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ORIGINAL ARTICLE

A modified global optimization method based on surrogate model and its application in packing profile optimization of injection molding process

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Abstract This article introduces a step-by-step optimization method based on the radial basis function (RBF) surrogate model and proposes an improved expected improvement selection criterion to better the global performance of this optimization method. Then it is applied to the optimization of packing profile of injection molding process for obtaining best shrinkage evenness of molded part. The idea is first, to establish an approximation function relationship between shrinkage evenness and process parameters by a small size of design of experiment with RBF surrogate model to alleviate the expensive computational expense in the optimization iterations. And then, an improved criterion is used to provide direction in which additional training samples could be added to better the surrogate model. Two test functions are investigated and the results show that stronger global exploration performance and more precise optimal solution could be obtained with the improved method at the expense of increasing the infill data properly. Furthermore the optimal solution of packing profile is obtained for the first time which indicates that the type of optimal packing profile should be first constant and then ramp-down. Subsequently, the discussion of this result is given to explain why the optimal profile is like that.

Keywords Injection molding · Shrinkage evenness · Packing profile · Radial basis function · Expected improvement

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1 Introduction

Injection molding process can be divided into three stages: filling, packing and holding, and cooling. During packing and holding stage, additional material is "packed" into the mold cavity at a high pressure to compensate for part shrinkage due to cooling and solidification until the gate is frozen [1]. Packing stage plays an important role on controlling part shrinkage and overcoming warpage defect led by uneven volume shrinkage of molded part, and therefore shrinkage evenness of part can be defined as an index for the optimization of packing profile.

It is commonly known that the larger the packing pressure, the smaller are the shrinkage and its evenness. But packing profile doesn't only refer to the magnitude of packing pressure, but also refers to the type of pressure curve, such as constant, ramp, and the combination of both. Thus, many researchers have furthered their studies on the optimization of the type of packing profile along with pressure magnitude. Chen et al. [2, 3] have studied optimal packing profile experimentally to achieve most uniform part quality, and the conclusion has been drawn that the ramp-down profile of the packing pressure is beneficial to reduce the cavity pressure difference and improve the part evenness. However, packing profile is restricted to ramp type, and the optimal solution obtained from design of experiment (DOE) is sketchy. Qiu et al. [4] have studied effects of packing profile on products surface quality with Moldflow software and found that profile as shown in Fig. 1 with the type first constant from t_f to t_c and then linear fall from t_c to t_e could lead to better surface quality. But this is not the optimal solution in design space, but only a conclusion drawn from qualitative analysis.

The optimal solution also called best design of process parameters can be obtained by classic Taguchi method [5]

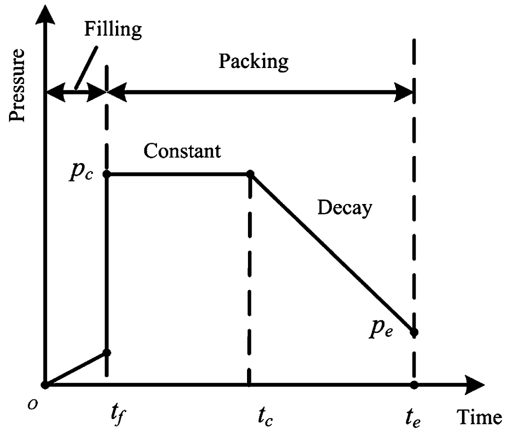

Fig. 1 Idealized sketch of packing profile

with the merit of easy implementation, but it is only the best combination of given process levels, and also not the optimal one in the design space. To solve this problem, evolution algorithms such as genetic algorithm [6] have been introduced. However, these strategies are regarded as too time-consuming to be used in practical applications because of the large number of objective functional evaluations with computer aided engineering simulation during the optimization process.

In order to reduce the computational cost, some researchers have employed surrogate models in optimization procedure, such as artificial neural network [7], kriging [8] and response surface model [9], to establish a mathematical approximation for replacing the expensive simulation analyses. However, a big size of DOE and additional validation samples are prerequisite for an accurate surrogate model to find the optimal solution in one step, which shadows practical applications of these methods.

Therefore, a small DOE size is expected in order to reduce computing expense, and consequently some step-by-step optimization methods have been proposed. A sequential optimization method has been proposed by [10] based on kriging surrogate model, which could improve the surrogate function using a current optimal solution in the each optimization iteration until the convergence criteria are satisfied. Thus, the requirement of substantive samples for modeling is needless, but it may easily get trapped in a local optimum with this method if the objective function is multimodal. To make the method with global search ability, a variance index for measuring uncertainty of predictor has been introduced by [11] to explore the unexplored space by finding additional training points. Similarly, expected improvement (EI) sample selection criterion has been introduced by [12] and it can be considered as a balance selection between optimization of the predictor and areas of maximum uncertainty, but this single infill sample method is not competent enough to optimize the complicated multimodal optimization problem.

In this paper, an improved EI samples selection criterion was proposed based on radial basis function (RBF) surrogate model for enhancing the global exploration performance of the method. With this criterion, several infill data were selected to improve the model, one of which was the optimum of current predictor and the others were from the most uncertain areas associated with the predictor. And subsequently, two simulation applications were investigated to show the advantage of this criterion compared with the original one. Finally, this method was applied to optimize the packing profile for ameliorating the shrinkage evenness of the molded part. Moreover, the optimal result was interpreted from technical aspect of injection molding.

2 EI selection criterion base on RBF surrogate model

2.1 Radial basis function interpolation [13, 14]

Given N designs $[x_1,x_2,...,x_N]$ and its corresponding responses $y=[y_1,y_2,...,y_N]$, a RBF predictor at any point x in design space is given by

$$\widehat{y} = \widehat{f}(x) = \sum_{i=1}^{N} \omega_i \phi(||x - x_i||) \tag{1}$$

where, ω_i is weight coefficient; $\phi(\cdot)$ is nonlinear basis function and $\|\cdot\|$ is Euclidean distance. Defining $\Phi_{i,j} = \phi\left(||x^{(i)} - x^{(j)}||\right) \quad i,j = 1,2,\cdots,N$ and provided the inverse of $\Phi_{i,j}$ exists, then a prediction $\widehat{y}_{N+1}$ made at x_{N+1} is

$$\widehat{y}_{N+1} = \phi\Phi^{-1}y^T \tag{2}$$

where, $\phi = [\phi(||x_{N+1} - x_1||), \cdots \phi(||x_{N+1} - x_N||)]$. Throughout this work, exponentially decaying Gaussian basis function

$$\phi(r) = \exp\left(\frac{-r^2}{2\sigma^2}\right) \tag{3}$$

is adopted to facilitate the deviation of EI function, and σ is an undetermined hyperparameter in (3).

2.2 Expected improvement selection criterion

Assuming that each deterministic response $y(x)$ is the realization of some Gaussian stochastic process $Y(x)$, then using the Gaussian distributions of the N responses y collected so far, the mean and the variance of the assumed stochastic process at x_{N+1} are (2) and

$$\sigma^2_{\widehat{y}_{N+1}} = 1 - \phi\Phi^{-1}\phi^T, \tag{4}$$

respectively, and σ is used for measuring the uncertainty of $\widehat{y}_{N+1}$ [15].

EI function is interpreted as the expectation for any point in design space to be promoted to the optimum. If the current best function value is $Y_{\min} = \min\{y_1, y_2, \cdots, y_N\}$, then the improvement at x is

$$I(x) = \max\{Y_{\min} - y(x), 0\}.$$

According to the hypothesis of Gaussian distribution,

$$E(I) = \int_{I=0}^{I=\infty} I\left\{\frac{1}{\sqrt{2\pi}\sigma(x)} \exp\left[-\frac{I - (Y_{\min} - \widehat{y}(x))}{2\sigma^2(x)}\right]\right\} dI.$$

By using integration by parts, equation above can be written as

$$E(I) = \begin{cases} (Y_{\min} - \widehat{y}(x))\Psi(u) + \sigma(x)\psi(u) & \text{if } \sigma(x) > 0 \\ 0 & \text{if } \sigma(x) = 0 \end{cases} \quad (5)$$

where, $\Psi(\cdot)$ and $\psi(\cdot)$are the standard normal distribution function and the standard normal density function, respectively, and $u = \frac{Y_{\min} - \widehat{y}(x)}{\sigma(x)}$ [16].

The first term of Eq. 5 called local term is the prediction deviation between the $Y_{\min}$ and $\widehat{y}(x)$, penalized by the probability of improvement. Hence, it is large where $\widehat{y}(x)$ is small. The second term called global term is large where $\sigma(x)$ is large and $\widehat{y}(x)$ is close to $Y_{\min}$. Hence, it is large where there is much uncertainty about whether y will be better than $Y_{\min}$. Therefore, EI function can be considered as a balance between seeking promising areas of the design space and the uncertainty in the model. EI selection criterion is just to pick out the point x that makes the value of EI function (5) maximized.

3 Improved EI selection criterion and its realization

3.1 Improved EI selection criterion

Though global exploration ability is enhanced by EI criterion, optimization process still easily gets trapped in a local optimum because only one sample is added into the training collection in the iteration, and it is a compromise between global exploration and local exploitation, and thus we may lose some promising seeking point in this way. An improved method presented by [13] to boost global exploration ability is to increase the weight of global term in (5), but it will bring about another problem that is how to choose the weight in practical application, which is also difficult to solve.

To boost the global exploration performance of EI selection criterion, an improved EI selection criterion featured by several infill data is put forward. One of these data is the promising point of current model obtained by optimizing the local term of Eq. 5 that is

$$LE(I) = (Y_{\min} - \widehat{y}(x))\Psi(u), \quad (6)$$

and the others are the most uncertain points obtained by optimizing the global term of Eq. 5 that is

$$GE(I) = \begin{cases} \sigma(x)\psi(u) & \text{if } \sigma(x) > 0 \\ 0 & \text{if } \sigma(x) = 0. \end{cases} \quad (7)$$

We call Eq. 6 and Eq. 7 as local expected improvement (abbreviated as LEI function) and global expected improvement (abbreviated as GEI function), respectively. Thus, the original EI function (5) is just split into LEI and GEI functions for optimization to find infill points with the improved criterion instead of one infill point in the original criterion, and therefore the improved EI selection criterion is more suitable for finding the optimum of multimodal function than the original criterion at the expense of more infill points.

3.2 Optimization procedure with improved EI selection criterion

The abovementioned surrogate model optimization procedure with improved EI selection criterion can be illustrated in Fig. 2 and summarized as below:

(1) Generate initial N samples with DOE method and get their corresponding objective function values. A random Latin hypercube experimental design [10] is used to build these initial samples, because it has advantages of small sample size and stable results.
(2) Determine the optimal hyperparameter σ of RBF with leave-one-out cross-validation procedure. After data normalization, the problem domain of searching for σ is over the range $[10^{-1}, 10^{1}]$, and 20 values of σ logarithmically spread over the range are considered to reduce the computation expense of applying leave-one-out method.
(3) Optimize GEI function with sequential quadratic programming (SQP) method and find n different x_g^i with the largest GEI function values, where x_g^i is a solution in the feasible region of GEI function and n is the number of global uncertain infill points. One hundred random initial points are selected for searching the maximums with SQP. Three of the solutions are selected after optimization with the largest GEI function values. Then reject x_g^i satisfying $\mathrm{GEI}(x_g^i) < \delta$ and finally get n x_g^i, where, $0 \le n \le 3$. The threshold δ can affect global exploration performance of optimiza-

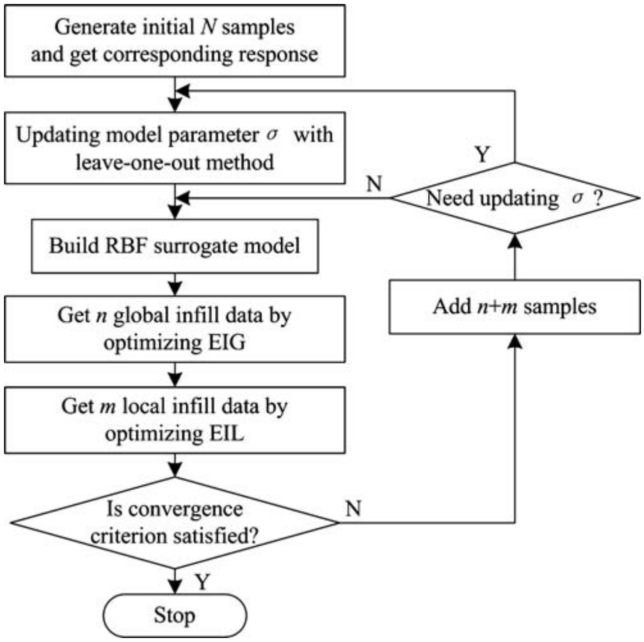

Fig. 2 Flowchart of iterative optimization with improve EI selection criterion

tion method. The larger δ, the weaker is the global performance.

(4) Optimize LEI function with sequential quadratic programming method and find x_l with the largest LEI function value, where x_l is a solution in the feasible region of GEI function. And then if $\mathrm{LEI}(x_l) > 0$ then $m=1$, and otherwise $m=0$, where m represents the number of local promising infill point and $0 \leq m \leq 1$. The optimization procedure is similar as done in step 3, except that 1,000 random initial points are selected to guarantee finding the global maximum because of the multimodal characteristic of LEI function.

(5) Update parameter σ of RBF model. Parameter σ has to be updated by leave-one-out method with the extension of training collection. However, it is unnecessary to update it in the each iteration, so we determine to renovate it after six data have been added into the collection since last renovation. Another situation that calls for renovation is when $m=0$, which means promising point doesn't exist under current approximate model.

(6) The optimization iteration should be terminated when no points could be filled for two consecutive times, or times of iteration exceed upper limit.

4 Simulation results

4.1 Example one

In this case, a two-variable modified Rosenbrock function [13] is considered for iteration optimization with both EI and improved EI selection criterion. We choose initial DOE size $N=20$ and threshold $\delta=0.01$, and the main optimization results are listed in Table 1, where three initial collections are adopted repeatedly due to the effect on optimization results from distribution of initial samples. As shown in Table 1, there is no obvious difference between these two criterions in the number of additional training points and optimal objective values under initial collection 1 and 2, but the optimal solutions of improved criterion are closer to real optimum. However, original criterion makes the solution trapped in local minimum with the distance 1.7747 from real global minimum under initial collection 3, whereas the improved criterion still works well.

4.2 Example two

In this case, a two-variable Ackley's path function [13] is considered for iteration optimization. We choose initial DOE size $N=30$ and threshold $\delta=0.02$, and the main optimization results are shown in Table 2. After iteration, all the solutions are near the global minimum, and those solved by improved criterion are much closer at the expense of increase of number of training points by no more than twice. However, this expense is much more less than the

Table 1 Comparison of two optimization methods

	Initial collection 1		Initial collection 2		Initial collection 3	
	EI	Improved EI	EI	Improved EI	EI	Improved EI
Iteration times	27	14	30	10	15	6
Additional training points	27	29/7/22[a]	30	29/7/22	15	24/6/18
Minimum objective values	−152.13	−153.85	−153.81	−153.9	−150.11	−153.12
Deviation from optimum	0.0349	0.0038	0.0072	0.003	1.7747	0.0438

[a] Additional training points of improved criterion is explained as total number/EIG's number/EIL's number

Table 2 Comparison of two optimization methods

	Initial collection 1		Initial collection 2		Initial collection 3	
	EI	Improved EI	EI	Improved EI	EI	Improved EI
Iteration times	22	15	30	14	22	23
Additional training points	22	38/10/28	30	37/8/29	22	32/13/19
Minimum objective values	0.2145	0.0532	0.1106	0.073	0.2154	0.0497
Deviation from optimum	0.0817	0.0163	0.0316	0.0215	0.0516	0.0254

traditional one-step modeling and optimization method that needs a mass of training data.

5 Optimization of packing profile

5.1 Optimization problem

The shrinkage evenness problem was simulated with Moldflow MPI 6.1, which is a commercial injection molding process simulation. A rectangular slab of 150 mm by 30 mm by 2 mm with fan gate shown in Fig. 3 was investigated for the research, and it was meshed with the fusion type of mesh. The total number of the elements was 1,950 containing 1,912 triangular elements, 38 beam elements, and 997 nodes. As a typical semicrystalline material, high-density polyethylene (Dowlex, IP-10) was selected for its large dimensional dependence on the packing pressure.

Shrinkage evenness of the slab could be expressed with variance of volumetric shrinkage results from Moldflow analysis. Since the length of the slab is much larger than width, the variance of eighteen locations along the flow path with approximately equal distance interval as shown in Fig. 4 was used to represent the evenness of the whole part. Thus, the shrinkage evenness is determined as

$$\text{Evenness} = \sqrt{\frac{\sum_{i=1}^{n}\left(d_i - \overline{d}\right)^2}{n-1}} \tag{8}$$

where, d_i is the volumetric shrinkage at location i; $\overline{d}$ is the average of the shrinkage at different locations; n is the total number of locations, which is 18 here. It is obvious, that a smaller value of Eq. 8 represents a better part evenness.

The packing profile is determined by four parameters, the packing duration t_e, the initial constant pressure p_c, the turning time t_c, and the end pressure p_e as shown in Fig. 1. Therefore, the optimization problem can be written as

$$\begin{array}{ll} \text{find} & x = [t_e, p_c, t_c, p_e] \\ \text{minmize} & \text{evenness}(x) \\ \text{s.t.} & 4.5s \le t_e \le 7s \\ & 100\text{MPa} \le p_c \le 120\text{MPa} \\ & 0 \le t_c \le t_e \\ & 0 \le p_e \le p_c \end{array} \tag{9}$$

Types of profile are restricted by constraint conditions of t_e and p_e to three kinds: constant, ramp-down, and first constant and then ramp-down. Moreover, t_e is considered as input of model as it can be effected by average holding pressure and its range is determined by gate seal time under maximum and minimum average holding pressure. Specially, negative reciprocal of evenness was used as actual optimization index to magnify tiny differences of evenness nearby optimum and consequently facilitate modeling and optimization.

5.2 Optimization results and discussion

As procedures mentioned in Section 3.2, 30 initial samples were firstly generated with Latin hypercube experimental design method, and then evenness was gotten with Moldflow software. Other process parameters besides shape parameters of packing profile are listed as follows: melt temperature is 220°C, mold temperature is 40°C, and injection velocity is

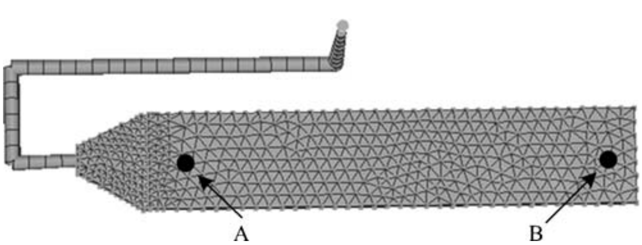

Fig. 3 Fusion model of rectangular product and its gating system

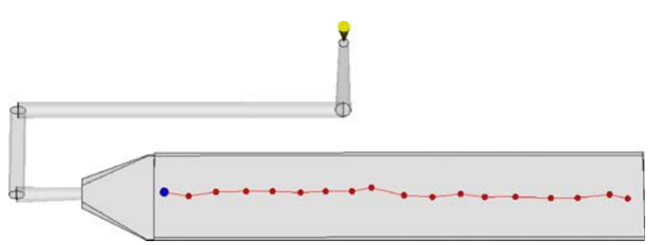

Fig. 4 Measured points on the part

Table 3 Number of training samples, model parameter, and minimum evenness among training samples for each step of iteration

	Cumulative samples	EIL/EIG	σ	E_{min}
1	30	1/3	1.58	0.03280
2	34	0/3	1.58	0.03280
3	37	1/3	0.89	0.02213
4	41	1/3	0.89	0.02213
5	45	1/3	0.89	0.02194
6	49	1/3	0.89	0.02194
7	53	0/2	0.89	0.02194
8	55	1/0	0.89	0.02141
9	56	–	–	0.02141
10	56	3/1	0.79	0.02141
11	60	1/1	0.79	0.02115
12	62	–	–	0.02115
13	62	1/0	0.71	0.02115
14	63	–	–	0.02004

40 mm·s^{-1}. Let threshold δ=0.01. Under the above settings, the optimal solution [7.0, 120.0, 5.5, and 60.8] was obtained after 14 times iteration with improved EI selection criterion. The results during iteration are listed in Table 3. The profile corresponding to the optimal solution is shown in Fig. 5 with the solid line, and its type is first constant and then ramp-down, with p_c=120 MPa, t_c=5.5 s, t_e=7 s, and p_e=60.8 MPa.

The practical significance of optimal profile is illustrated in Fig. 6, in which the long and short dashed lines represent the cavity pressure at points A and B of the part in Fig. 3 while exerting the optimal packing profile. The pressure starts to rise at about 4.5 s due to the partial solidification of part's edge and then the bottom edge of the part (right side of the point B) is about to solidify totally at 5.5 s, and before 5.5 s, constant holding pressure should be adopted to make the part with the least shrinkage. While from 5.5 s to gate seal (7 s), which is the solidification process of the whole part, ramp-down profile should be used to reduce the volume shrinkage difference between far gate and near gate parts of the molded part and consequentially make the part evener.

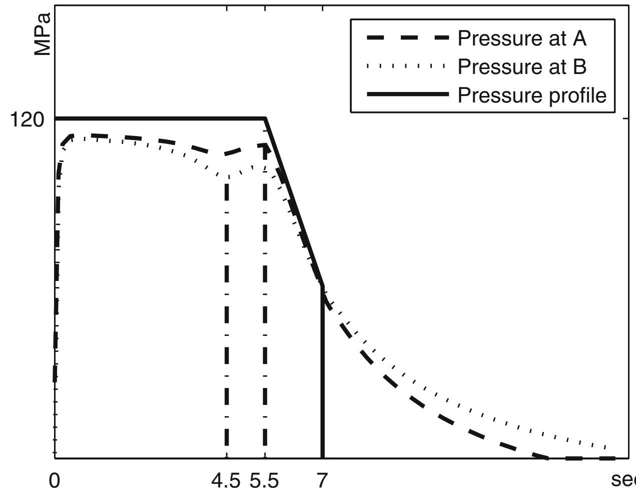

Fig. 6 Cavity pressure at points A and B of part while exerting optimal packing profile

However, actual gate seal time is not 7 s but 6.1 s from Moldflow analysis results. The reason for that can be explained by evenness pressure curves under two conditions of t_e=7 s and 6.1 s with p_c=120 MPa and t_c=5.5 s shown in Fig. 7, which are plotted from data generated by surrogate model. It can be seen that end pressures with minimum evenness corresponding to the minima of the

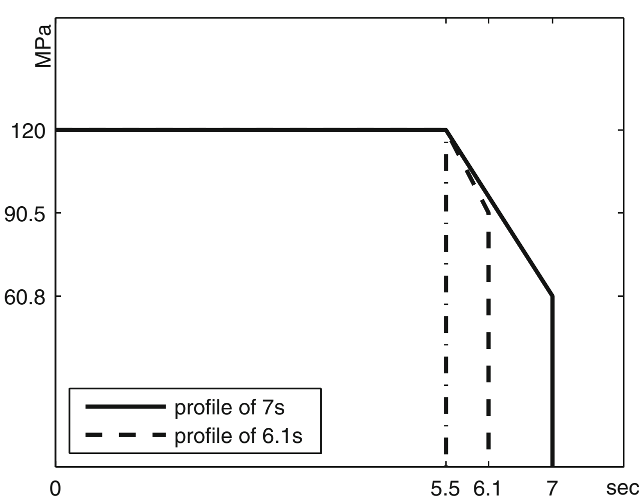

Fig. 5 The optimal packing profiles in the cases of t_e equal to 6.1 s and 7 s

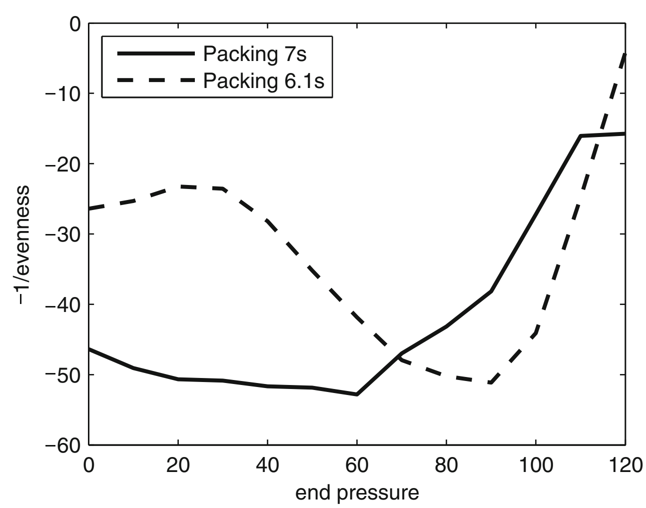

Fig. 7 Evenness curves with end pressure in the cases of t_e=6.1 s and 7 s with p_c=120 MPa and t_c=5.5 s

curves in Fig. 7 are both between 0 and 120. The optimal packing profile under t_e=6.1 s is plotted with dashed line in Fig. 5, and it can be known that the two curves nearly coincide with each other. And they are actually the same profile from technical analysis, since the volume shrinkage will not be affected by holding pressure after gate seal time. Therefore, it is easy to infer that infinite number of solutions exist between the duration 6.1 s and 7 s, whereas only the solutions under 7 s is found by this step-by-step optimization method with surrogate model driven by data. If the solution with the shortest packing duration 6.1 s is expected, more accurate model and more complicated optimal parameter setting have to be relied on.

6 Conclusions

In this study, a step-by-step optimization method based on RBF surrogate model and improved EI samples selection criterion is proposed and shown to be theoretically sound and practically applicable to the optimization of the injection molding simulation process. The modified criterion employs several additional samples with global exploration and local exploitation performance to improve the surrogate model in the each optimization iteration. From the results of the testing functions and packing profile optimization example, the modified method proposed can effectively establish the surrogate model with minimum computational resources and adaptively search for the global optimal solution for injection molding.

Based on the optimization results of shrinkage evenness, the type of optimal packing profile is first constant and then ramp-down: the initial constant holding pressure should be the upper limit of pressure; the packing duration should be more or equal to gate seal time; the turning time should be the solidification time of the tail end of filled part; end pressure should be lower than upper limit of pressure. In practical production, constant holding pressure can be calculated by the largest clamp force and effective projected area of part; packing duration can be identified as the time after which the part weight no longer increases with packing time; the optimal design of turning time and end pressure could be simply found by DOE method with shrinkage evenness or degree of warpage as the optimization index.

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