OPTIMAL SHAPE DESIGN OF A POLYMER EXTRUSION DIE BY INVERSE FORMULATION

°Su Yeon Na and Tai-yong Lee

Dep. of Chemical Engineering, Korea Advanced Institute of Science and Technology, Guseong-dong, Yuseong-ku, Daejon 305-701, KOREA

Abstract The optimum design problem of a coat-hanger die is solved by the inverse formulation. The flow in the die is analyzed using three-dimensional model. The new model for the manifold geometry is developed for the inverse formulation. The inverse problem for the optimum die geometry is formed as the optimization problem whose objective function is the linear combination of the square sum of pressure gradient deviation at die exit and the penalty function relating to the measure of non-smoothness of solution. From the several iterative solutions of the optimization problem, the optimum solution can be obtained automatically while producing the uniform flow rate distribution at die exit.

Keywords Polymer Processing, Extrusion Die, 3-D Model, Inverse Problem, Optimal Design

1. INTRODUCTION

Extrusion dies are used in polymer processing where the products of various crosssectional shapes are produced by the extrusion process. The extrusion dies for sheet or film production invented up to now can be classified into three kinds of dies, i.e., T-die, fish-tail die, and coat-hanger die, whose names come from the shape of the channel, referred as the manifold in extrusion die, that achieve the role of distribution of flow. Among the three kinds of dies, coat-hanger die is prevalently used in industry recently because its geometry has the more appropriate configuration to achieve the design objectives which provide the die of higher performance. The determination of optimum geometry of a coat-hanger die has become the main subject in the research area of polymer processing.

First, the design of coat-hanger die is considered by the analytic approaches that use the simplified model of die flow. Most of the analytic interpretations of the flow field in a coat-hanger die are based on the assumptions that the flows in the manifold and the slot are one-dimensional and there is no interaction between the two flows. The oversimplified flow model makes the design result of the one-dimensional model not to be accepted as an ultimate solution. Hence the higher dimensional models of flow in the die are developed to get the more practical analysis. Two-dimensional models are based on the lubrication approximation. Many different numerical solution methods have been applied to the two-dimensional models. Application of lubrication approximation can not be justified in the region of manifold where the crosssectional shape undergoes significant change. So the flows in the die are to be considered as three-dimensional in order to get more realistic results. Recently, three-dimensional model are used by many researchers. Most of the three-dimensional studies use the FEM as the numerical scheme.

The previous analyses of the coat-hanger die using three-dimensional model have focused only on the simulation with the given die. The optimal design problem has not been dealt with through the three-dimensional model. In this work, the design problem of the coat-hanger die is solved by the inverse problem where the automatic design is possible.

2. FLOW SIMULATION

The flow in the coat-hanger die is by nature three-dimensional due to the complex geometry. The flow in the die is assumed to be incompressible, creeping and isothermal. The gravitational force can be safely neglected in this case. Under these assumptions, the three-dimensional model equations which are the conservation equations of mass and momentum can be written as

$$\nabla \cdot \boldsymbol{u} = 0, \tag{1}$$

and

$$\nabla \cdot \boldsymbol{\sigma} = 0. \tag{2}$$

In this study the fluid in the die is assumed to be Newtonian fluid because the development of automatic design method is the main objective of this study in spite of the fact that the polymer melts processed by extrusion die usually show the shear thinning behavior that is accounted for by the various non-newtonian model.

In three-dimensional model the following boundary conditions are applied. At die inlet plane, the fully developed flow profile is assumed where the only axial velocity component exists. The no-slip boundary condition is applied at die wall. On the symmetry plane, the normal stress vector and the normal component of velocity vector are zero. At die exit plane, the free boundary condition of velocity is assumed except that the normal stress vector is zero and pressure is set to be constant as the reference value of zero.

The numerical solution of three-dimensional model equations is obtained using finite element method. The numerical domain is discretized using three-dimensional

Lagrangian element. The velocity and pressure variables are approximated by triquadratic basis function and discontinuous piecewise linear basis function respectively.

3. OPTIMIZATION PROBLEM

The objective of die design is to determine the optimum geometry satisfying the process requirement that is commonly the uniform flow rate at die exit. The distribution of flow in a coat-hanger die is wholly accomplished through the manifold. The design of a coat-hanger die is to determine the optimum profile of manifold geometry in the width direction, y, in our system. In this study the design problem of manifold is formulated as an inverse problem where the optimum geometrical variables of manifold are determined with the given objective as an uniform flow rate distribution at die exit.

3.1 Model of manifold geometry

The linearly tapered coat-hanger die shown in Fig. 1 has a linear boundary between the manifold and the slot section. This type of coat-hanger die is the most popular in industry. When the crosssectional shape of manifold is specified as the equilateral triangle, the manifold geometry can be defined completely by the function that represent the characteristic length of manifold crosssection as a function of lateral coordinate, y. That function can be written as

$$h = h(y) \tag{3}$$

where h is the square root of the crosssectional area of manifold.

There have been many works that suggest the analytic functions that determine the manifold geometry using one-dimensional model. Here, we do not search for the analytic functions but the profile of manifold is discretized on the grid of finite element mesh in y-coordinate. The profile of manifold geometry can be represented as

$$h = \sum h^i \phi^i \tag{4}$$

where h^i is the value of h at i-th node in y-coordinate and ϕ^i is a linear basis function. In interpolating manifold geometry, the quadratic element used for three-dimensional geometry is reduced to linear element so that the number of nodes for manifold geometry is about the half of that of numerical domain.

The preliminary calculation results show that the h^i is not appropriate for the optimal algorithm. The sensitivity of the objective function to h^i is so small that the update of geometrical variables from the gradient matrix is impossible. New variables have to be defined that have much relation with the objective function. Our idea is to decompose h^i's into summations of new variables H^i's as

$$h^i = \sum_{j=1}^{i} H^j. \tag{5}$$

These new variables have larger span of influence on manifold geometry in y-coordinate than the original variables

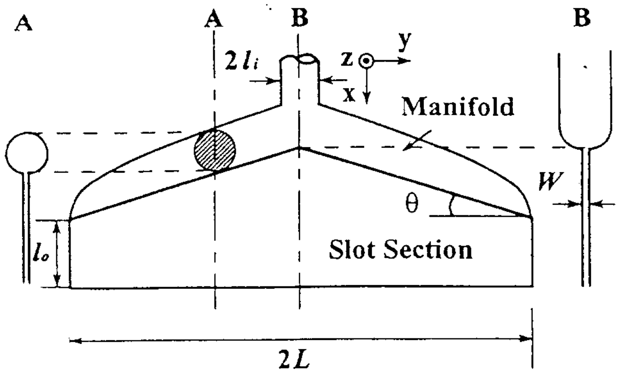

Fig. 1. Geometry of a linearly tapered coat-hanger die..

and are shown to be proper in optimization procedure.

3.2 Formulation of inverse problem

The coat-hanger die considered in this study is assumed to have the slot section of uniform thickness. If the slit opening is constant at die exit, the flow rate per unit width is the increasing function of pressure gradient, linearly for newtonian fluid. Uniform pressure gradient at die exit will ensure the maximum uniformity of flow rate distribution. From these considerations, the objective function of the optimization problem is defined as the square sum of pressure gradient deviations,

$$\Theta = \sum (p_g^i - \overline{p_g})^2. \tag{6}$$

where p_g^i is the pressure gradient in the i-th element lying on the bottom plane of numerical domain from the die center at die exit and $\overline{p_g^i}$ is the average of those values.

The inverse problem often exhibits the fluctuating solution due to its ill-conditioned feature. In this optimization problem, the fluctuation of solution is also found. The stabilizing functional is developed in inverse problem theory to eliminate this phenomena. In our study, the penalty function is introduced to the original objective function. The penalty function has to be defined to improve smoothness of the manifold geometry. Among the stabilizing functionals defined in the Solenov space, the penalty functional is selected as the square sum of third order gradient of the profile of manifold geometry along the y-coordinate that is written as

$$\Omega = \sum_i \left(\frac{d^3 h}{dy^3}^i \right)^2 \tag{7}$$

where $\left(\frac{d^3 h}{dy^3}^i \right)$ is the third order gradient in i-th domain. This penalty function is called stabilizer of third order and the third order gradient is calculated numerically in each domains that cover the whole y-coordinate.

The design problem of a coat-hanger die has become the optimization problem whose objective function is the linear combination of the square sum of pressure gradient deviation and the penalty term relating to the smoothness of solution. The final objective function of this optimization problem can be written as

$$M = \Theta + \alpha\Omega \tag{8}$$

where α is the regularization parameter. The determination of regularization parameter is a part of solution procedure of inverse problem. We use the formula for the optimum regularization parameter given in [3] as

$$\alpha_{op} = \inf_{\alpha} \left\| \alpha \frac{d H_\alpha}{d\alpha} \right\| \tag{9}$$

where H_α is the solution vector of the optimization problem for regularization parameter of α. The optimum geometrical variables can be obtained by the solution of Eq. (8) with the optimum regularization parameter determined by Eq. (9).

3.3 Solution of optimization problem

The optimization problem, Eq. (8) is solved using the three-dimensional flow simulator developed in the previous section. The optimum geometrical variables, H^i, are to be found that minimize the objective function given in Eq. (8). The solution of this inverse problem can not be directly obtained. The iterative optimization technique should be emploied.

The square sum of pressure gradient deviations is represented as a quadratic function of the geometrical variables, H^i. The penalty function can be also easily expressed as a quadratic function of the geometrical variables. The upper and lower bounds of update magnitude are imposed on each geometrical variables and the lower bound for the sum of all H^i is applied so that the minimum value of h at die side end is greater than zero. The quadratic optimization problem with a number of inequality constraints is solved using the subroutine, **qprog**, that is included in the commercial math library, **IMSL**.

4. RESULT AND DISCUSSION

The extrusion die considered in this study is the linearly tapered coat-hanger die. The ratio of die width to slot thickness is set to 100. The manifold angle is 15°. The numerical domain is a quarter of the total flow domain due to the symmetry of the die geometry. The bird-eye's view of three-dimensional mesh is shown in Fig. 2. We used the muti-block scheme in discretizing the numerical domain into the finite element mesh because the geometry of the manifold is very different from that of slot.

The geometrical variables, h^i, is defined along the y-direction at each node point resulting from the finite element discretization neglecting the node locating inside the quadratic element. h is set to be constant at die center. This means we fixed the initial magnitude of manifold crosssection in y-direction.

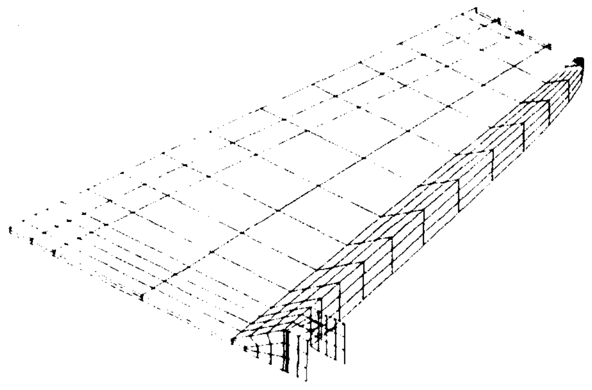

Fig. 2. Bird-eye's view of three-dimensional mesh.

Our optimization algorithm shows good convergence for the given process conditions that has been tried. Two kinds of initial guess, the uniform profile and the one determined by one-dimensional design equation, are considered. Here we used the one-dimensional design given by Liu *et al.*[1] who considered the same geometry of die used in this study. The value of h at die center calculated by one-dimensional design is used as the uniform initial guess. The optimum regularization parameter is determined. Then the optimum design result corresponding to the optimum regularization parameter is investigated. From the solutions of the optimization problem with the various reguarization parameters, the optimum regularization parameter is determined to be 0.01 for this inverse problem.

The most simplest initial guess that can be conceivable is the manifold that has constant crosssectional area. Even with this crude initial guess, our optimization algorithm easily converges to the optimum solution. The evolution of the profiles of flow rate distribution into the uniform one are shown in Fig. 3. It takes only 4 number of iterative solutions of optimization problem to reach the optimum solution. The flow rate distribution of the optimum solution has the flat profile suggesting the fully developed flow in the slot section.

The one-dimensional design equations are the only ones that have be developed. But the three-dimensional simulation results have shown that the die designed according to the one-dimensional design can give the uniform flow rate under the specific process condition[2]. Here the manifold geometry given by the one-dimensional design is used as the initial guess. After only two solution of optimization problem, the optimum solution is converged. The two flow rate distributions are compared in Fig. 4. The remarkable improvement of uniformity of flow rate distribution can be noticed. The corresponding change of profile of manifold geometry is shown in Fig. 5. In the region of manifold inlet and end, there is update of geometry. Fig. 4 and 5 suggest that small difference in the profile of manifold geometry can result the significant change of flow rate distribution. This emphasize the importance of our optimization algorithm that can correct the manifold geometry in detail.

5. Conclusion

The automatic design algorithm for the coat-hanger die is developed based on the three-dimensional flow model. The design of die is a shape optimization problem which exhibits poor convergence and ill-conditioned feature. A novel method is devised and successfully applied to accelerate the convergence. The regularization method is introduced to alleviate the ill-conditioned feature. When this automatic design algorithm is applied to the initial guess given by the one-dimensional design, the uniformity of flow rate distribution is significantly improved by only two solutions of the optimization problem. This automatic design algorithm can be considered as the new approach which employ the concept of inverse problem in the area of the die design study.

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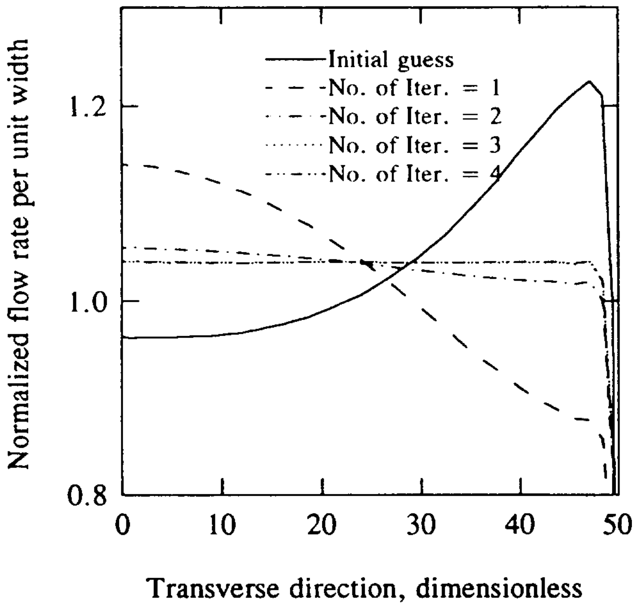

Fig. 3. Flow rate distribution with the number of iterative solutions of optimization problem.

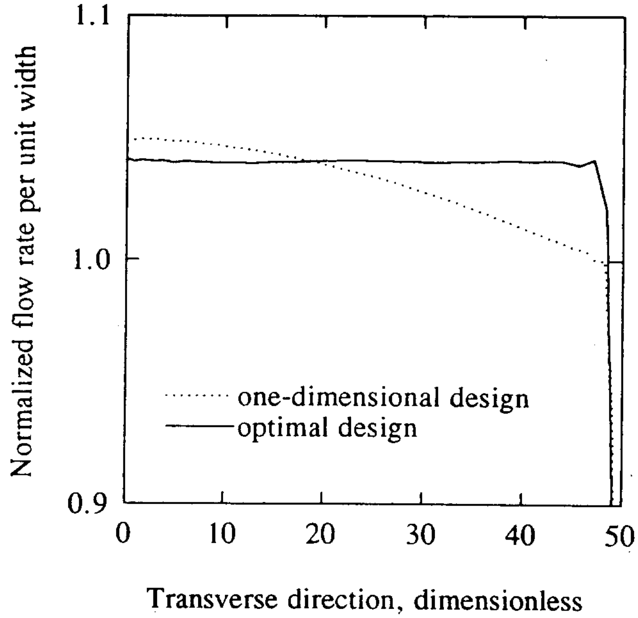

Fig. 4. Comparison of profiles of flow rate distribution between optimal design and one-dimensional design.

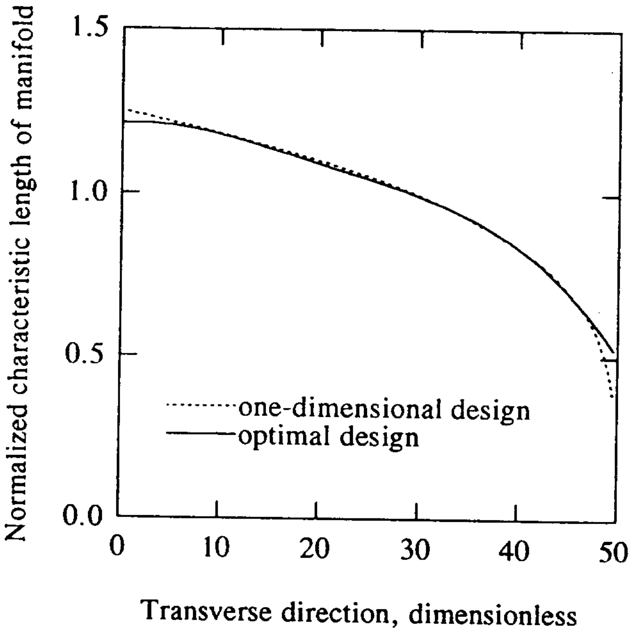

Fig. 5. Comparison of profiles of manifold geometry between optimal design and one-dimensional design.