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Identification of Cross-WLF Viscosity Model Parameters Using Optimization Technique

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최적화기법을 이용한 Cross-WLF점도 모델 계수 추정

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Abstract Predicting the behavior of rheological polymers is highly shear rate- and temperature-dependent. The Cross-WLF viscosity model has become a powerful solution that describes the shear rate- and temperature-dependent characteristics. To estimate the behavior of polymers in computational simulations, the coefficients of the Cross-WLF model should be well identified. An identification technique was proposed to determine the Cross-WLF viscosity model coefficient. The assumption is that the Cross-WLF viscosity model well describes the real characteristics of polymers when the calculated viscosity with the parameters is identical to the reference data. In this study, Auto-desk Moldflow data were used as a reference. The numerical examples showed that the proposed method accurately identifies the Cross-WLF viscosity model coefficients.

요 약 본 논문은 최적설계기법을 적용하여 Cross-WLF 모델의 계수 값을 효과적으로 추정하는 것이다. 사출성형 공정의 해석에서 주로 사용되는 Cross-WLF 점도 모델은 온도와 전단율의 영향이 민감한 고분자의 유변학적 특성을 잘 모사하는 모델로 널리 사용되고 있다. 정확한 폴리머 유변학적 특성 예측을 위해서는 정확한 Cross-WLF 계수 값의 추정은 필수이다. 실험적으로 획득한 데이터의 점도 값과 Cross-WLF의 계수 값을 설계변수로 가정하여 계산한 점도 값이 일치한다면, 최적화기법을 통해 정의된 Cross-WLF모델이 실험 데이터를 정확하게 모사하는 것이라 할 수 있다. 이러한 Cross-WLF 모델을 통해 계산된 점도와 실험 데이터의 차이를 최소화하는 목적함수로 Cross-WLF의 계수 값을 설계변수로 정의하여 연구를 수행하였다. 본 논문에서 제시한 최적화기법의 타당성으로 확인하기 위하여 몇개의 소재를 대상으로 하여 Moldflow에서 제공하는 Cross-WLF 계수 값과 본 논문에서 제안한 방법으로 획득한 계수 값을 비교하여 잘 일치함을 확인하였다. 또한, Moldflow Plastic Lab의 실제 측정 데이터를 활용하여 추정한 결과 제안한 방법의 효율성 및 타당성을 입증하였다.

Keywords : Cross-WLF viscosity model coefficients, Identification, Optimization procedure, Sensitivity analysis, Injection molding

1. Introduction

Computational simulations have been significantly important tools for the investigation of part design such as mold design and processing parameters in injection molding in terms of their cost effectiveness and immediate responses. Since the viscosity of melt polymer has been wide variations and is highly nonlinear behavior depending upon temperatures and shear rates. In order to accurately predict the viscosity for specifically thermoplastic materials with respect to shear rate, the Cross-WLF viscosity model is widely

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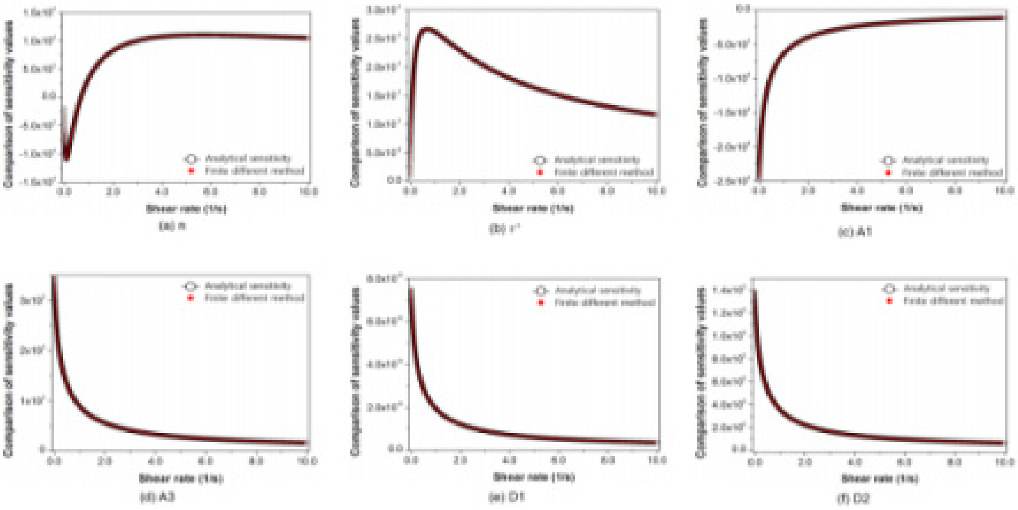
and mostly used [1-2]. There are ultimately 7 coefficients describing the Cross-WLF viscosity model and those parameters should be accurately identified in order to improve simulation accuracy. It requires a very long during and very expensive in order to identify the parameters of a new materials. In the literature survey, there are also not many journal papers published to identify those unknown design parameters of Cross-WLF viscosity model.

A line search method is recently adopted identifying the coefficients of Cross-WLF viscosity model using central differential method [3]. Although the method provides reasonable results, the final optimal points might be less accuracy and the optimization procedure could be less efficiency because of the central differential method. A couple of research papers have also investigated to find design parameters of a prediction model. A direct nonlinear optimization and sub-optimal methods are adopted to find the parameters of viscoelastic damping materials [4]. A structural joint identification method in a real structure in which the differences between calculated FRFs and measured FRFs are minimized using a gradient-based optimization method was proposed [5]. It is also proposed an efficient identification method of the viscoelastic damping material parameters using an optimization technique and showed its applicability through numerical and experimental examples [6-7].

In this research paper, an identification procedure identifying Cross-WLF viscosity model coefficient is proposed with a gradient-based optimization algorithm. It is assuming that the design parameters of Cross-WLF viscosity model are accurately identified when calculated viscosity models by changing the model parameters are identical to the reference data. Thus, minimizing the discrepancy between the calculated viscosity model with parameters and reference data is the objective function and the parameters are considered as design variables. For robustness and efficiency, analytical sensitivity formulae are derived for the minimization of optimization procedure. Estimating the proposed numerical algorithm, Autodesk Moldflow data would be adopted by comparing the coefficient of Cross-WLF viscosity model and objective function values.

The remainder of this paper is organized as follows. Section 2 illustrates the proposed method in order to identify Cross-WLF viscosity model coefficients using optimization technique. Numerical examples demonstrate the proposed procedure in Section 3. Section 4 summaries the proposed identification method.



(a) n (b) τ^* (c) A1 (d) A3 (e) D1 (f) D2

Fig. 1. The comparison of sensitivity values between analytical and finite difference method

2. A new identification technique for Cross-WLF viscosity model coefficients

2.1 The Corss-WLF viscosity model

The Cross-WLF viscosity model could be described as follow:

$$\eta = \frac{\eta_0}{1+\left(\frac{\eta_0\dot{\gamma}}{\tau^*}\right)^{1-n}} \tag{1}$$

where is the melt viscosity, is zero shear viscosity or Newtonian limit meaning that the viscosity approaches a constant at very low shear rates and is shear rate. n and are coefficients. The zero shear viscosity could be expressed as follows:

$$\eta_0 = D_1\exp\left[-\frac{A_1(T_1-T_{ref})}{A_3+(T_1-T_{ref})}\right] \tag{2}$$

where T_{ref} is an absolute reference temperature and could be expressed as $T_{ref}=D_2+D_3 \cdot P$. P is pressure. In most cases, pressure effect on viscosity is neglected so D_3 is not a design parameter. D_3 is considered as zero meaning that the pressure influence is ignored for the numerical examples. Here, A_1, A_3, D_1 and D_2 are design variables. Therefore, total 6 design variables, n, τ^*, A_1, A_3, D_1 and , D_2 should be carefully identified for accurately describing the Cross-WLF viscosity model.

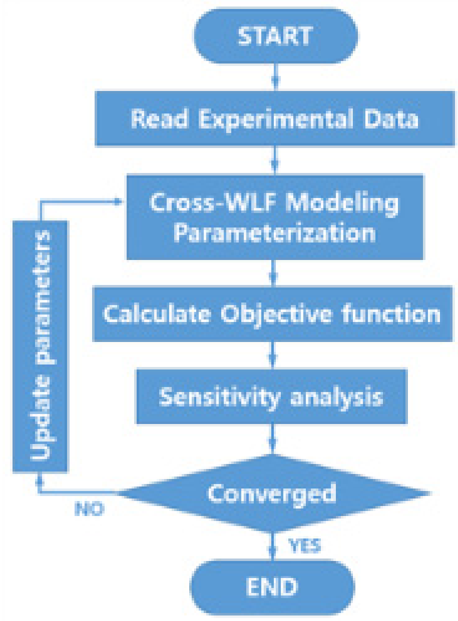


Fig. 2. The flow chart of optimization procedure

2.2 Proposed identification method by minimizing residual

In order to accurately and efficiently find the coefficients of Cross-WLF, it is assuming that the parameters would be “true” values as minimizing the discrepancy between reference data and the one that numerically reproduced by the parameters. The coefficients of Cross-WLF viscosity model would be considered as design variables. It is well-known technique in engineering problems that a least-square error between two different data is considered as an objective function in this study. The summation of square of the discrepancy between two different data－reference data and calculated data by the design variables over a wide range of shear rate－could be considered as identification index as follows:

$$g(b)=\sum_{j=1}^{M}\sum_{i=1}^{N}\left(\eta^{s}_{i,j}-\eta^{ref}_{i,j}\right)^2 \tag{3}$$

where {b} would be n, τ^*, A_1, A_3, D_1 and D_2 as design variables. N is the number of samples with respect to shear rate at a temperature and M is the number of

Table 1. The lower and upper boundaries of parameters

Design parameters	Lower boundary	Upper boundary
n	0.000e+00	1.000e+00
τ^*	1.000e+01	1.000e+07
A1	1.000e+00	1.000e+02
A3	1.000e+00	1.000e+02
D1	1.000e+10	1.000e+16
D2	1.000e+01	1.000e+03

different temperature conditions. The superscripts s and ref are calculated data and reference data respectively. To identify the parameters of Cross-WLF viscosity model, the formulation of optimization as follows:

$$\begin{aligned} &Minimization\ g(b) \\ &\text{subject to } b_{l,i} \le b_i \le b_{u,i} \end{aligned} \tag{4}$$

where $g(b)$ is the objective function and there is no constraint, which is an unconstrained optimization formulation. The $b_{l,i}$and $b_{u,i}$are the lower and upper boundaries of $i-th$ design variables respectively. The lower and upper values are reasonably determined by the user based on understanding the physical meaning of each parameter.

2.3 Sensitivity analysis of Cross-WLF model

A gradient-based optimization method is adopted to minimize the identification index. Generally gradient-based techniques are most effective and accurate even though they may provide a local minimum value. Thus, design sensitivity analysis is necessary. The parameter sensitivity analysis is the gradient of the objective function with respect to each design variable. As an alternative method, a finite different method could be used to calculate the sensitivity information. However, the finite different method would be much more expensive and less accurate, which causes into a slow convergence. In this study, a direct differentiation method [6] is applied to the discrete system equations in order to obtain an analytical sensitivity formula with respect to the Cross-WLF viscosity model coefficients as follows:

$$\frac{\partial g(b)}{\partial b} = 2.0\left(\eta_{i,j}^{s} - \eta_{i,j}^{ref}\right)\frac{\partial \eta_{i,j}^{s}}{\partial b} \tag{5}$$

where $\partial g(b)/\partial b$ is the sensitivity of objective function with respect to design variables. The partial derivative of the calculated Cross-WLF viscosity model, $\partial \eta_{i,j}^{s}/\partial b$, should be ultimately obtained. It is imperative to show the accuracy of the analytical sensitivity formulation. The forward difference method would be used in order to compare the analytical sensitivity formulation with respect to the model parameters. For the forward difference method, 0.1 percentage perturbation of design variable is considered. Temperature, T_1, is 400°C as an environmental condition. For calculating the sensitivity analysis, it would be adopted for the coefficients of Cross-WLF viscosity model [3].

Fig. 1 shows the comparison the sensitivity values between the analytical sensitivity and 0.1 percentage perturbed finite different calculation with a wide range of shear rate, 0.001 to 10.0. The red line with square dot represents the finite different values; meanwhile, the black line with circular dot represents the analytical sensitivity value. As shown in Fig. 1, both values are almost identical which means that the analytical sensitivity formulation would be accurately obtained. The number of sensitivity comparison graph is only 6 because D_3 would not be considered as design variables in this study.

3. Numerical examples

In order to prove the proposed optimization technique identifying the coefficients of Cross-WLF viscosity model, Autodesk Moldflow [8] data would be adopted; 1) Ultramid b3k6, 2) Trirex 30221R, 3) Lexan HF 1140R and 4) Lupilon s-2000. Since n and τ^* are the most important coefficients, the above mentioned 4 different viscosity model are considered. Parameters n makes an important role of shear thinning. Because of these important effectiveness, Ultramid b3k6 and Trirex 30221R polymer materials are considered; would be either the biggest or lowest value among Autodesk Moldflow data. Lexan HF 1140R and Lupilon s-2000 were also chosen due to τ^*. In terms of optimization procedure, significantly different curved-shape data maybe have some difficulties for obtaining proper optimal values. Ultimately, 3 different data and 2 objective function values are carefully compared. Firstly, 200 discrete numerical data are from Autodesk Moldflow as reference data, which are viscosity values with respect to shear rate. Secondly, Cross-WLF viscosity model calculated with coefficient values provided from Autodesk Moldflow. Lastly, Cross-WLF viscosity model with optimal values. Thus, it is required to compare parameters between the commercial software provided and the optimal values throughout the optimization procedure. The objective functions are compared between reference viscosity and the ones calculated from Autodesk Moldflow coefficients and between reference viscosity and the ones calculated from optimal design variables. Autodesk Moldflow usually provides 200 discrete data points, which are 4 different temperature conditions and each temperature condition includes 50 viscosity data according to shear rate with the design parameters values. For the optimization procedure, the data from Autodesk Moldflow would be considered as reference.

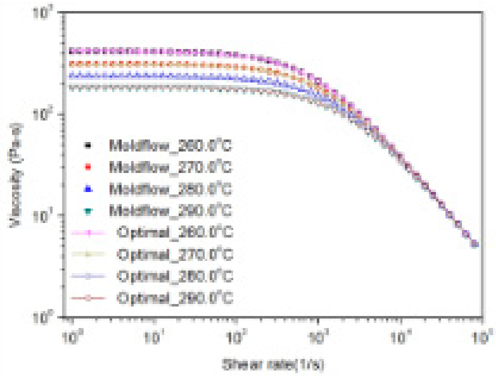


Fig. 3. The comparison of Cross-WLF viscosity model between optimal values and the ones from Autodesk Mold flow; Ultramid B3K6

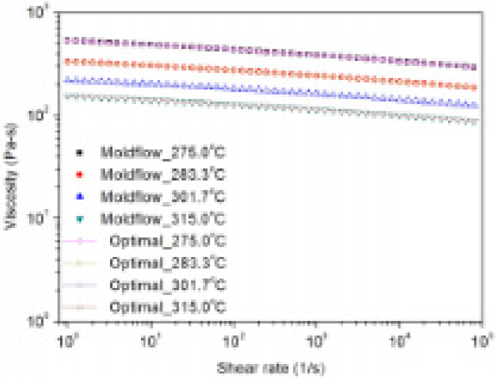


Fig. 4. The comparison of Cross-WLF viscosity model between optimal values and the ones from Autodesk Mold flow; Trirex 30221R

Additionally, Cargill Dow LLC-MAT2238 was also considered in which experimental viscosity data would be provided and the coefficients of Cross-WLF viscosity model identified by Moldflow Plastics Labs[10]. Based on the provided experimental data, the parameters would be identified and then compared with the ones obtained by Moldflow Plastic Labs.

The optimization procedure would be explained. Firstly, it is required that the data provided from Autodesk Moldflow would be read as reference data. Secondly, the Cross-WLF viscosity model with initial

Table 2. The comparison the optimum design variables and coefficient provided from Autodesk Moldflow; Ultramid B3K6

Design parameters	Lower boundary	Upper boundary
n	1.131e-05	1.000e-05
τ^*	4.318e+05	4.318e+05
A1	3.699e+01	3.707e+01
A3	5.169e+01	5.160e+01
D1	2.455e+15	2.628e+15
D2	3.332e+02	3.332e+02

Table 3. The comparison the optimum design variables and coefficient provided from Autodesk Moldflow; Trirex 30221R

Design parameters	Lower boundary	Upper boundary
n	8.948e-01	8.948e-01
τ^*	2.059e+05	2.060e+05
A1	2.972e+01	2.539e+01
A3	4.263e+01	5.160e+01
D1	5.714e+12	6.720e+12
D2	4.114e+02	4.172e+02

design variables would be investigated at the same shear rate with Autodesk Moldflow data. Thirdly, the objective function would be calculated, which is the discrepancy between reference data and the Cross-WLF viscosity model calculation with design variables. Fourthly, the sensitivity analysis should be obtained at the given parameters. Then a convergence condition would be checked. If the convergence criterion is met, the procedure would be terminated. Unless the iteration procedure is going to keep until the convergence condition would be met by minimizing the objective function. Those optimization flow is shown in Fig. 2.

It is also noted that normalization, in other words scaling, often desirable to eliminate wide variations in the magnitudes of design variables as follows:

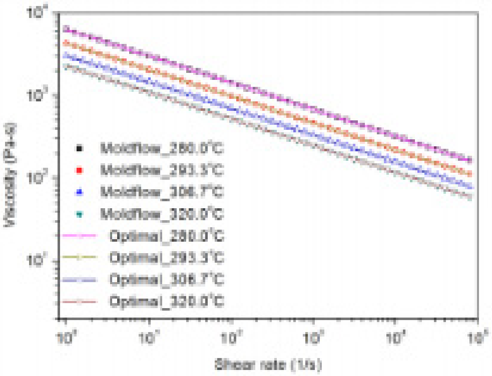


Fig. 5. The comparison of Cross-WLF viscosity model between optimal values and the ones from Autodesk Mold flow; Lupilon S-2000

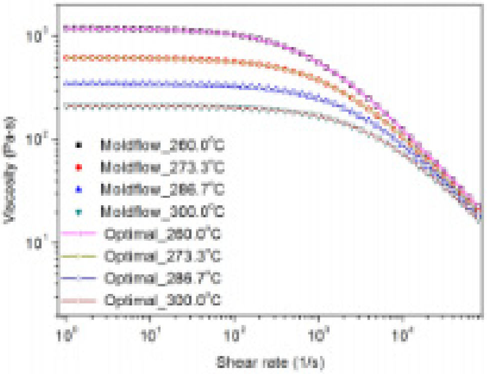


Fig. 6. The comparison of Cross-WLF viscosity model between optimal values and the ones from Autodesk Mold flow; Lexan HF 1140R

$$\frac{\triangle g(b)/g(b)}{\triangle b/b} = \frac{b}{g(b)} \cdot \frac{\partial g(b)}{\partial b} \qquad (6)$$

Normalization technique is very important to the Cross-WLF viscosity model because of the wide magnitude design sensitivity values. For instance, the order of magnitude of design sensitivity values of n is 4; however, the order of magnitude of design variables D_1 is -9 which is almost zero and not significantly affect into Cross-WLF viscosity model. Since a wide magnitude design sensitivity values, normalization should be considered in this study. The global optimization toolbox in Matlab is adopted for an optimizer with both global minimum, GlobalSearch class, and multiple starting point, MultiStart class, for gradient-based unconstrained problem. Considering only a local optimizer, *fmincon*, sometimes provide local minimum point which means the final design parameters are significantly dependent upon the given initial values. All other parameters for optimization in Matlab are set as default [9].

Table 4. The comparison the optimum design variables and coefficient provided from Autodesk Moldflow; Lupion S-2000

Design parameters	Lower boundary	Upper boundary
n	6.703e-01	1.000e-05
τ^*	8.361e+01	4.318e+05
A1	3.039e+01	3.707e+01
A3	5.070e+02	5.160e+01
D1	6.103e+14	2.628e+15
D2	4.193e+02	3.332e+02

Table 5. The comparison the optimum design variables and coefficient provided from Autodesk Moldflow; Lexan HF 1140R

Design parameters	Lower boundary	Upper boundary
n	1.300e-01	1.300e-01
τ^*	1.020e+06	1.020e+06
A1	2.891e+01	2.910e+01
A3	5.003e+01	5.160e+01
D1	6.405e+11	6.620e+15
D2	4.189e+02	4.172e+02

3.1 Ultramid B3K6 vs. Trirex 30221R

As the first example, Ultramid b3k6 and Trirex 30221R polymer materials were chosen in order to identify the design coefficient of Cross-WLF viscosity model with the proposed optimization technique.

For the optimization procedure, it is important to limit the lower and upper values of each design variables. It is shown that the design variables a very wide ranges; however, some of them have narrow bands such as n; from 0 to 1. The prediction of the range of design variables is not easy so the boundaries are considered widely enough as shown in Table 1. The initial values are not very significant since global optimization algorithm and multiple starting points are considered. The initial values are the same as the lower boundary values of each design variables in this study. Table. 2 shows the comparison between the optimal design variables and coefficient from Autodesk Moldflow of Ultramid B3K6 material. Most of design variables is very similar to each other. However, n obtained from optimal result is a slightly different from the one provided by Autodesk Moldflow. It is very hard to conclude which one is proper value. In order to compare which parameters are better, the objective function was calculated. The objective function with optimal values is 1.500E-05 and the one with Autodesk Moldflow is 1.210E-05. In terms of objective function comparison, the objective function with optimal values is approximately 30 percent larger than the one with Autodesk Moldflow. However, the order of magnitude of objective function is -5 which is almost close to zero and the comparison is meaningless. Since the design variables are quite close to each other, the Cross-WLF viscosity models are also very similar as shown in Fig. 4. Both optimal and Autodesk Moldflow cases are plotted for four different temperature cases; 260, 270, 280 and 290℃. When the shear rate is larger than 10^3, the viscosity values are drastically dropped at all different temperature cases due to lower value of n. On the contrary, the viscosity values are not significantly dependent upon the shear rate change as shown in Fig. 5, which shows the comparison of Cross-WLF viscosity model for Trirex 30221R. The n is 8.948E-01 for both, which is very different value from the one of Ultramid B3K6. Table 3 presents the final optimal design variables and the design coefficient provided from Autodesk Moldflow as well.

Since A_1,A_3 and D_1 parameters are slightly different in this case, it is necessary to compare the objective function calculated from both optimal values and Autodesk Moldflow. The objective function value with the optimal values is 3.339E+00 and the one with Autodesk Moldflow coefficient is 7.682E+00. The value with optimal points is approximately 43% compared to the one with Autodesk Moldflow coefficient. Both cases are not huge values; however, the objective function with the optimal value provides 43% lower which means that Cross-WLF viscosity model with optimal values is more accurately described the reference data than the ones from Autodesk Moldflow.

3.2 Lupilon S-2000 vs. Lexan HF 1140R

For the second example, Lupilon S-2000 and Lexan HF 1140R polymer materials are chosen. As mentioned in the previous section, τ^* is one of the most important coefficient describing the Cross-WLF viscosity model; therefore, it was selected either the biggest or lowest value among Autodesk Moldflow data－Lupilon S-2000 and Lexan HF 1140R. The optimization procedure is the same with the previous example such as optimizer, initial and lower/upper boundary values.

Fig. 6 shows the comparison the Cross-WLF viscosity Lupilon S-2000 model with optimal coefficients obtained from the proposed method and the ones from Autodesk Moldflow at four different temperature conditions; 280.0, 293.3, 306.7 and 320.0°C. The comparison graph shows there is no difference between optimal and Autodesk Moldflow data. The design coefficients of both are presented at Table 4. Except for A_3, other design parameters are almost identical. The objection function values with

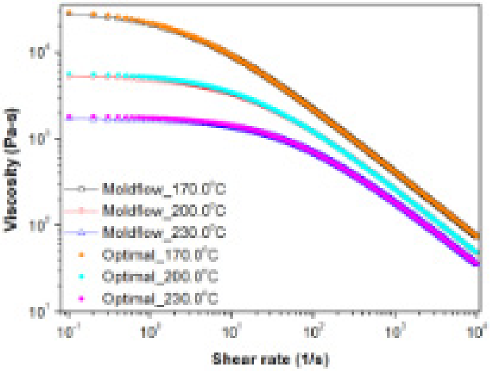


Fig. 7. The comparison of Cross-WLF viscosity model between optimal values and the ones from Autodesk Mold flow; MAT 2238

Table 6. The comparison the optimum design variables and coefficient provided from Moldflow Plastic Labs : MAT 2238

Design parameters	Lower boundary	Upper boundary
n	2.5402e-01	2.500e-01
τ^*	9.603e+04	1.009e+05
A1	3.495e+01	2.910e+01
A3	3.137e+02	5.160e+02
D1	7.465e+15	3.317e+09
D2	3.494e+02	3.373e+02

optimal and Autodesk Moldflow are 1.001E+02 and 1.430E+02 respectively. The residual with optimal data is 42.9% less than the other one, which is optimal data would more properly describe the Cross-WLF viscosity model than the other.

Table 5 shows the optimal and Autodesk Moldflow data for Lexan 1140R, which are almost identical and comparison graph is presented in Fig. 7. Even though τ^* is very different value from the one of Lupilon S-2000, the optimal design parameters well describe the Cross-WLF viscosity model compared to the ones from Autodesk Moldflow. The objective functions with the optimal and Autodesk Moldflow are 1.372E+01 and 3.605E+01 respectively. In this case, the objective function with optimal data is approximately 72% less than the other one, which means that the optimal data more accurately describe the Cross-WLF model than Autodesk Moldflow one.

3.3 Cargill Dow LLC-MAT2238

It has been investigated to identify the coefficient of Cross-WLF viscosity models provided from Autodesk Moldflow software. Those data–reference data in this study–are extracted from well described Cross-WLF viscosity model. However, it is very important to identify the coefficient of Cross-WLF viscosity model from experimental data. Some experimental data would be slightly or significantly different from the ones described by Cross-WLF viscosity model and the number of data should be very limited. Because of those difficulties, we should try to identify the coefficients from experimental polymer materials in order to show the robustness and effectiveness of the proposed method. As reference data, Moldflow Material Testing Report [10] would be adopted in which viscosity experimental data and the coefficients are provided. It seems that a polymer company would submit their own experimental data to Moldflow plastic labs then the labs would provide design parameters of the model and others such as thermal conductivity, shrinkage and so on. “Calculated viscosity data” from the report would be used as reference data for optimal procedure and the results are compared in Table 6. Most design coefficients are almost identical except for D_1. Even though D_1 is very different from each other, the comparison of viscosity graph is quite similar as shown in Fig. 7 due to a very low sensitivity value of D_1.

4. Conclusion

It is imperative to identify the coefficients of Cross-WLF viscosity model for predicting the behavior of polymer materials. Usually there are 6 design coefficients which should be accurately identified in order to describe the behavior of polymer materials in simulation analysis. The assumption is that the 6 design coefficient would be well described the real polymer materials when the calculated Cross-WLF viscosity model with those design parameters is the same with the reference data. An identification method is proposed in order to find the coefficients of Cross-WLF viscosity model based on analytical sensitivity analysis. The analytical sensitivity of the design parameters are compared with the FDM, which are very good in agreement. For the identification procedure, the discrepancy between the reference viscosity data and the ones obtained by design variables is considered as objective function. By minimizing the objective function, the Cross-WLF model with design variables should be close to the real data.

The proposed identification method was applied to 4 different Cross-WLF viscosity model provided by Autodesk Moldflow and 1 experimental data from Moldflow Plastics Labs. Throughout the numerical examples, the proposed methods are well identified those design variables and the Cross-WLF viscosity models are almost identical with the ones obtained by Autodesk Moldflow. Some cases the proposed method provides better design variables in terms of the objective function comparison. Additionally, it has been investigated to identify the design coefficient of the model from experimental data. A report from Moldflow is adopted as reference. The design coefficients provided by the company and the ones obtained by the proposed method are good in agreement and the viscosity graph is almost identical.

An optimization technique is proposed in order to identify the Cross-WLF viscosity model parameters. It has shown that the proposed method is very effective and robust by comparing design coefficients and viscosity graph obtained from reference. With the methodology, even a small-business company would effectively and efficiently identify the Cross-WLF viscosity model parameters which could improve their competitiveness.

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