dimensional analysis are required, numerical methods are required. There are three basic classes of numerical techniques that are commonly used to solve complex fluid flow problems (Fig.2). They are: the finite difference method (FDM), the finite element method (FEM), and the boundary element method (BEM). Each of these methods has its own advantage and disadvantages and, therefore, one may be preferred for certain type of process or material. Each technique has been adapted in some form for specific problems encountered in polymer processing.

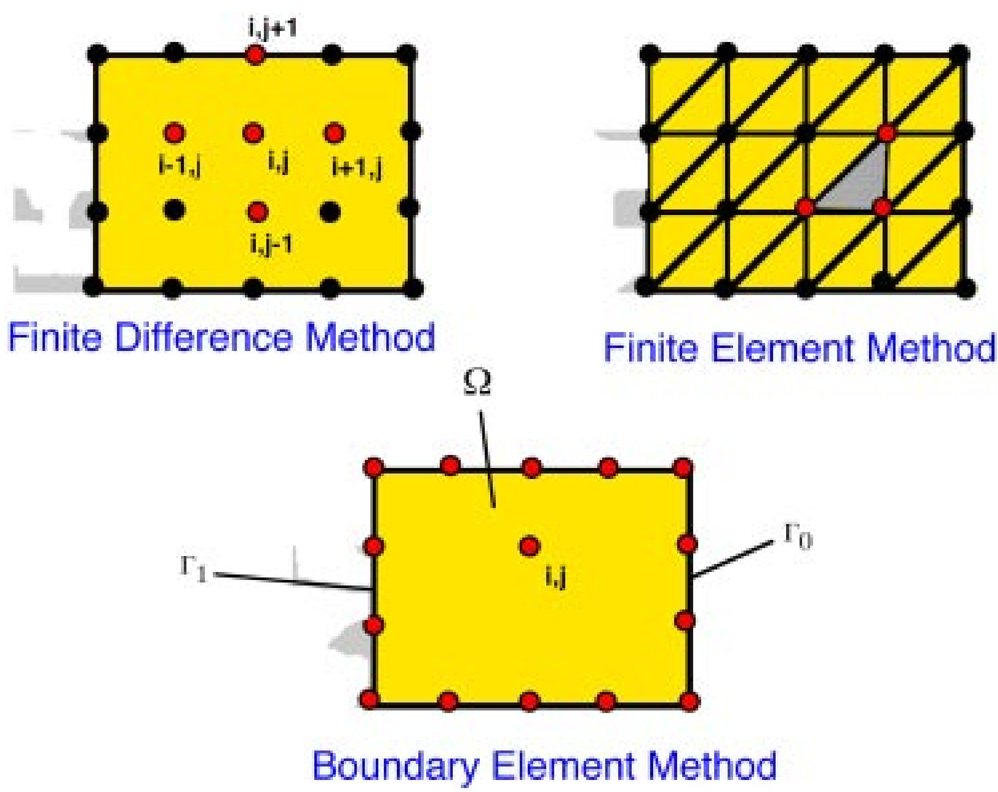



*Figure 2. Comparison between various numerical techniques*

## 3.1 Finite Difference Method

The finite difference method started gaining prevalence in the 1930's for use in hand calculations and is the simplest to use and understand. Figure 2 shows the grid that would be constructed to represent the geometry of a two-dimensional domain. Once the grid is created, the governing differential equations are rewritten in a discretized form and then applied at each nodal point. The resulting system of algebraic equations can then be solved for by standard Gaussian elimination or more elaborate numerical algorithms. Because of the simplicity of the method, it can implemented in a wide variety of problems. The method discretizes the governing equations at the start of the analysis, and it lends itself to model non-linear problems. The finite difference method is also easy to program and computer simulations can provide quick computation times. The first consideration when implementing the FDM is that it is best suited for cases that have relatively simple geometries. Even though more complex geometries can be modeled with special differential equations or coordinate transformations, there are still limitations that exist, and the other methods presented in this paper often prove to be more efficient. However, for a quick assessment of a process or product performance, often a 1D simplication of the process can yield useful results. Such is the case with the simplified solution of injection mold filling presented in Fig.3.

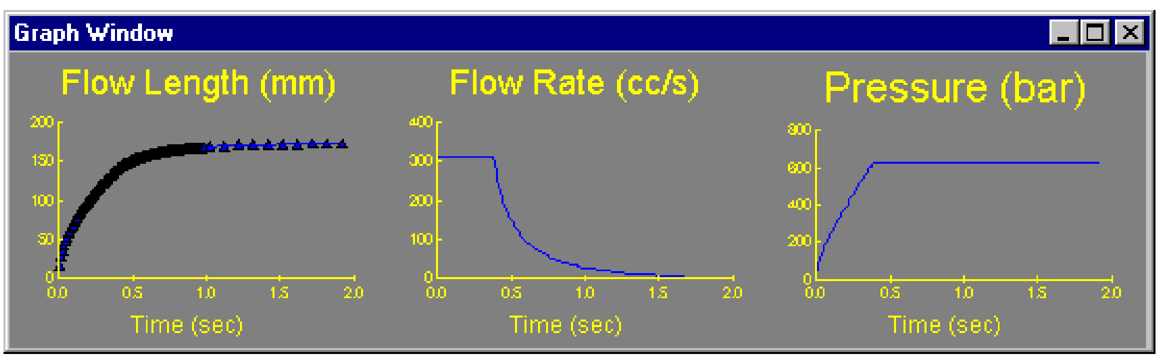



*Figure 3. Flow length, flow rate and pressure prediction during injection molding using a 1D FDM simulation program.*

## 3.2 Finite Element Method

In contrast to the FDM the finite element method is a relatively new technique used for solving fluid flow problems. Popularized in the 1960's along with the advent of digital computers, the finite element method has become the basis for most commercial structural dynamic and fluid flow simulation programs. Like

FDM, FEM is a domain method in which the entire geometry to be modeled must be discretized into nodes and elements. The mesh shown in Fig. 2 represents the discretization required for FEM to model a two-dimensional geometry. Although several different methods are available to obtain the final equations, the Galerkin method of weighted residuals is normally preferred in fluid flow problems. Once the mesh has been created, the governing differential equations are then expressed in integral form and numerically integrated to obtain an algebraic system of equations. Because of the nature of the finite element method, it is capable of modeling much more complex geometries than FDM. It can also provide quite accurate solutions to the field variables, such as fluid velocities or pressures, for a wide variety of problems that include non-linear flows. However, higher order derivative solutions, such as velocity gradients, tend to be less accurate. Without complex adaptive meshing techniques, FEM is also difficult to use for problems with moving solid boundaries. Since the governing equations are approximated with the Galerkin method, they have a certain amount of intrinsic error even before numerical errors are accounted for, which is carried throughout the computation. This can cause the FEM to become unstable in highly non-linear situations. Although this can be partially alleviated by special upwinding techniques it nonetheless increases the amount of computation effort. In addition, since the solution is computed only at the nodes and the velocity field must be interpolated, the tracking of particles in the flow field in not easily accomplished with FEM.

However, FEM is extensively used when simulating processes that are highly non-linear such as flow of viscoelastic materials. For example, Fig.4 shows predicted extrudate swell of HDPE flowing through a converging die [4]. Mitsoulis [4] predicted the flow of various materials through dies of different geometry using the K-BKZ model. His numerical results compared well with experiments.

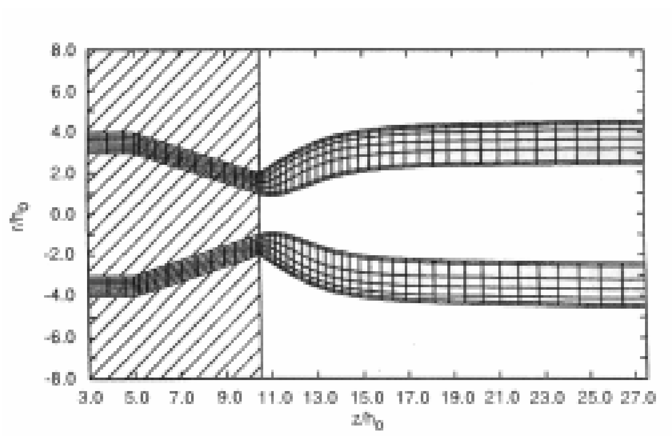



*Figure 4. Predicted extrudate swell of HDPE flowing through a converging die.*

The finite element has also proved to be ideal when simulating mold filling processes, fiber orientation, shrinkage and warpage of thin plastic parts. The major difficulty which arises when simulating molding processes (and other moving boundary processes) is tracking the transient free surface (or solid moving boundaries during mixing). The material constantly changes shape as it flows and is deformed inside the cavity, making it necessary to redefine the geometry of the domain of interest after each successive time step. Redefining the finite element mesh or finite difference grid is the most tedious part of simulations when dealing with moving boundary problems and many times makes it unreasonable to simulate.

Kouba and Vlachopoulos [5] and deLorenzi and Nied [6] developed a technique to model membrane stretching during blow molding and thermoforming. Although the processes are basically three-dimensional, they can be represented with two-dimensional plate elements oriented in three-dimensional space.

Tadmor, Broyer and Gutfinger [7-8] used a spatial finite difference formulation to solve two-dimensional flow problems in complex geometrical configurations. Using a Hele-Shaw [9] formulation to simulate the flow; their method is applicable to flows in narrow gaps of variable thickness, such as injection molding of thin parts and flows inside certain extrusion dies. This technique is known as the flow analysis network (FAN), and works well for Newtonian and non-Newtonian fluids. The method uses an Eulerian grid of cells that covers the flow cavity. A fill factor is associated with each cell, a number that varies between zero and one. A fill factor denotes an empty cell, and a fill factor of one denotes a cell that is full of material. A local mass balance is made around each cell, which results in a set of linear algebraic equations with pressures at the center of the cells as the unknown parameters. The pressure field that results from solving the set of equations is used to calculate the flow distribution between the cells, which in turn is used to advance the flow inside the cavity by updating the cell fill factors. A major disadvantage of this technique is that relatively fine meshes are required, especially if curved boundaries are present in the geometry. This disadvantage can be overcome by using finite difference operators, however, this makes the simulation awkward and difficult to use.

Osswald and Tucker [10] and Wang et al. [11] modified the flow analysis network to model the non-isothermal flow of non-Newtonian fluids inside thin three-dimensional cavities using finite elements. The technique, which is commonly known as the control volume approach (CVA) requires that the three-dimensional molding surface be divided in flat three- or four-noded finite elements. Cells or control volumes are generated by connecting element centroids with element mid-sides. When applying the mass balance to each cell, the resulting equations are the same than those that result from applying the Galerkin method to the governing equation for pressure. This allows the use of standard finite element assembling techniques when generating the set of liner algebraic equation. A typical configuration of elements and nodal control volume is shown in Fig. 5. In the figure the solid lines denote element sides and the dashed lines represent the control volume boundaries. The hashed area represents the control volume for node *i*. This technique remains the dominant form of modeling mold filling processes such as compression and injection molding.

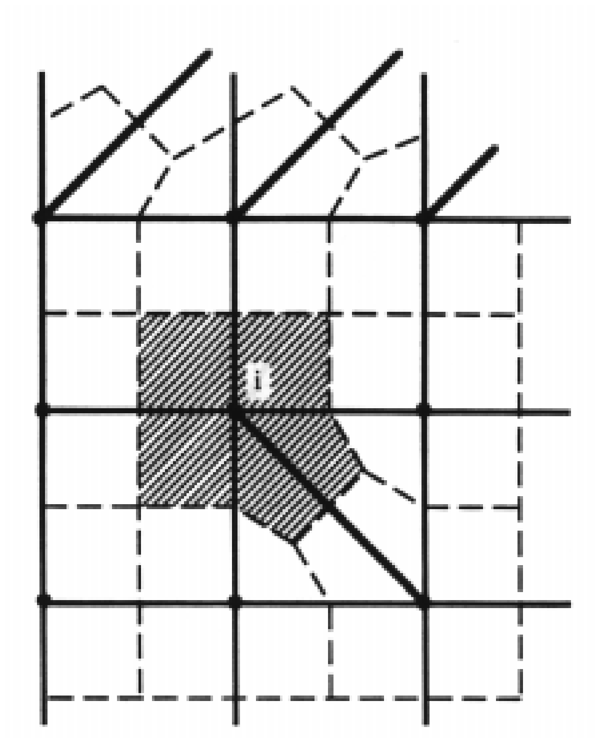



*Figure 5. Finite element / control volume configuration*

Commercially available software packages all use this technique to track the flow fronts during mold filling. As an example Fig. 6 presents the mold filling pattern during mold filling of a compression molded SMC part represented with the mesh shown in Fig.7. Figure 8 presents the fiber orientation distribution within the compression molded fender shown in Figs.6-7. Mold filling simulation programs have shown good agreement with experimental results. Work still needs to be done when predicting mold filling of very thin injection molded products. Since the industry is constantly reducing part thickness, this issue remains a top research priority for the injection molding community.

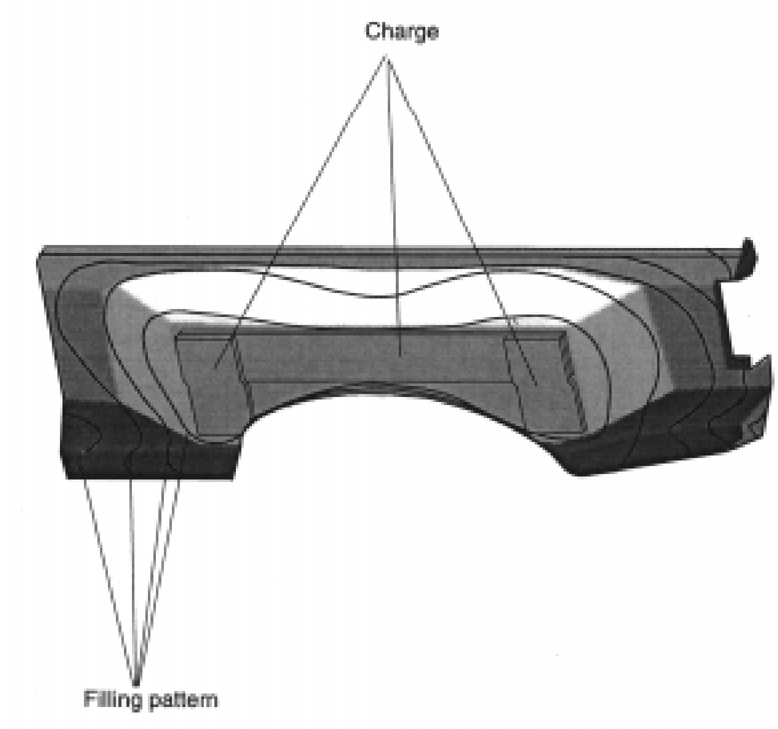



*Figure 6. Simulated mold filing pattern during compression molding of an automotive SMC fender.*

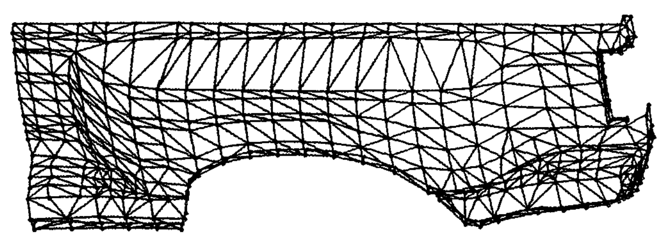


*Figure 7. Finite element mesh of the automotive fender*

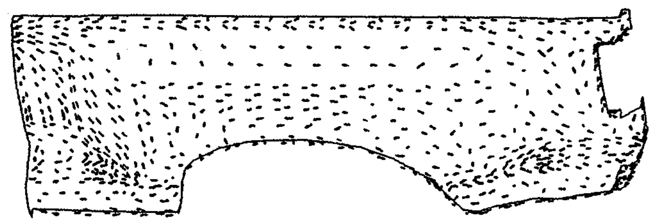
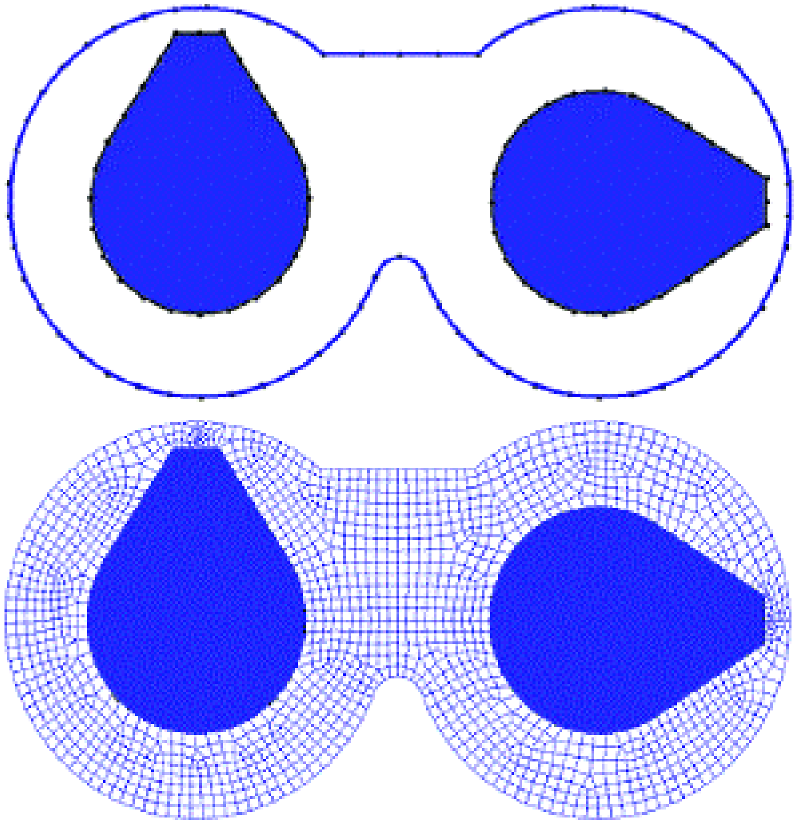


*Figure 8. Fiber orientation prediction within the compression mold automotive fender*

### 3.3 Boundary Element Method

In contrast to both the finite difference and finite element methods, the boundary element method (BEM) only requires that the boundary or surfaces of the geometry be discretized. As shown in Fig. 2, a two-dimensional geometry only requires a discretization of the curve that makes up the boundary of the part. In essence, the order of analysis being made is reduced by one. Figure 9 compares FEM and BEM discretizations of a two dimensional model of an internal batch mixer [12].

BEM also gained prevalence around the same time as FEM, but because of the relatively complex mathematics involved with BEM, it has been relatively slow to gain the same level of acceptance that FEM did in the engineering community, and has been primarily used by mathematicians. The formulation of the boundary element method begins with a different form of the governing equations, which are expressed in terms of domain integrals. These integrals are manipulated by Green-Gauss transformations until they are reduced to boundary integrals. The integrals are then numerically evaluated to yield an algebraic system of equations. Interestingly, up to the point of evaluating the integrals, no approximations have been made in the governing equations. Thus, the boundary element method, unlike the FDM or FEM, does not introduce any error to the solution until the boundary is discretized – the boundary element solution is *exact* up until the geometry is meshed. Another advantage of BEM is that the accuracy of higher order derivatives is excellent. This becomes extremely important when trying to calculate heat transfer effects or track particles. Here, the boundary element is well suited to track particles in the flow of material since the solution at any location in the fluid can be obtained quite easily and very accurately.



*130 nodes*

*4921 nodes*

*Figure 9. BEM and FEM discretization of a 2D (completely filled) internal batch mixer*

A typical simulated mixing history inside the above internal batch mixer is presented in Fig. 10[13]. It is important to point out that, up to date, all mixing analyses performed on internal batch mixers assume a full mixing cavity. However, a mixing process greatly depends on the fill factor of the mixer. This remains an area of research of the polymer processing research community, and can be eventually addressed using BEM.

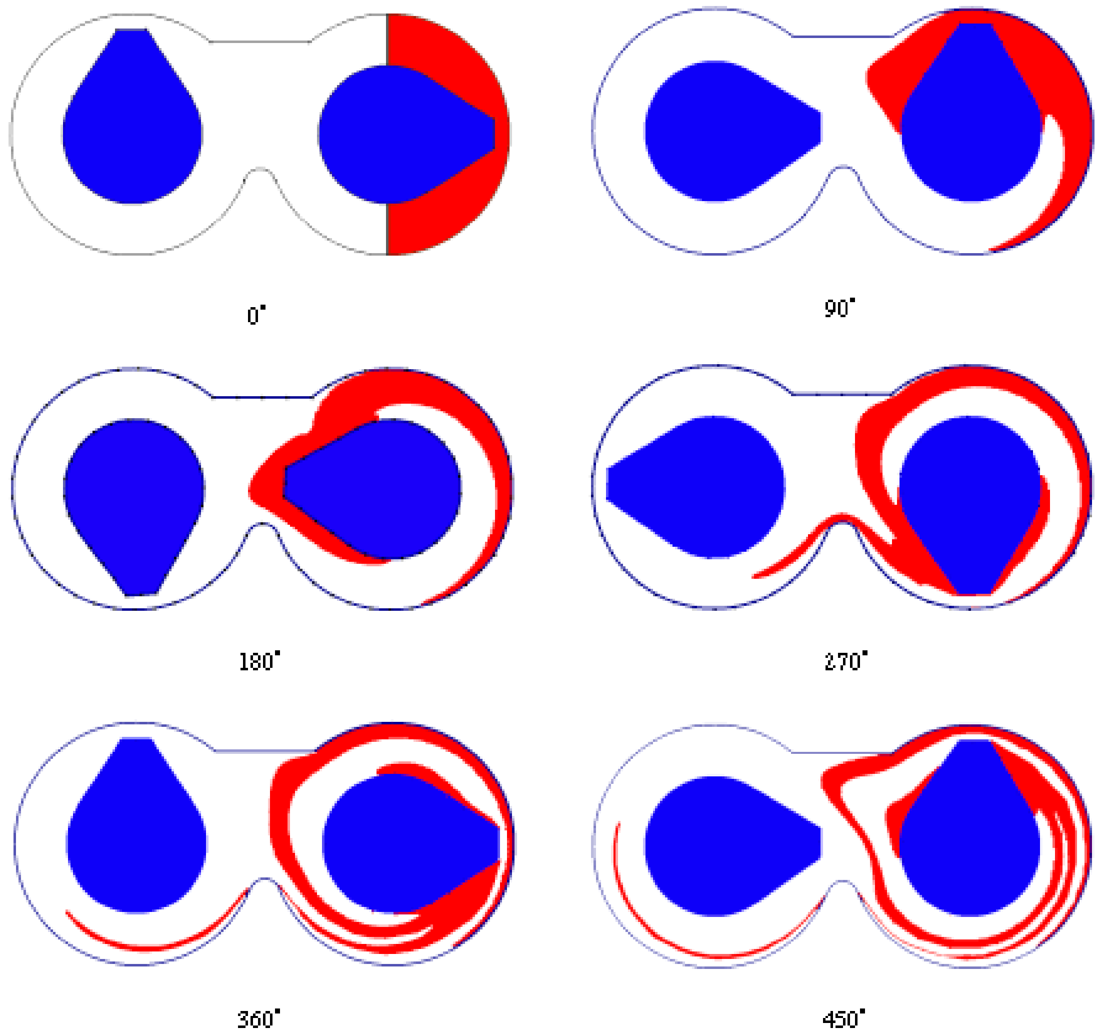



*Figure 10. Simulated domain deformation during mixing.*

Other areas where BEM is being applied are complex three dimensional flows such as shown in Fig.11 below. Here, a double flighted co-rotating twin screw extruder was simulated using a 3D BEM simulation {Krawinkel]. Although BEM has proven very versatile when dealing with complex geometries, the technique is still primarily being used to simulate linear problems such as linearly elastic stress strain problems or Newtonian flow problems. However, research is underway to simulate non-linear problems with BEM and still maintain the boundary only discretization. Since BEM generates full unsymmetric matrices it does not bring a great gain in computational savings. However, the greatest advantage of BEM is the ease with which a complex geometry is generated and simulated, significantly reducing problem preparation time and practically eliminating the need of user interaction.

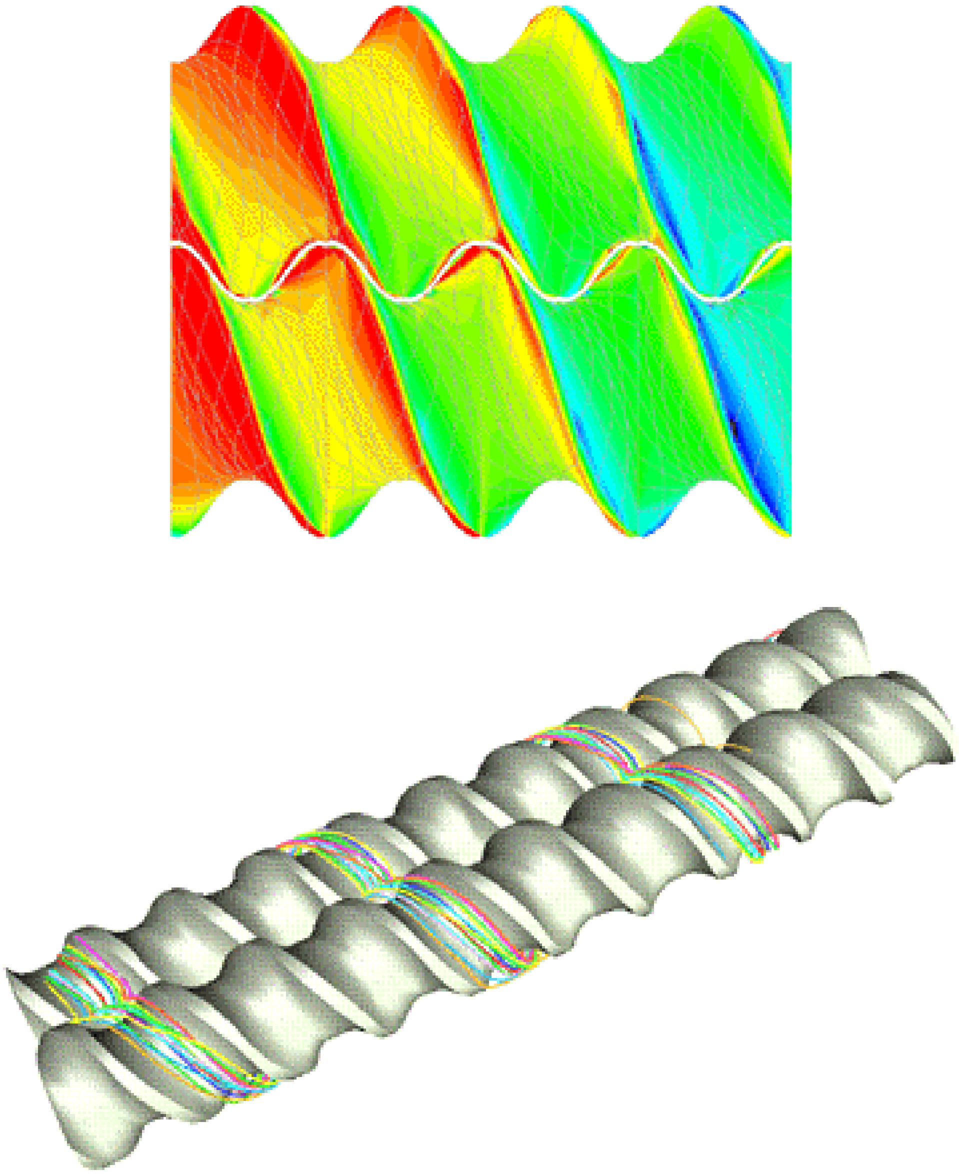


*Figure 11. Pressure distribution on the screw surfaces and particle trajectories inside a twin screw extruder.*

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