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3차원 흐름 모사와 비뉴톤 유체 모델을 이용한 고분자 압출 다이의 형상 최적화

Shape Optimization of Polymer Extrusion Die Using Three-Dimensional Flow Simulation and non-Newtonian fluid models

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Abstract Three-dimensional optimum design of coat-hanger die is performed using power-law and Carreau models. It is found that the three-dimensional optimum design algorithm shows good convergence with the non-Newtonian fluids. The more realistic optimum design is accomplished by employing Carreau model with the three-dimensional design method. The effect of viscosity models is investigated by comparing the optimum manifold profiles and flow rate distributions of power-law and Carreau models. Through the accurate viscosity representation of Carreau model, the effect of total flow rate on the optimum manifold profile is investigated.

Keywords Polymer, Extrusion, Three-Dimensional, Optimization, non-Newtonian

1. INTRODUCTION

A coat-hanger die is widely used in polymer process for production of films or sheets. Fig.1 shows the schematic geometry of a coat-hanger die. Many researches have been performed to get the optimum geometry of coat-hanger die which generates the uniform flow rate distribution at die exit. Since the product quality is governed by thickness uniformity, much efforts has been devoted to the shape optimization problem of coat-hanger die in polymer processing industry.

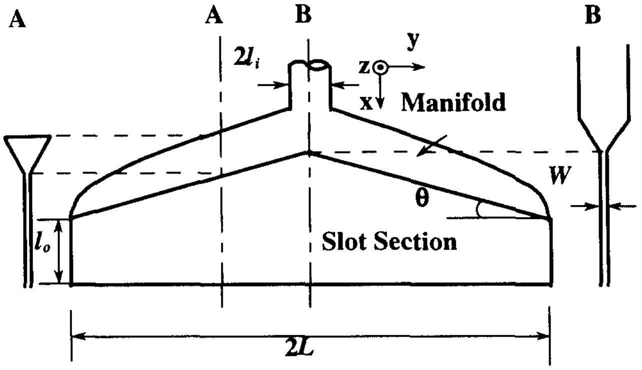


그림 1 옷걸이형 다이의 형상.

Fig. 1 Schematic geometry of a coat-hanger die.

The optimum design of coat-hanger die has been achieved by many researchers using one-dimensional flow model. The accurate and complicated analyses of die flow have been achieved using more rigorous flow models such as two- and three-dimensional flow models. Although many numerical analyses of coat-hanger die have been accomplished using two- and three-dimensional flow models, they were limited to the inductive simulation for a given die geometry. A systematic design algorithm was implemented to the numerical flow analysis based on two- or three-dimensional flow model in order to develop an optimum design tool which efficiently utilizes the precise flow information. Recently, Na and Lee[4] developed an optimum design method of coat-hanger die based on three-dimensional flow modeling.

Carreau model is effective and accurate in representing the non-Newtonian viscosity of polymer melts as a function of shear rate. If elastic effect is negligible, the non-Newtonian viscosity of polymer melts can be represented accurately by Carreau model in the whole range of shear rate. Matsunaga et al.[3] showed that in creeping flow dominated by the shear deformation the velocity fields calculated by the pure viscous non-Newtonian and viscoelastic models coincide with each other if both models have the same shear viscosity. In their analysis, Carreau model was used for the representation of non-Newtonian viscosity.

In spite of the fact that the viscosity behavior of polymer melts is accurately represented by Carreau model, the optimum design has not been accomplished using the model. In this work, the three-dimensional design method developed by Na and Lee[4] is applied to a linearly tapered coat-hanger die with power-law and Carreau models. An important merit of the design method is that any fluid models can be used for polymer melts in the optimum design process as long as the three-dimensional flow simulation is feasible with those models. By using the three-dimensional design method with Carreau model, more realistic design results are obtained. The optimum manifold profile and flow rate distribution of power-law model are compared with those of Carreau model to reveal how the accuracy of viscosity model affects the optimum design results.

2. DIE FLOW MODELING

In flow modeling, the die flow is assumed to be incompressible, creeping, and isothermal. The effect of gravitational force is negligible in this process. Application of these assumptions gives the governing equations of three-dimensional model as

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

and

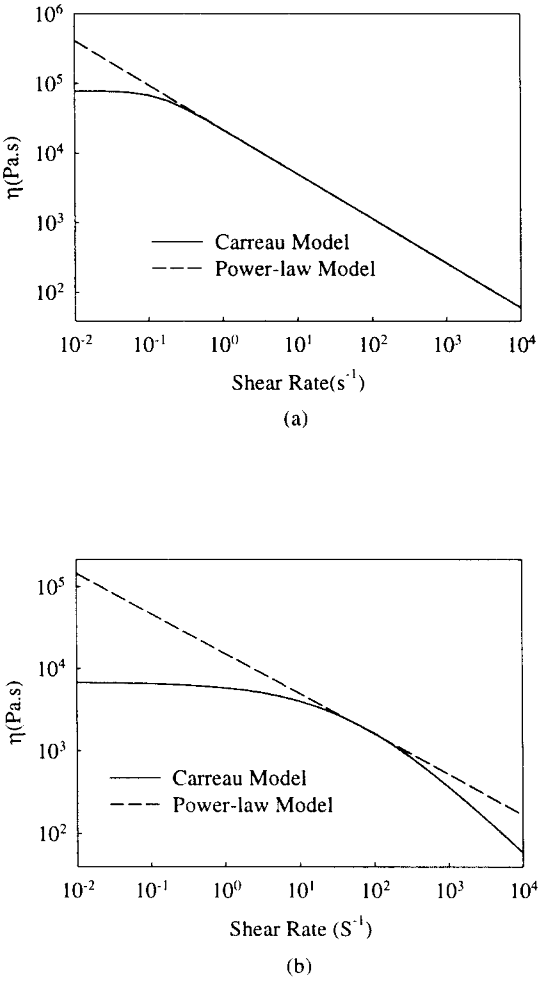
$$\nabla \cdot \sigma = 0 \tag{2}$$

where σ is a stress tensor. In general, polymer melts are non-Newtonian fluids. It is necessary to use a generalized Newtonian model whose viscosity is a function of shear rate.

In modeling of polymer melt flow, an appropriate viscosity model is necessary to represent the non-Newtonian behavior of polymer melts. The result of flow modeling is severely dependent on the viscosity model. The simple and widely used model in die analysis is power-law model In this study, Carreau model is also employed to get more realistic representation of non-Newtonian viscosity of polymer melts. Carreau model uses four parameters for fitting of viscosity vs. shear rate data, while power-law model uses two parameters.

In this study, the fluid property data given by Arpin et al.[1] are applied. They experimentally obtained viscosity data of HDPE and LLDPE and calculated the parameters of power-law and Carreau models from curve fitting method. Their viscosity master curve showed that Carreau model was a quantitatively accurate representation of experiment data.

To compare the two viscosity models, the viscosity curves of power-law and Carreau models are plotted together in Fig. 2. The two models agree well with each other for HDPE except in the range of shear rate less than 1.0. In the case of LLDPE, the two models are significantly different from each other in the whole range of shear rate. In both materials, power-law model shows a considerable deviation from Carreau model for low shear rate. As shear rate increases, the two models nearly coincide for HDPE but the deviation of power-law model from Carreau model does not disappear for LLDPE. The results indicate that the reliability and accuracy of the optimum design result can be improved by application of Carreau model.



(a)

(b)

그림 2 점도 곡선. (a) HDPE (b) LLDPE

Fig. 2 Viscosity curve. (a) HDPE (b) LLDPE

3. THREE-DIMENSIONAL OPTIMUM DIE DESIGN

The optimum design method employed in this study is briefly outlined to help understand the optimum design results. Details of the design method are given by Na and Lee[4].

The schematic geometry of a linearly tapered coat-hanger die considered in this study is shown in Fig. 1. The characteristics and performance of the coat-hanger die are determined by the distribution of manifold cross-sectional area in the transverse direction. The manifold geometry is represented by the profile function,

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

where h is the characteristic length of manifold cross-section, and y is the lateral coordinate as shown in Fig. 1. The manifold profile function is discretized into finite data points, (h_i, y_i), from $i = 0$ at die center to $i = N_I$ at die side end. The complete manifold profile is obtained using the cubic spline interpolation of the finite data points. Then the manifold geometry is determined by the finite number of geometrical variables, h_i's.

The design variables are defined using h_i's as

$$H_0 = h_0,\ H_i = h_i - h_{i-1} \text{ for } i \geq 1 \tag{4}$$

which efficiently represent the effect of the manifold profile on the flow rate distribution at die exit. The sensitivity of flow rate distribution with respect to design variables is greatly improved by using H_i's. The characteristic length of manifold cross-section at die inlet, h_r, is fixed as a reference point of the manifold profile to guarantee the uniqueness of the optimum solution.

The optimum solution of the design variables is obtained from the quadratic optimization problem which is developed through the inverse formulation. The design objective function, Θ, is defined as the square sum of pressure gradient deviations at die exit. The ill-conditioned nature of the inverse problem is eliminated using the penalty function, Ω, defined as the square sum of third-order derivatives of the manifold profile function. The total objective function of the optimization problem is defined as

$$M = \Theta + \alpha\Omega \tag{5}$$

where α is the regularization parameter which controls the effect of the penalty function on the optimum solution profile.

4. RESULTS AND DISCUSSION

In this study, a linearly tapered coat-hanger die shown in Fig. 1 is considered. The slot thickness, which is 0.01m, is chosen as characteristic length scale, and all the dimensions are given in dimensionless values from now on. Half the die width, L, is 50. The manifold angel, θ, is 5°. Half the inlet width, l_i, is 4, which is small enough not to influence the die flow field. The length of slot region, l_o, is 10. The cross-sectional shape of manifold is assumed to be an equilateral triangle, and the characteristic length of manifold cross-section, h, is defined as the side length of triangular cross-section.

The optimum design method, which is going to be applied in this study, employs a three-dimensional flow simulator based on finite element method to get realistic die flow field[4]. In the three-dimensional simulation, characteristic velocity, u_c, is defined as the mean velocity at die inlet of a standard case. As the standard case, u_c is taken as 0.01m/s. Hence, the dimensionless mean velocity at die inlet, u_m, of the standard case is 1.0. u_c and u_m are defined separately to control the total flow rate by changing u_m.

In the optimum design method, there are two parameters to be provided prior to the shape optimization process, the number of interpolation points of the manifold profile, N_I, and the regularization parameter, α. N_I does not affect the optimum design results if it is large enough to represent the curvilinear manifold profile function sufficiently. But the computational load increases with the number of interpolation points. In this study, it is decided to be 8, and its effect on the optimum manifold profile is investigated. Since the desirable optimum manifold profile is a smooth function, it is unnecessary to use a large number of interpolation points. Na and Lee[4] determined the optimum regularization parameter as 1.0E-8 in the development of the optimum design method. The optimum regularization parameter can be safely used in this study because the optimum design scheme is formulated to be independent of the process conditions[4]

4.1 Convergence of optimum design algorithm for power-law and Carreau models

The variations of total objective function are plotted in Fig. 3 with the number of iterations for power-law and Carreau fluids of HDPE. The uniform manifold profile is used as the initial guess to test the robustness of convergence of the optimum design algorithm. In both cases, the optimum solution is obtained by about five iterations. It is shown that the convergence of the optimum design algorithm is nearly independent of the fluid model as long as the flow simulation is performed precisely during solution process.

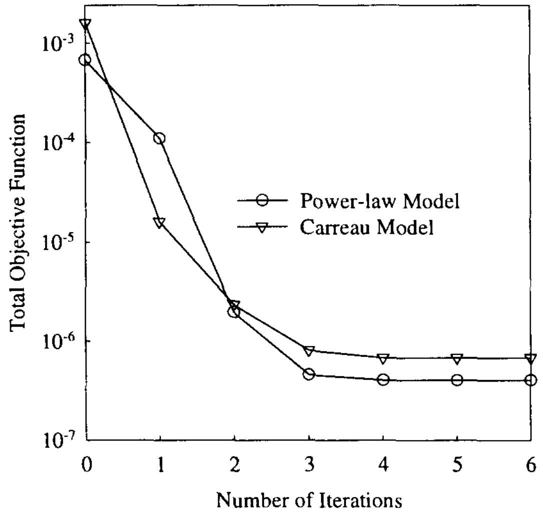
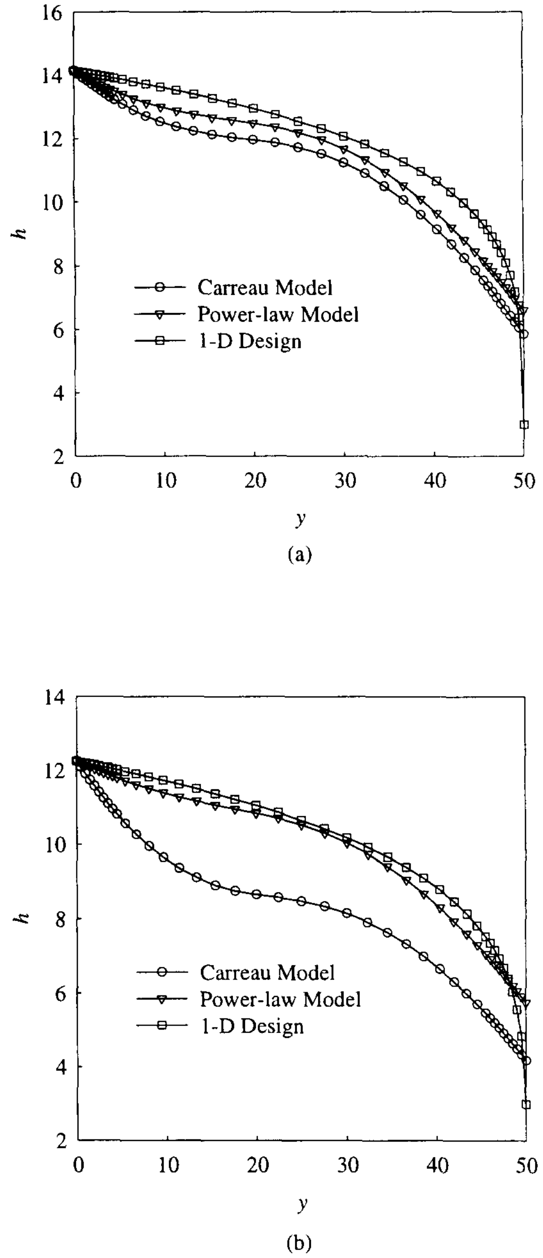


그림 3 최적화 문제의 반복해에 따른 목적함수의 변화.

Fig. 3 Change of total objective function with iterations.

4.2 Optimum manifold design for power-law and Carreau models

In Fig. 4, the optimum manifold profiles of Carreau and power-law models are compared for HDPE and LLDPE. In both calculations, the reference characteristic length of manifold cross-section, h_r, is taken as the one given by one-dimensional design based on power-law model[2]. The manifold profiles of Carreau model are lower than those of power-law model in the whole range for both cases. The difference is more significant for LLDPE than HDPE. It is in accordance with the fact that power-law model deviates more significantly from Carreau model for LLDPE. In the viscosity curves shown in Fig. 2, Carreau model gives smaller viscosity than power-law model. It is the reason the manifold profile of Carreau model is lower than that of power-law model.



(a)

(b)

그림 4 최적 매니폴드의 비교. (a) HDPE (b) LLDPE

Fig. 4 Comparison of optimum manifold. (a) HDPE (b) LLDPE

4. 3 Effect of total flow rate on flow rate distribution

The shear rate of the die flow increases with the total flow rate at die inlet. Since the viscosity behavior of polymer melts is dependent on the shear rate, the effect of the total flow rate on the optimum manifold profile must be investigated. By using Carreau model, we can identify the effect of the total flow rate on the die flow field, consequently the optimum manifold profile. In contrast, power-law model cannot represent properly the effect of the total flow rate on the die flow field since the characteristics of viscosity vs. shear rate is constant throughout the whole range of shear rate.

The dimensionless mean velocity, u_m, at die inlet of the standard case is 1.0 which was used in the previous calculations. As u_m is increased, the flow rate distributions are calculated using the constant die which is optimized for $u_{ni}=1.0$. Change of flow rate distributions is shown with u_{ni} for both materials in Fig. 5. For comparison, the flow rate distribution of power-law fluid is displayed together.

The two materials show significantly different behaviors of the flow rate distributions. In the case of HDPE, the flow rate distribution converges to that of power-law fluid by a small increase of total flow rate. It results from the fact that Carreau and power-law models are nearly coincident for HDPE except in the narrow range of shear rate less than 1.0 as shown in Fig. 2. As the total flow rate increases, the shear rate increases up to such a level that the two fluid models give the same viscosity in the whole flow domain. If power-law model represents viscosity of polymer melts correctly except for low shear rate, power-law model can give realistic design results for the higher total flow rate. But it may be recommendable to choose a fluid model as accurate as possible in the optimum design stage, if available.

In Fig. 5, the flow rate distribution changes more severely with the total flow rate for LLDPE than HDPE.It can be explained by the fact that the characteristics of viscosity vs. shear rate relationship of LLDPE varies greatly with the shear rate as shown in Fig. 2. LLDPE shows the similar trend to HDPE in that the flow rate distribution becomes closer to that of power-law fluid as the flow rate is increased. This result indicates that the discrepancy between Carreau and power-law models becomes smaller as the shear rate increases. The flow rate distribution, however, does not converge to that of power-law fluid even when the total flow rate is increased by order of ten. For the fluid whose viscosity deviates significantly from power-law model as LLDPE, Carreau model has to be used to get the practical optimum design results. Through the accurate representation of viscosity behavior of polymer melts, the effect of process conditions must be taken into account in the optimum design stage.

5. CONCLUSION

Three-dimensional optimum design of coat-hanger die is successfully accomplished for power-law and Carreau model fluids. The design method shows good convergence even from the rough initial guess of uniform manifold profile. The effect of viscosity model and other process conditions on optimum manifold profile is investigated thoroughly.

By using Carreau model, we obtain more practical design result with the three-dimensional design. The effect of viscosity representation on the optimum manifold profile is clearly identified by comparison between power-law and Carreau models. Power-law model shows higher manifold profile than Carreau model for both materials, HDPE and LLDPE, considered in this study. Optimum manifold profile is affected more severely when power-law model shows more deviation from Carreau model.

Total flow rate is varied to see its effect on the flow rate distribution using Carreau model. For HDPE, the flow rate distribution converges to that of power-law model as total flow rate is increased. The flow rate distribution of LLDPE is more influenced by total flow rate but does not converge to that of power-law model.

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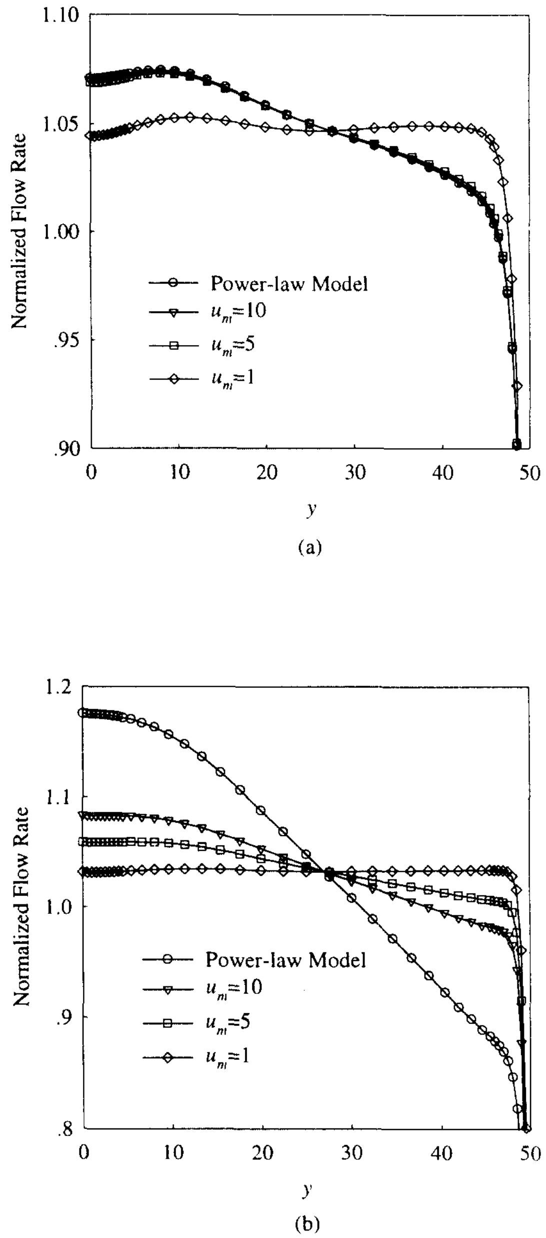

(a)

(b)

그림 5 전체 유량에 따른 유량 분포의 변화. (a) HDPE (b)LLDPE
Fig. 5 Change of flow rate distribution with total flow rate.
(a) HDPE (b) LLDPE