Investigation of non-linear flows in polymer mixing

B.A. Davis, W.F. Florez, T.A. Osswald

Polymer Processing Research Group,
Department of Mechanical Engineering,
University of Wisconsin-Madison, Madison, Wisconsin 53706, USA

ABSTRACT

Two alternatives for the solution of non-linear problems using boundary integrals are presented. First the dual reciprocity method is presented for both flow and heat transfer problems in polymer processing. The technique proved to work well for heat transfer but only marginally for non-linear flow problems. The second form of dealing with non-linearities is a cell integration method. This technique was successfully applied to polymer flow problems which included the shear thinning effect, the most important non-linearity in this type of problems.

INTRODUCTION

Numerical simulation of polymer mixing is complicated by the spectrum of flow behavior exhibited by polymer melts. The molecular structure of polymers is the underlying reason for the non-linear behavior that is observed during flow. This conduct results in properties that are highly dependent on the flow field such as strain rate dependent viscosity. Since the morphology of polymer blends is directly dependent on the deformation and stresses induced in the flow field, the non-linear effects cannot be neglected.

The labor intensity and requirements on computer performance when simulating processes with complex material behavior is complicated by the presence of moving boundaries. The most complex process which involves solid moving boundaries is the intermeshing twin screw extruder. Here, the polymer is constantly changing shape as the screws, mixing heads and kneading blocks rotate. The narrow gaps created by the self-wiping arrangement of these systems adds to the numerical complexity of the problem.

Unfortunately, the available numerical methods are not particularly well suited to fully optimize mixing flows. Non-linear flows can be simulated with domain-type methods, such as finite elements or finite differences, but when moving boundaries are introduced, these methods become cumbersome to implement. They require that the user create a discretization of the domain at every time step due to the change of geometry. Interpolation between these different geometries introduces error when tracking points in the flow field. Boundary-type methods, such as boundary elements, can easily simulate moving boundaries as well as accurately track points during flow. Unfortunately, the traditional boundary element theory is only applicable to linear problems. To take the best of both methods would produce a simulation ideally suited to optimize mixing problems.
To investigate non-linear flows on mixing, a simulation that can accurately and efficiently deal with the complex moving boundaries as well as the non-linear behavior of polymer melts was developed and is presented in this paper. The boundary element method has proven itself capable of modeling moving boundary problems with ease but cannot accommodate non-linear flows as a boundary-only simulation. The dual reciprocity boundary element method was applied to non-linear polymer flows to alleviate the shortcomings of traditional simulation methods. The technique works well in the solution of heat transfer problems in polymer processing but did not prove successful when solving non-linear flow problems. Non-linear flow problems were solved using a boundary integral/cell integration method. The simulation was applied to various problems in polymer processing, and the results were excellent.

MATHEMATICAL MODEL

In order 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, conservation of momentum, and conservation of energy as shown in Eqs. 1-3.

\[ U_{a,a} = 0 \]  
\[ \rho \left( \frac{\partial U_a}{\partial t} + U_a \cdot \nabla U_a \right) = \nabla \cdot \mathbf{S} \]  
\[ \rho C_v \left( \frac{\partial T}{\partial t} + U_a \cdot \nabla T \right) = -q_{a,a} - \nabla \cdot \left[ \mathbf{S} \right] U_a + \tau_{a,b} U_{a,b} + \dot{S} \]

In addition to the three conservation equations there may also be one or more constitutive equations which describe material properties. Since these equations may also be coupled together, e.g. temperature dependent viscosity, the solutions can become even more complex. The goal of the modeler is to take a physical problem, use these mathematical equations and solve them to predict the flow phenomena. Although analytic 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 necessary.

THE BOUNDARY ELEMENT METHOD

There are three basic classes of numerical techniques that are commonly used to solve fluid flow problems: the finite difference method (FDM), the finite element method (FEM), and the boundary element method (BEM). Both the finite difference and finite element methods are domain methods which require the domain of the geometry to be discretized. In comparison, the boundary element method only requires discretization of the boundary and offers a substantial advantage for moving boundary problems.
The boundary element method gained prevalence around the same time as FEM, but because of the relatively complex mathematics involved with BEM, it has been slow to gain acceptance as well as FEM. The boundary element method begins with a different form of the governing equations that are expressed in terms of domain integrals. These integrals are then 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. Up to the point of evaluating the integrals, no approximations have been made in the governing equations. Therefore, the boundary element method, unlike FDM or FEM, only introduces error into the solution from numerical sources. Another advantage of BEM is that the accuracy of higher order derivatives is excellent. The boundary element method is also ideally suited to track particles in the flow since the solution at any internal location can be obtained quite easily. The reduction of dimensionality is a key advantage to modeling polymer flows in complex geometries with the boundary element method. Since only the boundary of the domain needs to be defined and discretized, the amount of work for the modeler is dramatically reduced. This boundary only method also can easily handle moving solid boundary problems.

The boundary element method has proven to be an extremely useful tool for modeling polymer processing applications. Gramann [1] has solved numerous problems concerning mixing flows of two dimensional systems. Later, Biswas et al. [2] have extended the 2-D simulation to three dimensions and have solved for the complex flow phenomena within the single screw extruder. Although these simulations have yielded excellent results that agree well with experimental data, they are only valid for Newtonian viscosity in Stokes flows. Since polymers behave as non-Newtonian fluids, the prior simulations are only accurate for qualitative measurements. In order to obtain quantitative results, the full non-Newtonian flow must be analyzed.

DUAL RECIPROCITY BOUNDARY ELEMENT METHOD

Although the BEM is an elegant technique for linear problems, it looses many of its advantages when non-linear problems are investigated. The standard BEM is only able to handle non-linearities by using domain meshing, thus eliminating the boundary only discretization. More recently, Nardini and Brebbia [3] have developed a variation of the BEM, known as the dual reciprocity method (DRM), which has the ability to solve non-linearities with a boundary only formulation. The application of the dual reciprocity method to polymer processing fluid flow applications is still an open problem.

Since the standard BEM is not capable of including the non-linearities from the non-Newtonian viscosity, an alternative method must be used. In order to retain the convenience and elegance of a boundary-only formulation, the use of a dual reciprocity boundary element method is proposed.

DRBEM FOR FLOW EQUATIONS

The equation of continuity from Eq. 1, and a slightly different form of the conservation of momentum shown in Eq. 4 constitute the starting point for the
boundary integral formulation. All of the extra terms found in Eq. 2 can now be lumped in the single term, $b_\alpha$, of Eq. 4. The motivation for this will become evident during the rest of the derivation.

$$\sigma_{a,\beta} = b_\alpha$$  \hfill (4)

By integrating Eq. 4 over the domain and then performing several Green-Gauss integrations and mathematical manipulation one can obtain the following governing integral equation shown in Eq. 10.

$$c_\alpha U_\kappa + \int t^{*}\alpha U_\alpha d\Gamma - \int t_a U^{*}_a d\Gamma = \int b_\alpha U^{*}_{a} d\Omega$$  \hfill (5)

Thus far, Eq. 5 is the solution to the classical derivation of the boundary integral equations for Stokes flows by Lorentz [8]. For a Newtonian fluid the domain integral on the right hand side disappears and the standard BEM can be used. For the non-linear flows being considered, however, the domain integral does not vanish.

The problem of solving the right hand side of Eq. 5 is analogous to finding a particular solution that satisfies the right hand side of Eq. 6.

$$\hat{\sigma}^{x}_{a,\beta} = b_\alpha$$  \hfill (6)

It is virtually impossible to find a continuous solution to Eq. 6, particularly for non-linear or transient problems. Instead, one can use a series of particular solutions $\left(\hat{\sigma}^{x}_{a,\beta}\right)_j$ instead of the single function $\hat{\sigma}^{x}_{a,\beta}$. It is then possible to further define the following approximation for the function $b_\alpha$. This formulation is similar to mathematical collocation functions.

$$b_\alpha = \left(\sum_{j=1}^{2(N+L)} \beta_j f_j\right)_\alpha$$  \hfill (7)

Next, one assumes that the particular solutions and approximating functions are linked through the relation given in Eq. 8.

$$\left(\hat{\sigma}^{x}_{a,\beta}\right)_j = (f_j)_\alpha$$  \hfill (8)

Now, by substituting Eq. 7 and 8 into the governing integral equation, Eq. 9 is obtained. Note that the summation on right hand side of Eq. 9 can be taken outside of the integral and the resulting form is identical to the domain integration of Eq. 9.

$$c_\alpha U_\kappa + \int (t^{*}\alpha U_\alpha - t_a U^{*}_a) d\Gamma = \int \left(\sum_{j=1}^{2(N+L)} \beta_j \left(\hat{\sigma}^{x}_{a,\beta}\right)_j\right) U^{*}_{a} d\Omega$$  \hfill (9)

Now the dual reciprocity method can be used in which both sides of the weighted residual equation are treated with multiple applications of Green-Gauss integrations to obtain the following boundary integral equation:

$$c_\alpha U_\kappa + \int [t^{*}\alpha U_\alpha - t_a U^{*}_a] d\Gamma = \sum_{j=1}^{2(N+L)} \beta_j \left(\hat{U}^{x}_{\alpha}\right)_j + \int [t^{*}\alpha \left(\hat{U}^{x}_{\alpha}\right)_j - (\hat{t}^{x}_{a})_j U^{*}_{a}] d\Gamma$$  \hfill (10)
The left hand side of Eq. 10 is the same as Eq. 9, but now the right hand side has been replaced with the dual reciprocity formulation. The new terms on the right hand side, $\hat{U}$ and $\hat{t}$, are the velocity and traction solutions to Eq. 6. These terms and the unknown coefficients $\beta$ can all be determined once $f_j$ is specified. By choosing a radial basis function for $f_j$ it guarantees non-singular solutions and is relatively simple to implement numerically. The comparatively simple function can be expressed as the power series:

$$F_j = 1 + r_j + r_j^2 + r_j^3 + \cdots + r_j^m$$  (21)

The important point to make is that now the problem has been reduced to only boundary integrals. After discretizing the boundary and numerically integrating, Eq. 11 can be obtained. After the boundary conditions have been specified, Eq. 11 reduces even further to a solvable system of linear algebraic equations.

$$[H][U] - [G][t] = ([H][\hat{U}] - [G][i])[F]^{-1}[b]$$  (16)

**DRBEM FOR THE ENERGY EQUATION**

The two-dimensional equation of energy for an incompressible flow with constant thermal conductivity, and including convection and viscous dissipation is given by:

$$k\nabla^2 T = \rho c_v \left( \frac{\partial T}{\partial t} + v_x \frac{\partial T}{\partial x} + v_y \frac{\partial T}{\partial y} \right)$$

$$-2\mu \left( \left( \frac{\partial v_x}{\partial x} \right)^2 + \left( \frac{\partial v_y}{\partial y} \right)^2 \right) - \mu \left( \frac{\partial v_x}{\partial x} + \frac{\partial v_y}{\partial y} \right)^2$$  (17)

where $k$ is the thermal conductivity, $T$ temperature, density, and $c_v$ specific heat, $v_x$ and $v_y$ are velocity components, and $\mu$ is the viscosity. The above equation can be written in the form of a Poisson-type equation as follows:

$$\nabla^2 T = b(x, y, t, T)$$  (18)

where $b$ is a function of the coordinates $x$ and $y$, time $t$ and temperature $T$.

By using the DRBEM, a particular solution for Eq. 18 can be found and it is of the form:

$$b_1 = \sum_{j=1}^{N+L} \beta_j F_j$$  (19)

where $N$ is the number of boundary nodes and $L$ the number of internal collocation points.

Furthermore, in matrix notation, Eq. 19 can be expressed as:

$$b = \beta F$$  (20)

Patridge and Brebbia suggested using a radial functions for approximating the functions $F_j$ locally. The power series $F_j$, as used above, can be applied as a localized particular solution, by assuming that the distance function $r$ accurately describes the temperature distribution. Thus, after applying conventional
Boundary Elements

reciprocity techniques, Eq. 17 can be transform into the following set of boundary integral equations:
\[ c_i T_i - \int_{\Gamma} T^* q \, d\Gamma + \int_{\Gamma} q^* T \, d\Gamma \]
\[ = \sum_{j=1}^{N+L} \beta_j \left( \int_{\Gamma} T^* \hat{q}_j \, d\Gamma - \int_{\Gamma} q^* \hat{T}_j \, d\Gamma - c_i \hat{T}_j \right) \]
(22)

where \( T^* \) is a Green's fundamental solution with the following form:
\[ T^* = -\frac{1}{2\pi} \ln(r) \]
(23)
And \( q^* \) is the fundamental solution for the heat flux:
\[ q^* = -\frac{1}{2\pi} \frac{\partial r}{\partial \eta} \]
(24)

To solve Eq. 22 numerically, a discretization of the boundary into quadratic elements can be used, and this leads to a set of linear equations which can be written as:
\[ \begin{array}{c}
H^T - \frac{1}{\alpha} \left( v_x \frac{\partial F}{\partial x} + v_y \frac{\partial F}{\partial y} \right) F^{-1} T - Gq \\
= S \left[ 2 \frac{\mu}{k} \left( \frac{\partial v_x}{\partial x} \right)^2 + \left( \frac{\partial v_y}{\partial y} \right)^2 \right] + \frac{\mu}{k} \left( \frac{\partial v_x}{\partial x} + \frac{\partial v_y}{\partial y} \right)^2 \end{array} \]
(25)

where the matrix \( S \) is defined by:
\[ S = \left( G \hat{Q} - H^T \right) F^{-1} \]
(26)

It must be pointed out that for the case of isoparametric quadratic elements, the matrices \( H^T, S \) and \( F \) are constructed on a nodal base, thus they have dimensions \((N+L)\times(N+L)\). In contrast, the dimension of matrix \( G \) is \((N+L)\times(3NE+L)\) because it is constructed on an element base.

CELL INTEGRATION

As has been previously mentioned, the DRM is a very elegant approach, that uses a sum of approximating particular solutions to transform the domain integral to the boundary. However, this method is not always accurate enough, specially when dealing with highly non-linear problems. As an alternative for solving that kind of problems, there is the cell integration technique in which the domain must be discretized and the non-linear integrals are numerically evaluated. Although cell integration hinders the boundary-only advantage of BEM, it is a very accurate method for solving non-linear problems.

The most transparent way of computing the domain term in Eq. 5 is by subdividing the region into a series of internal cells and numerically integrating them with Gauss quadrature. Although by discretizing the domain the boundary element method appears superficially similar to FEM, the advantage of the cells is that there is no strict connectivity requirement as with finite elements. The
governing integral equation from Eq. 5 can be rewritten with all of the non-linear terms lumped into the \( b_a \) term. The resulting integral equation can then be rewritten as

\[
C_i U_i^x + \int_{\Omega} t_a^x U_a d\Omega - \int_{\Gamma} U_a^x t_a d\Gamma = \int_{\Omega} b_a U_a^x d\Omega = I_i
\]

with the value of the domain integral \( I_i \) being evaluated for every source point \( i \). The domain integral for each source point is evaluated by numerically integrating the product of the non-linearity and the fundamental solution over each cell.

If eight node quadratic isoparametric cells are chosen to discretize the domain, then Gaussian quadrature can be used to numerically evaluate the integral. Here, the global cell is transformed into a local coordinate system that has the origin in the center of the element and the intrinsic coordinates \( \xi \) and \( \eta \) oriented as shown in Fig. 1.

![Figure 1 - Schematic of a quadratic isoparametric cell used to evaluate domain integrals.](image)

The domain integral is then evaluated for each source point over every cell. By calculating the non-linear term \( b_a \) and the fundamental solution \( U_a^x \) at each Gauss point, the value of \( I_i \) can be obtained by numerically integrating over the cell. Also, for truly non-linear problems an iterative algorithm is required. For the case of non-Newtonian viscosity, the iteration algorithm can be represented by Fig. 2. Here, the initial Newtonian problem is solved and then used to compute the current stress gradients within the cells. The cells are integrated with Gauss quadrature to solve for the new velocity solution and the process is repeated until convergence is attained.
RESULTS

Gravitational Forces In Stokes Flow

As an initial check to determine the accuracy of the DRBEM flow formulation, a gravitational term was modeled. Consideration of gravity forces results in a constant term for $b_\alpha$ which can be written as

$$b_\alpha = -\rho g \alpha.$$  \hspace{1cm} (28)

Although gravity is not a non-linear term, it causes the Stokes equation to become non-homogeneous and necessitates the use of DRBEM. Since $b_\alpha$ is a known constant, the DRBEM governing equation can be solved for velocities and
tractions. Figure 3 shows an inclined trough geometry with gravitational forces. The trough was chosen to have a thickness $\delta=10$ mm and an angle of inclination $\beta=45^\circ$. Gravity is assumed to be acting downward with $g=9.81$ m/s$^2$ as the acceleration constant. A Newtonian fluid with density $\rho=1.0$ kg/m$^3$ and viscosity $\mu=1.0$ Pa-s is allowed to flow down the inclined surface from the resulting gravitational forces.

The analytical solution for the fluid velocity $v_z$ can be expressed as

$$v_z(x) = \frac{\rho g \delta^2 \cos \beta}{2\mu} \left[ 1 - \left( \frac{x}{\delta} \right)^2 \right]$$

where $x$ is the coordinate through the thickness of the fluid and $z$ is the direction of flow. Solving the trough flow by using the DRBEM, one can choose any number of terms from the approximation function $f$. This results in a disturbing property that is exhibited by the flow DRBEM formulation. The accuracy of the method is dependent upon the choice of $f$ and the number of internal points used to collocate the particular solutions. As Fig 4 illustrates, the DRBEM solutions for the gravitational trough flow problem varies depending on the specific collocation function $f$. 

Figure 3 – Trough flow of a Newtonian fluid with gravity forces.
For this case, acceptable accuracy is obtained by retaining the first three terms from the radial function. By retaining any higher-order terms, no improvement in accuracy was observed. If only two terms were retained, however, the accuracy deteriorates and errors of 12% were observed. This was somewhat improved to 3-5% error if the number of internal points was increased. Unfortunately, by increasing the number of collocation points the problem requires more computational effort. This deficiency of the dual reciprocity method for fluid flow becomes more pronounced as the order of non-linearity increases.

Spatially Varying Viscosity

To determine if the DRBEM is feasible to handle non-linear cases, a spatially varying viscosity is proposed. Here, the viscosity can be written as

$$\eta(y) = \frac{\mu_o}{(\delta - y + 1)^a}$$  \hspace{1cm} (30)

where \(y\) is the dimension through the gap, \(\delta = 50\, \text{mm}\) is the gap height, \(\mu_o = 1000\, \text{Pa} \cdot \text{s}\) is the viscosity at the lower surface, and \(a\) is an integer that can be used to increase the degree of non-linearity. Figure 5 shows the relevant dimensions of the geometry being considered for spatially varying viscosity.
This effect causes the $b_{\alpha}$ term from the governing equation to be written as

$$b_{\alpha} = -(\tau_{\beta\alpha,\beta})_{\text{extra}} = -[\eta(y)\dot{\gamma}_{\alpha\beta}]_{\beta}.$$  

(31)

An alternative to approximate the extra stress term in Eq. 31 is to use a dual reciprocity formulation to approximate the derivatives. In this case, the extra stress term can be written as the following.

$$\tau_{\alpha\beta} = \eta(y)(U_{\beta,\alpha} + U_{\alpha,\beta}).$$  

(32)

If one uses a similar approach as the dual reciprocity method, the velocity can be approximated by

$$\{U\} = [F]\{\phi\}.$$  

(33)

Furthermore, one can then rearrange Eq. 31 to be written as

$$\{\phi\} = [F]^{-1}\{U\}.$$  

(34)

The spatial velocity derivatives can then be expressed as

$$\{U\}_{\beta} = [F]_{\beta}[F]^{-1}\{U\}.$$  

(35)

where the derivative has been transferred from the unknown velocity to the known approximating function $f$. By evaluating the derivatives in Eq. 34 and then grouping them in proper order, the DRM formulation for the strain rate $[\dot{\gamma}]$ can be obtained. Then the DRM formulation for the extra stress $[\tau]$ can be obtained at each collocation point as

$$[\tau] = [\eta(y)][\dot{\gamma}]$$  

(35)

where $[\eta(y)]$ is a diagonal matrix with the diagonal made up of values from Eq. 30. However, since the stress derivative is required, the stress can be treated with DRM in the same manner as the velocity derivatives. The final non-linear term $\{b\}$ for the prescribed viscosity gradient can then be written as

$$\{b\} = [F]_{\beta}[F]^{-1}[\eta(y)][\dot{\gamma}].$$  

(36)

It should be noticed that $\{b\}$ is a function of the velocity solution and iteration must be used to solve the final form of the governing equation.
An additional requirement on the numerical solution of Eq. 37 is that the approximating function \( f \) must contain at least second order terms because of the presence of its derivatives.

The sample problem introduced in Fig. 5 was solved using the dual reciprocity formulation of Eq. 37. Here, the geometry was modeled using 24 boundary elements and 67 internal points. Fifty of the internal points were randomly distributed within the domain and the remaining 17 were equally spaced through the thickness and used to ascertain the velocity profile. Initially, the distance function was chosen as \( f = 1 + r + r^2 \) but needed to be revised as the degree of non-linearity increased. The analytical solution to the velocity through the thickness can be expressed as

\[
v_x(y) = \left[ (\delta + 1)^{(a+1)} - (\delta - y + 1)^{(a+1)} \right] \frac{V}{(\delta + 1)^{(a+1)} - 1^{(a+1)}}
\]

where the velocity of the upper plate was chosen to be \( V = 1.0 \text{ m/s} \). Here, the role of the variable \( a \) from Eq. 30 is evident. By increasing \( a \), higher degrees of non-linearity can be investigated with DRBEM.

The results from the dual reciprocity boundary element simulation of the prescribed viscosity gradient were accurate for low orders of non-linearity, but error increased with the value of \( a \). Figure 6 shows the results from the simulation for the various degrees of non-linearity compared with the analytical solution. As shown in the figure, for values of \( a \) greater than \( a=2 \), the DRBEM solution loses accuracy. Additionally, upon closer inspection, one observes that to obtain an accurate DRBEM solution the order of the distance function \( f \) must be at least of the same order as the analytical solution for velocity.
A Generalized Newtonian Fluid Using Cells

As an alternative to the dual reciprocity, domain cell integration was applied to a Couette flow problem. The domain was discretized with 14 boundary elements and 144 quadratic domain cells as shown in Fig 7.

Figure 6 – Dual reciprocity solution for the velocity distribution in parallel plates with a prescribed spatially varying viscosity. The values of $a$ in the plot refer to the exponent in the prescribed viscosity. Note that the solutions for DRM were obtained with different approximations for the distance function $f$.

$$\eta(y) = \frac{\mu_o}{(\delta - y + 1)^a}$$

$\circ$ a=1 $\left( f = 1 + r + r^2 \right)$

$\bullet$ a=2 $\left( f = 1 + r + r^2 + r^3 \right)$

$\square$ a=3 $\left( f = 1 + r + r^2 + r^3 + r^4 \right)$

$\blacksquare$ a=4 $\left( f = 1 + r + r^2 + r^3 + r^4 \right)$

Figure 7 – Domain cell discretization of the Couette flow geometry.
Results for the cell BEM solution of the Couette flow are given in Fig. 8. The results observed in the figure show excellent agreement with the analytical solutions. Note, also that the solution to the Couette flow was not dependent upon the details of the internal cell discretization. Acceptable accuracy was achieved for the initial discretization from Fig. 7.

The solution obtained from the domain cells was found to be convergent and accurate. A relaxation technique was used on the extra stress term. By using relaxation, coupled with the smoothly varying solution for velocity, convergence was usually attained within 8 iterations. The convergence criteria was chosen to be less than a 1% change of the residuals for viscosity and stress.

**Static Mixer**

In order to further test the effectiveness of the domain cell BEM simulation, a static mixer was considered. Static mixers or motionless mixers are pressure-driven continuous mixing devices through which the melt is pumped, rotated and divided, leading to effective mixing without the need for movable parts and mixing heads. One of the most commonly used static mixers is the twisted tape static mixer schematically shown in Fig. 9.
Figure 9 – Schematic representation of a Kenics static-type mixer.

Here, a 2-D section is taken through the mixer to study the recirculation flow. The physical geometry of the static mixer was an outer diameter of 100 mm and a through put corresponding to a rotation of the outer surface of 100 rpm. Since this mixing section is actually stationary, equivalent boundary conditions can be obtained by simulating the relative motion between the tube wall and the mixing element. The flow of high density polyethylene at 180° C was simulated using the cell BEM and compared with a 4-node quadrilateral finite element analysis. Figure 10 shows how the geometry was discretized with 64 boundary elements and 436 cells compared with 1232 finite elements.

Figure 10 – Discretizations used to describe the geometry of the static mixer using (a) cell BEM and (b) FEM. Note that the cells for BEM are not required to be discretized all the way to the boundary.

As figure 11 shows, the results are in good agreement between the cell BEM solution and the FEM solutions. However, since the boundary element formulation allows discontinuous tractions, the contours near the corner are smoother than the finite element solution. Additionally, it can be noticed that the influence of the power-law fluid causes subtle changes in the velocity field which become more evident in the strain rate.
Figure 11 – Velocity contours for a Newtonian fluid and HDPE in the static mixer as computed by cell BEM compared with FEM.

The flow field inside the mixer is of great importance when quantifying the mixing during the process and to maximize the mixing efficiency. To analyze the process, the magnitude of strain rate and vorticity tensors and the flow number were examined. The parameter is defined as:

$$\lambda = \frac{\dot{\gamma}}{\gamma + \omega}$$  \hspace{1cm} (38)

where $\dot{\gamma}$ is the magnitude of the strain rate tensor and $\omega$ is the magnitude of the vorticity tensor. The parameter varies between 0, for pure rotational flow, and 1, for pure elongational flow, and a valued of 0.5 signifies simple shear flow. Flow number contours are depicted in figure 12. Note how the majority of the mixing section is characterized by shear flow, with a thin region of high elongation and high rotational flow in the central region of the section. Also, figure 13 shows that the central region of the section has a very low strain rate as well as a low value of vorticity. Therefore, although the flow in the center region is computed as elongational, its dispersive mixing effectiveness is low.
Figure 12 – Flow number contours for HDPE in the static mixer as computed with cell BEM.

Figure 13 – Strain rate contours for HDPE in the static mixer as computed with cell BEM.
The function of the static mixer is to distribute or blend the material through reorientation by the staggered mixing sections. Therefore, in addition to the flow number, the main parameter that defines the effectiveness of mixing is the total strain. Since strain at any time is related to the integral of strain rate. Fig. 12 illustrates regions of high strain rate. Another outcome from the simulation of the static mixer is that the relative viscosity in the section can be computed and displayed as shown in Fig. 14. The results displayed in the figure are a measure of the non-linear effects in this specific application. By considering both the strain rate and the flow number, one can make reasonable conclusions on the effectiveness of mixing— even with a Newtonian simulation.

![Viscosity contours for HDPE in the static mixer as computed with cell BEM.](image)

**Figure 14** – Viscosity contours for HDPE in the static mixer as computed with cell BEM.

**Single Rotor Mixer**

The single rotor mixer geometry is another device in the polymer industry and is used primarily for dispersive mixing. The geometry of the mixer consists of a single lobed rotor within a cylindrical barrel. The physical geometry of the single rotor mixer used in this simulation consisted of an outer barrel with a diameter of 11.76 cm and the mixer rotating at 100 rpm. In this case, it is possible to consider the equivalent boundary conditions of the outer cylinder rotating around the fixed lobed rotor. Here, the flow of PA–66 was simulated under isothermal conditions of 290°C. The mixer was discretized as shown in Fig. 15 with 100 boundary elements and 152 internal cells. The solutions of the velocity field and power law
viscosity inside the single rotor mixer are shown in Fig. 16 and Fig 17, respectively.

Figure 15 – Discretization used to describe the geometry of the single rotor mixer using cell BEM

Figure 16 – Velocity contours of PA-66 in the single rotor mixer using cell BEM
The results for the velocity contours shows the recirculation patterns that are present. The corresponding strain rates in the recirculation region cause an increase in the viscosity. However, the high strain rates near the rotor tip, create a region of low viscosity.

The resulting flow number distribution of Fig. 18 shows the effect of the power law viscosity on the type of flow. The Newtonian simulation predicts more elongational flow than the actual power law fluid. This difference, in itself, illustrates the effects induced by non-linear viscosity.
The strain rate distributions for the polyamide, shown in Fig. 19, also reveal some deviation from the Newtonian analysis. The shear thinning behavior of the melt generates regions of high strain rate—even higher than predicted by Newtonian analysis.

Dispersive mixing is concerned with the stress that can be applied by the mixing device. A shear thinning fluid, such as polyamide, has a non-homogeneous viscosity and the resulting stress field is complex. The predicted stress field in the Newtonian fluid is shown in Fig. 20. The maximum predicted stress near the rotor tip is found to be nearly 85 kPa. The non-Newtonian analysis
shows that the Newtonian prediction is over four times too high. Therefore, if the Newtonian analysis were used to predict agglomerate break-up, it would over-predict the ability of this mixer.

Figure 20– Stress invariant as predicted by a Newtonian fluid.
The irregularities of the stress contours around the outer edge of the single rotor mixer are related to small numerical errors and the coarse discretization used. In the comparison of the Newtonian and power law solutions for stress, the second invariant of stress was used. As an additional consideration, the Newtonian analysis was used to obtain an estimate of the power law stress field. Here, the Newtonian solution for the strain rate was used to approximate the equivalent power law viscosity. The product of this estimated viscosity and the Newtonian strain rate were used to ascertain the estimated non-Newtonian stress field as shown in Fig. 22. This analysis yielded a maximum stress of 15 kPa and a distribution that compares favorably with the full non-linear solution of Fig. 21. Thus, the distribution of stress is more accurate than the simple Newtonian prediction. This outcome shows that it possible to obtain an estimate of the actual stress from a Newtonian analysis.
CONCLUSIONS

The research presented in this paper resulted in a boundary integral simulation of non-linear flows. First, a Newtonian quadratic boundary element formulation that predicts linear mixing flows was developed. Through the use of quadratic elements and discontinuous tractions, accurate solutions for the flow field, strain rates, particle deformation, and flow number can be assessed for a wide variety of mixing problems.

To alleviate the linear restriction of the BEM, the dual reciprocity method has been implemented to solve several non-linear problems. However, the DRBEM was not sufficient to fully model highly non-linear polymer flows. Therefore, an alternative domain cell boundary element method was applied to several non-linear flows. The results and comparisons with analytical solutions prove the accuracy of the cell BEM.

REFERENCES


