Transactions on Modelling and Simulation vol 3, © 1993 WIT Press, www.witpress.com, ISSN 1743-355X

# Simulating flow and heat transfer in polymer processing using BEM/DRM

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## INTRODUCTION

In a variety of processes in the plastic industry, such as extrusion, injection molding, and mixing, the knowledge of the temperature field and the amount of heat generated by viscous dissipation is of great importance. Due to the strong temperature dependence of the viscosity, the temperature field is necessary to predict the non-isothermal flow of polymer melts. In polymer flow through narrow geometries, vast amounts of mechanical energy are converted irreversibly into heat due to internal friction. The viscous dissipation may increase the overall bulk temperature of the fluid significantly, which may lead to thermal degradation of the polymer. In fact, 50-80% of the energy required for plastication comes through viscous heating. In order to maintain product quality, short cycle times are in conflict with possible thermal degradation. The temperature field is also significant in typical polymer processes to predict solidification and melting.

To solve for the temperature field in typical polymer flow problems, the equation of energy and the equation of motion have to be solved simultaneously, taking into account the temperature dependence of the viscosity. The convective and viscous dissipation terms of the equation of energy require the velocity field and its gradients. Finding an exact solution for the coupled differential equations is extremely difficult even for simple problems. More complex geometries must be solved numerically, applying the finite difference method (FDM), the finite element method (FEM), or the boundary element method (BEM). Some attempts have been made to simulate polymer flow problems using FDM and FEM [1-5]; none of them took the viscous dissipation into account. However, Nunn and Fenner [6] and Winter [7-8] investigated channel flow of a power law fluid considering viscous dissipation by applying a central finite difference scheme. Their algorithms took into account the influence of the temperature on the velocity profile. Zienkiewicz and Gallagher [9] solved the slit flow problem with FEM. However, both the FDM and FEM are domain methods which require a complex domain discretization into elements or cells. This is a tedious and time consuming process, especially when moving boundaries, common in polymer processing, are considered.

Hence, boundary element solutions are preferred to the other numerical techniques when moving boundaries, such as in mixing, are involved. With domain methods, generating the required meshes necessary to compute a full cycle becomes complicated and time consuming. Here, the mesh has to be re-shaped after each consecutive time step to fit the geometry of the new domain. The boundary element method was applied to steady incompressible thermoviscous flow in a moderate Reynolds number range by Dargush and Banerjee [10], but the viscous dissipation effects were neglected. The nonlinear convective terms were treated with volume integrals which required a domain discretization, thus, losing the advantage of a boundary element scheme. Gramann and Osswald [11] developed a boundary element simulation to solve the isothermal Navier - Stokes equation. They used their simulation to model mixing in various processes, but neglected viscous heating and its effect on the viscosity.

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This paper presents the solution of the equation of energy for flow problems using the boundary element dual reciprocity method (DRM). To solve for velocities and velocity gradients needed in convection and viscous dissipation problems, the boundary integral equation for creeping flow are presented as well. In all cases the numerical and analytical results are in very good agreement making the dual reciprocity method superior to domain type methods including BEM with domain integration.

## BOUNDARY ELEMENT EQUATIONS

### Heat Transfer Equations

The two dimensional equation of energy in full length assuming incompressible flow and constant thermal conductivity is given by:

$$k\nabla^2 T = \rho c_v \left(\frac{\partial T}{\partial t} + v_x \frac{\partial T}{\partial x} + v_y \frac{\partial T}{\partial y}\right) - 2\mu \left[\left(\frac{\partial v_x}{\partial x}\right)^2 + \left(\frac{\partial v_y}{\partial y}\right)^2\right]$$
$$- \mu \left(\frac{\partial v_y}{\partial x} + \frac{\partial v_x}{\partial y}\right)^2 + \Phi \qquad (1)$$

where, k represents thermal conductivity, T temperature, $\rho$ density, $c_v$ specific heat, $v_x$ and $v_y$ velocity components, $\mu$ Newtonian viscosity and $\Phi$ an arbitrary internal heat generation term. Equation (1) can be written into a general form of a Poisson type equation as a function of the coordinates x and y, time t, and temperature T.

### Boundary Integrals Using the Dual Reciprocity Method

The body term of the general Poisson equation for two-dimensional applications can be expressed using a particular solution. The particular solution is usually difficult to evaluate for nonlinear and time-dependent problems. For general field problems Partridge and Brebbia [12] introduced the dual reciprocity method which applies a series of localized particular solutions. Applying this method [15] to Eq. (1) reduces to:

$$\nabla^2 T = \sum_{j=1}^{N+L} \beta_j \nabla^2 \hat{T}_j \qquad (2)$$

where, the right-hand side represents a series of localized particular solutions. A boundary integral equation can now be derived for both sides of Eq.(2) using a direct or indirect formulation. The indirect formulation is based on Galerkin's method and weighted residuals. The derivation of the boundary integrals that satisfy Eq.(1) and the boundary conditions is explained in detail by Gipson [13] and Brebbia [14]. The resulting equation is as follows [15]:

$$c_i T_i - \int_\Gamma T^* q \, d\Gamma + \int_\Gamma q^* T \, d\Gamma$$
$$= \sum_{j=1}^{N+L} \beta_i \left( \int_\Gamma T^* \hat{q}_j \, d\Gamma - \int_\Gamma q^* \hat{T}_j \, d\Gamma - c_i \hat{T}_j \right) \qquad (3)$$

where $c_i$ is 1/2 for a point on the boundary, 0 for a point outside the domain and 1.0 for a point inside. The term $T^*$ and $q^*$ are fundamental solutions:

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$$T^* = -\frac{1}{2\pi}\ln(r) \tag{4a}$$

$$q^* = -\frac{1}{2\pi r}\frac{\partial r}{\partial n} \tag{4b}$$

Here r represents the distance from the point of the potential to the point under consideration. A numerical solution of Eq.(3) requires a segmentation of the domain and of the boundary into elements. The temperature and the normal derivative of the temperature are assumed to be constant over the elements and equal to the value at the midpoint. In matrix form Eq.(3) can be written as:

$$\mathbf{H'T} - \mathbf{Gq} = (\mathbf{G\hat{Q}} - \mathbf{H'\hat{T}})\boldsymbol{\beta} \tag{5}$$

The matrices **G**, **H'**, $\mathbf{\hat{Q}}$, and $\mathbf{\hat{T}}$ are all of the size (N+L)x(N+L). The vectors **T** and $\boldsymbol{\beta}$ are of the size (N+L), while the size of the vector **q** is restricted to the boundary nodes (N) [15]. The elements of the coefficient matrices **G** and **H** are integrated using the Gaussian quadrature technique [15]. Matrix **F**, which is based on the distance function r. According to Partridge and Brebbia [12], a higher order of the series expansion does not result in a noticeable increase in accuracy.

**Flow Equations**

Neglecting variations in the third dimension and the compressibility of the polymer, the continuity equation simplifies to:

$$\nabla \cdot \mathbf{u} = 0 \tag{6}$$

Assuming a Newtonian fluid where the viscous forces are much larger than the inertia effects, the momentum balance of a typical mixing problem reduces to:

$$\nabla P + \mu \nabla^2 \mathbf{u} = \mathbf{F} \tag{7}$$

For complex geometries, as is the case in most polymer processes, this equation cannot be solved analytically. Here, we chose the boundary element method to solve the governing equations for any given geometry and boundary conditions. It should be noted that two boundary conditions on each boundary are known and two conditions are always unknown, and must be solved for. The boundary conditions can be either a known traction, $t_\alpha = \bar{t}_\alpha$ or velocity, $U_\alpha = \bar{U}_\alpha$. During the formulation of the boundary integral equation, Eqs.(6) and (7) must be satisfied and the required boundary conditions must be met. The following boundary integral equation for Newtonian, isothermal creeping flows results from a weighted residual statement that satisfies Eq.(6) and boundary conditions [16]:

$$C_i U^i_\kappa + \int_\Gamma \left[ t^\kappa_\alpha U_\alpha - t_\alpha U^\kappa_\alpha \right] d\Gamma = 0 \tag{8}$$

In Eq.(8) $t^\kappa_\alpha$ and $U^\kappa_\alpha$ are fundamental solutions which represent velocities and tractions in the 1 and 2 directions in an infinite domain, caused by the concentrated forces acting in the two perpendicular directions $\kappa$=1,2 on a singular point "i". The fundamental solutions for velocity and traction are as follows [17]:

$$U^\alpha_\kappa = \frac{-1}{4\pi\mu}\left[\delta^\alpha_\kappa \ln(r) - \frac{\partial r}{\partial x_\alpha}\frac{\partial r}{\partial x_\kappa}\right] \tag{9a}$$

$$t^\alpha_\kappa = -\frac{\partial r}{\partial x_\kappa}\frac{\partial r}{\partial x_\alpha}\frac{\partial r}{\partial n}\frac{1}{\pi r} \tag{9b}$$

Since the integrals in Eq.(8) cannot be evaluated analytically, the boundary is discretized into a finite number of elements. This analysis utilizes constant boundary elements where the values of $U_\alpha$ and $t_\alpha$ are assumed to be constant on each element and equal to its value at the midpoint, which reduces Eq.(8) to a set of linear algebraic equations.

## RESULTS

### Transient Heat Conduction

The time dependent heat conduction equation is:

$$\nabla^2 T = \frac{1}{\alpha}\frac{\partial T}{\partial t} \qquad (10)$$

Using the general dual reciprocity Eq.(5), results in [15]:

$$\left(\mathbf{H'} - 2\frac{\mathbf{S}}{\alpha\Delta t}\right)\mathrm{T}_1 - 2\mathbf{G}\mathrm{q}_1 = \left(2\frac{\mathbf{S}}{\alpha\Delta t} - \mathbf{H'}\right)\mathrm{T}_0 \qquad (11)$$

where $\mathbf{S} = (\mathbf{G}\hat{\mathbf{Q}} - \mathbf{H'}\hat{\mathbf{T}})\mathbf{F}^{-1}$. After the S matrix is assembled, Eq. (11) can be evaluated. The only remaining unknowns are the vector **T**, which contains the temperatures, and the vector **q**, which contains the temperature gradients. If initial temperatures and the boundary conditions are known, Eq. (11) can be converted into a linear system of equations.

Recently, Mätzig [15] investigated the accuracy of the DRM and the impact of the position and number of the internal nodes the method was applied to the cooling of a square domain, where the initial temperature is 30°C and all four sides are cooled instantaneously down to 0°C, at t = 0. The exact solution to the two-dimensional problem is given by Bruch and Zyvoloski [19]. The thermal diffusivity is set to be $\alpha_x = \alpha_y = 1.25$.

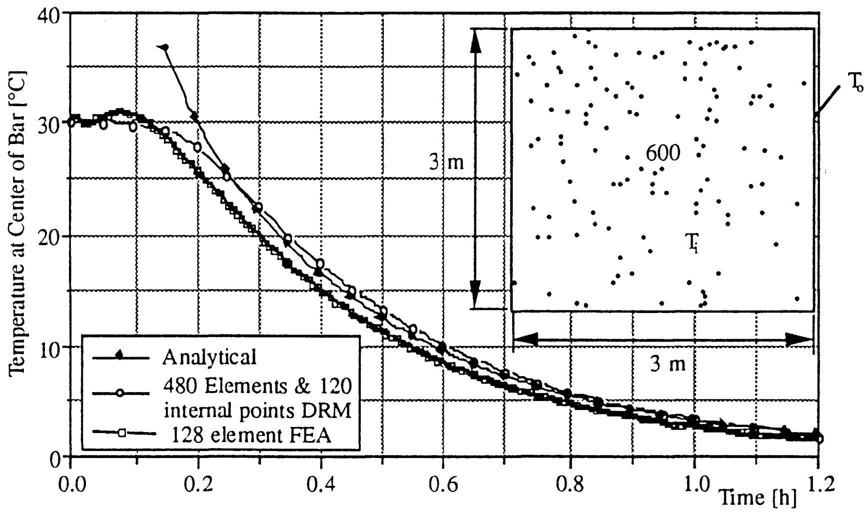


Figure 1. Transient heat transfer results comparing DRBEM, FEM to analytical.

As a demonstration of the accuracy of the transient heat transfer DRBEM, the results of a highly refined discretization are shown in Fig. 1. The discretization used for this figure consisted of 480 boundary elements and 120 randomly distributed internal points. This solution was obtained from a version of the program that was coded to run on a parallel computer by Davis and Osswald [20]. This version offers substantial speed-up over the serial version and allows problems with very large numbers of elements to be computed in a short amount of CPU time. Figure 1 shows that the initial oscillations at small times have been eliminated and the solution is in excellent agreement with the analytical result. For reference, the results from a finite element analysis using triangular elements are also shown in Fig. 1. The FEA used 128 elements and an Euler time stepping scheme to offer a comparison to the DRBEM. It should be pointed out that to avoid spurious oscillations, the FEA needed a time step twenty times smaller than the DRBEM. In addition, Fig. 1 shows that even with the small time step, the FEA solution is less accurate than the DRBEM.

**Combining Viscous Dissipation and Convection**

Non-isothermal flow phenomena between parallel plates and in tubes was studied by several authors [6-8,21-22]. The solution of the coupled, nonlinear differential energy equations is fairly complicated for even one dimensional flow problems. Comparing the numerical results of convection effects combined with viscous dissipation between parallel plates to an exact solution as presented by Ybarra and Eckert [21] is challenging when real material data is used. This is explained with the following arguments: first, the conduction term in flow direction cannot always be neglected as it was assumed when the eigenvalue solution was derived; second, the length, l, must be "infinite" to achieve thermal equilibrium, which is cumbersome to simulate. Mätzig [15] used DRM to study viscous effects and convective effects separately and collectively to validate the method with analytical solutions. The next step within the project was use the combined viscous dissipation and convection effects to solve realistic problems which do not have analytical solutions. The DRM equations considering viscous dissipation and convection terms are derived in the following section and results are shown for non-isothermal flow inside a single rotor mixer, where the velocities and the velocity gradients were computed with the flow portion of the boundary element program [11,17]. Combining the DRM equations considering viscous dissipation and convection [15], results in

$$\left[H' - S\frac{1}{\alpha}\left(v_x\frac{\partial F}{\partial x} + v_y\frac{\partial F}{\partial y}\right)F^{-1}\right]T - Gq = S\left\{2\frac{\mu}{k}\left[\left(\frac{\partial v_x}{\partial x}\right)^2 + \left(\frac{\partial v_y}{\partial y}\right)^2\right] + \frac{\mu}{k}\left(\frac{\partial v_y}{\partial x} + \frac{\partial v_x}{\partial y}\right)^2\right\} \qquad (12)$$

If the velocity and the velocity gradients are known, the equation can be converted into a system of linear independent equations and the temperature and its gradient can be solved for.

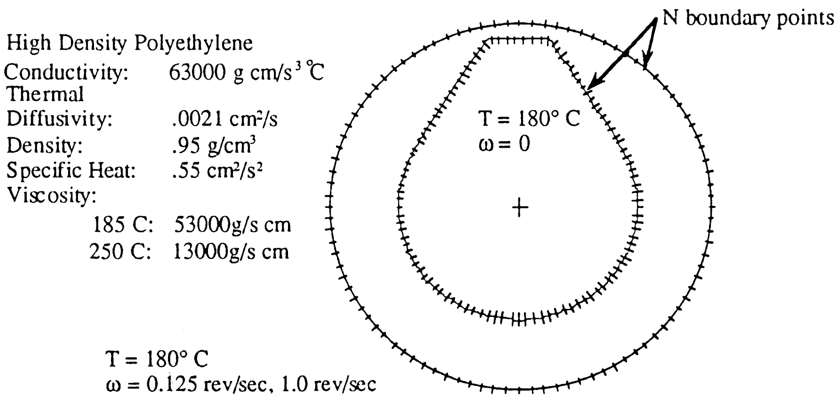


Figure 2. BEM discretization for the single rotor mixer.

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To be able to simulate more complicated flow problems, where the velocities and the velocity gradients cannot be computed analytically, a flow [11] and the heat transfer algorithm [17] were combined. To test the coupled flow and heat transfer equations, the mixing inside the single rotor mixer shown in Fig. 2 was simulated. The streamlines shown in Fig. 3 were computed using the flow simulation described in the previous sections. Here, the recirculation and

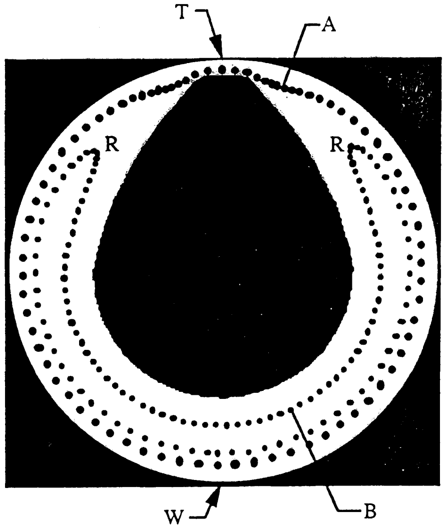


Figure 3. Streamlines for the single rotor mixer computed by BEM.

stagnation areas can be clearly seen. The accuracy of the boundary element method can also be seen by the repeated return of the particles to their starting points after they complete a full cycle on their streamline. To increase the efficiency of mixing, the geometry of mixers are changed to increase the strain rate that the fluid undergoes. The high strain rates present during the mixing process generate heat by viscous dissipation, greatly influencing the temperature of the polymer inside the cavity. The importance of the energy generated by viscous dissipation and its transport by convection become more significant as the rotor speed is increased. The boundary conditions and material properties used to analyze the temperature of the point shown in Fig. 3, are shown in Fig. 2. The internal points needed for the dual reciprocity method are those that make up the streamlines shown in Fig. 3 which were calculated using the flow portion of the program. The viscosity corresponds to the average temperatures in the system, requiring an iterative procedure for its computation. The temperature increase and variations caused by viscous dissipation and the influence of convection are shown in Figs. 4 and 5.

When the rotor speed is 0.125 rev/sec the viscous dissipation causes a $7^{o}C$ rise in temperature; Fig. 4. As expected, the temperature profile caused by viscous heating is symmetric on both sides of the rotor. In the wide gap area of the mixer, "W", the temperature of the fluid is close to the barrel wall temperature. This is due to the low viscous heating in this area and direct heat conduction to the barrel wall. The high temperature areas of the graph correspond to the two recirculation areas of the mixer, "R." Although, the viscous heating is significant in the area of the rotor tip, "T", the heat conduction to the barrel wall lowers the temperature of the fluid due to the narrow gap. When the energy transport by convection is included the temperature profile is slightly shifted with more variation in temperature in the recirculation area. However, because of the low rotational speed, the energy transported by convection is small; resulting in two similar temperature profiles.

Increasing the speed of the rotor to 1.0 rev/sec the temperature increase caused by viscous dissipation can be as high as $90^{o}C$; Figs. 5. It should be noted that in this case the viscosity of the fluid was lowered to 13 MPa-s. Again, it should be pointed out that a low Nahme-

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Griffith number was assumed, and therefore, a constant viscosity throughout the domain. This assumption is no longer valid for the high temperature variations. However, the results are of qualitative value when studying the effects of viscous dissipation and convective energy

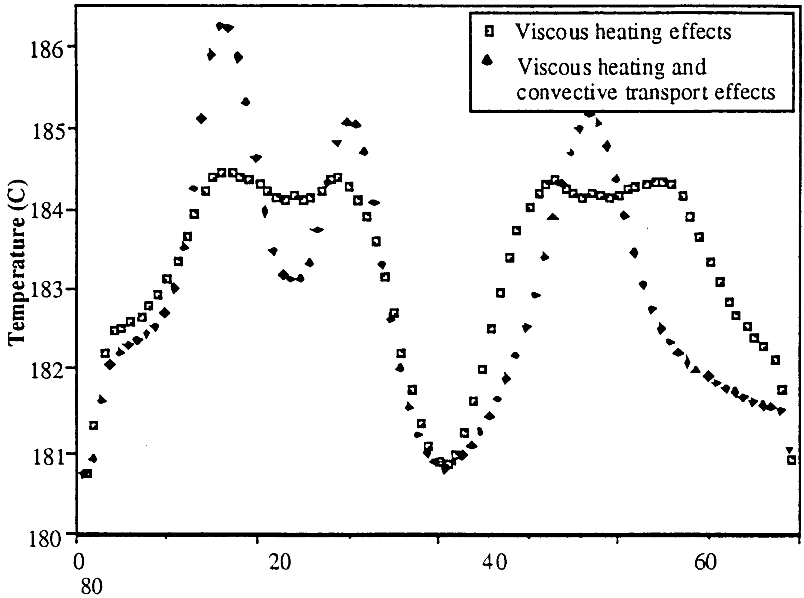


Figure 4. Temperature of a particle traveling on streamline "A" caused by viscous heating with and without convective transport. ω=0.125 rev/sec

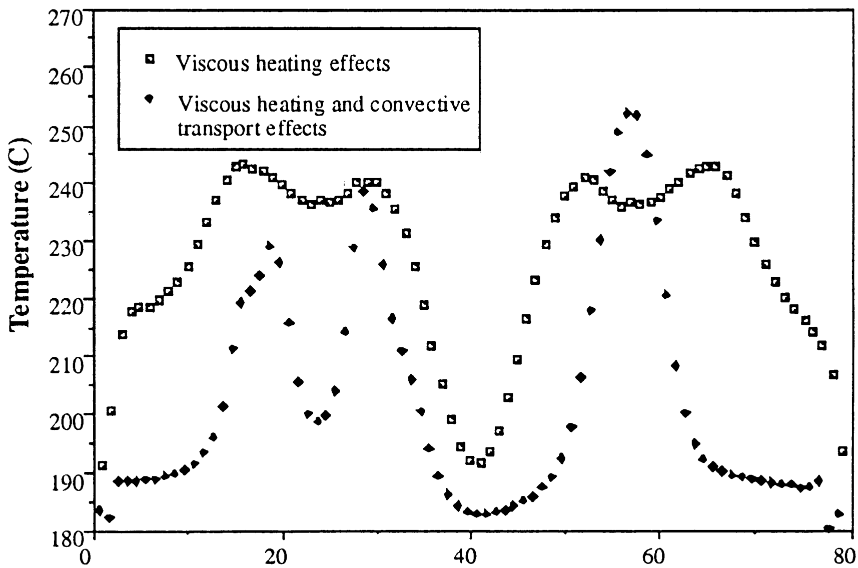


Figure 5. Temperature of a particle traveling on streamline "A" caused by viscous heating with and without convective transport. ω = 1.0 rev/sec.

transport. When compared to the 0.125 rev/sec rotor speed results, the temperatures increase maintaining a similar profile. However, when the effects of energy transport by convection are included, the temperature profiles significantly decrease with highest variation in the recirculation regions. From a numerical standpoint it is important to mention that the ratio of convective to conductive energy transport for the 1 rev/s case was on the order of 10,000. Most numerical solutions are unstable at those high values; as a result, requiring up-winding techniques as in the finite element method. The measure of the convection to conduction ratio is most commonly referred to a the Graetz number and for this problem is defined by

$$Gz = \frac{\text{convective transport}}{\text{conductive transport}} = \frac{\Omega X^2}{\alpha} \qquad (13)$$

where $\Omega$ is the rotational speed of the mixer, X a characteristic dimension and $\alpha$ the thermal diffusivity.

## OUTLOOK

We are currently able to solve three-dimensional fluid flow problems and work is underway in developing DRM to allow the simulation of non-linear flow problems. We will be able to use this to simulate realistic polymer processing flows as shown in Fig.6. The figure depicts a single screw extruder where 9 points were tracked using the flow BEM program and compared with experimental results [23].

## CONCLUSION

Several variations of the equation of energy for problems encountered in polymer processing were solved using the boundary element method; a technique which requires simpler problem discretization than the finite difference and the finite element method. For problems such as the homogeneous Laplace equation the boundary element method needs only a discretization of the boundary and not the domain. For time dependent problems, the nonlinear terms were treated with the dual reciprocity method with randomly distributed internal nodes. The dual reciprocity method appeared to be superior in accuracy over domain type formulations with no need for domain integration, which is very cumbersome when moving boundaries are involved. Since the dual reciprocity method is a general applicable technique, algorithms for heat generation during exothermic cure reaction, viscous dissipation, convection, and viscous dissipation combined with convection were developed. The results agreed well with analytical and exact solutions. Oscillations in the convection problems were avoided by increasing the number of elements on the boundary. Heat transfer problems involving more complicated fluid flow were computed using an existing boundary element code that solves the Navier-Stokes equation and the results are plausible.

## ACKNOWLEDGMENTS

The authors would like to thank the German Academic Exchange Service (DAAD) for partial support of Mr. Mätzig's studies, the National Science Foundation under grant number DDM-9158145 and 3M Engineering Systems and Technology for their financial support. Acknowledgment is also made to the University-Industry Research program of the University of Wisconsin-Madison for supporting this research project in its early stages.

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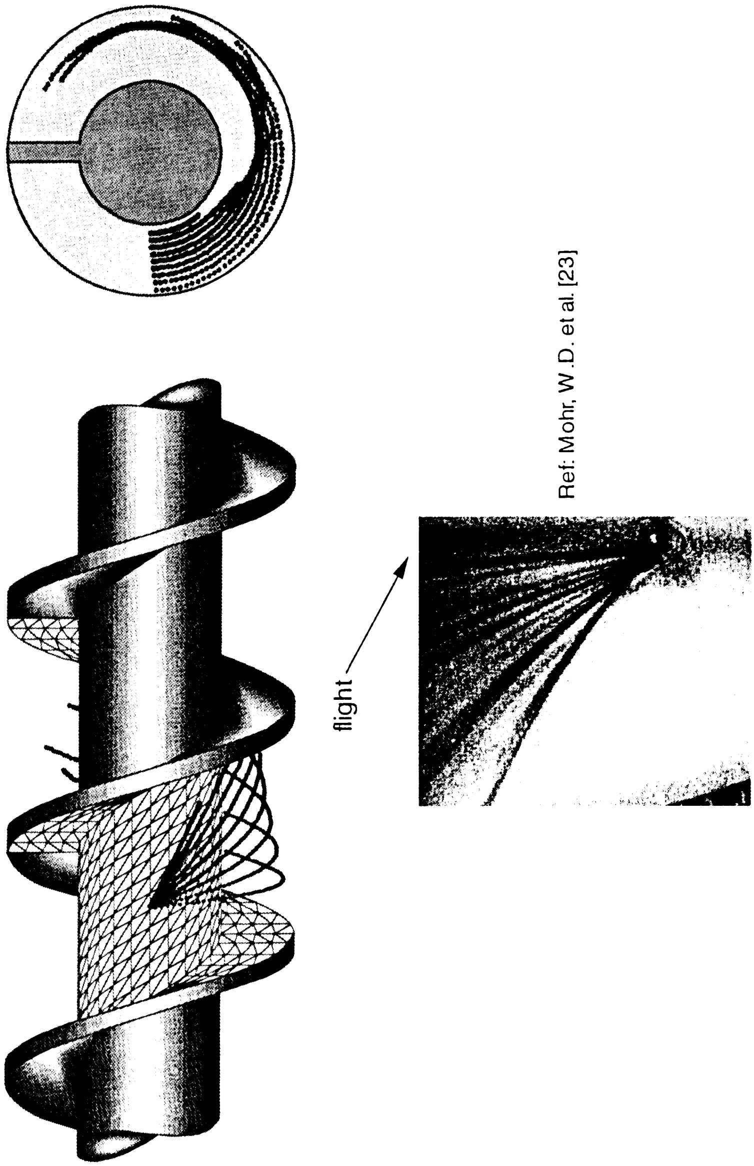


Figure 7. Comparison between the boundary element flow simulation and experimental results [23] of the flow through a single screw extruder.

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