Proceedings of ASME 2011 International Design Engineering Technical Conferences & Computers and Information in Engineering Conference IDETC/DTM 2011 August 28-31, 2011, Washington, DC, USA

DETC2011-48505

A NEW APPROACH FOR EXPLICIT CONSTRUCTION OF MOLDABILITY BASED FEASIBILITY BOUNDARY FOR POLYMER HEAT EXCHANGERS

Timothy Hall Department of Mechanical Engineering University of Maryland College Park, MD 20742 Email: timrhall@umd.edu Madan Mohan Dabbeeru Department of Mechanical Engineering University of Maryland College Park, MD 20742 Email: mmd@umd.edu

Satyandra K. Gupta Department of Mechanical Engineering & Institute for Systems Research University of Maryland College Park, MD 20742 Email: skgupta@umd.edu

ABSTRACT

Incorporating manufacturing feasibility is a very important consideration during the design optimization process and this paper is interested in investigating the molding feasibility of polymer heat exchangers. This application requires the explicit construction of the boundary, represented as a surface based on the parameter space, which separates the feasible and infeasible design space. The feasibility boundary for injection molding in terms of the design parameters is quite complex due to the highly nonlinear process physics, which, consequently, makes molding simulation computationally-intensive and time-consuming. Moreover, in heat exchanger applications, the optimal design often lies on the feasibility boundary. This paper presents a new approach for the explicit construction of a moldability-based feasibility boundary for polymer heat exchangers. The proposed approach takes inspiration from intelligent design of experiments and incorporates ideas from the field of active learning to minimize the number of computational experiments needed to construct the feasibility boundary. Our results show that the proposed approach leads to significant reduction in the number of computational experiments needed to build an accurate model of the feasibility boundary.

1 INTRODUCTION

The utilization of polymers in heat exchangers is attractive due to their relatively low cost and weight, lower fabrication energy and lifecycle energy usage than equivalent metal heat exchangers [1], and corrosion and fouling resistance [2]. DuPont developed the first polymer heat exchanger in 1965 using flexible Teflon[®] tubing in a shell-and-tube configuration [3]. The introduction of new thermally-enhanced polymer composites and manufacturing processes has led to renewed interest in polymer heat exchangers and emerging applications previously supported only by heat exchangers made of exotic metallic alloys. Industrial applications which utilize seawater as a cooling medium for heat exchangers traditionally require exotic alloys to survive the corrosive environment, leading to dramatically increased costs and processing requirements. Polymer composites utilizing thermally-enhanced fillers, such as pitch-based carbon fiber, have led to orders of magnitude improvement in overall thermal conductivity, making them competitive with corrosion-resistant metals such as titanium and copper-nickel alloys. [4]

Injection molding is one of the most widely used manufacturing methods for polymer components and its rapid cycle times and ability to create complex geometries makes it an attractive solution for many applications. The complex physical behavior of injection molding has led to the use of methods such as finite element analysis and other computer-aided engineering (CAE) techniques in order to analyze mold filling [5], an essential feasibility consideration when evaluating a potential component design. Additionally, since in many design situations it is highly likely that the optimal solution will be found at the boundary defining feasibility and therefore it is useful to know both the feasibility of a proposed design and the feasibility boundary. Incorporating manufacturing feasibility is a very important consideration during the design and optimization processes and the complex nonlinear physics that govern many manufacturing processes require computer simulation to determine manufacturing feasibility. While such simulation has proven invaluable to the field of injection molding and other manufacturing applications, it is computationally expensive and therefore not suitable for design exploration and optimization situations.

The application of metamodeling techniques, which predict response values based on a set of design experiments [6], has been successful in applications ranging from the optimization of the air flow rate in aircraft jet engines, in which [7] described experiments requiring a day to two weeks to complete, to crash simulation, which Ford Motor Company reports takes 36-160 hours per simulation [8]. Metamodeling is an integral component in these and other computationally-expensive applications and this study proposes a method of developing a metamodel for predicting the moldability of polymer heat exchangers.

1.1 Injection Molding and Moldability

One of the primary concerns when designing products for injection molding is moldability, whether the use of injection molding is feasible for a given design, primarily from the point of view of mold filling. Moldability is especially important for potential polymer heat exchanger applications which have very large components and relatively expensive materials for which a failure to fill could have dramatic cost effects. Additionally, the unusual properties of the thermally-enhanced polymers utilized, including high viscosity and thermal conductivity, combined with the large scale and thin wall thickness of the investigated heat exchanger designs introduce further complexity into the mold filling process. Finally, since conductive heat transfer increases as thickness decreases [9], the optimal heat exchanger design often occurs at the minimum thickness that is feasible for mold filling and therefore it is very useful for the designer to know the location of the feasibility boundary.

Based on the requirements described above, there are two primary design criteria that should be considered when analyzing the moldability of a polymer heat exchanger and in general applications where constrained optimization is utilized: As discussed previously, CAE techniques such as finite element analysis are commonly applied to analyze mold filling in injection molding [5], but they are computationally expensive and consequently the development of a method for predicting moldability is beneficial for applications which require numerous simulations, such as optimization.

1.2 Application of Metamodeling Techniques

The development of a computationally-fast metamodel is an apt approach for approximating moldability, although the goal of both predicting feasibility and accurately estimating the feasibility boundary may be challenging. Traditional statistical metamodeling involves collecting a range of experiments across the design space and then applying a model to the discovered response values to approximate the response space.

Traditionally, standard design of experiments (DOE) methods have been applied to ensure that the developed model is useful across the entire design space. Methods include fractional or factorial design of experiments, Central Composite Designs, or space filling methods such as Latin Hypercube sampling. [10] argues that the consensus of the metamodeling community is that space filling methods should be used for deterministic, nonrandom computer simulations. While these techniques are useful for creating a representative model across the space, they may not collect enough local information for constructing an accurate estimation of the feasibility boundary. It is therefore advisable to have a more directed approach to performing simulations in order to ensure that adequate local information is collected for accurately determining the feasibility boundary.

There are many possible models that can be applied to the collected experiments. Fitting a response surface is the traditional choice but more advanced mathematical models such as non-uniform rational B-splines (NURBs) and Kriging have successfully been applied to metamodeling applications [6, 11, 12]. While fulfilling the design criteria of giving both the design feasibility and feasibility boundary, statistical metamodeling assumes that a regular function can be fit to the highly complex mold filling behavior for polymer heat exchangers, for which it may not be feasible to do so. Advanced methods of sequential or adaptive sampling have been shown to improve the accuracy of statistical metamodeling [6, 13, 14], but they still rely on the application of regular functions and therefore may not be suitable for application to mold filling of polymer heat exchangers.

1.3 Classification Methods

Since the primary goal of this study is determining mold filling feasibility of a candidate design, classification techniques from the field of machine learning are a potential alternative to traditional metamodeling. Possible methods include Neural networks, Bayesian networks, decision trees, or Support Vector Machines (SVMs) [15–17]. These methods use complex learn-

^{1.} Is the design feasible?

^{2.} Where is the feasibility boundary located, explicitly?



FIGURE 1: Comparison between classification methods and proposed method, noting implicitly vs explicitly discovered feasibility boundary and adaptive design of experiments.

ing techniques to devise a model for classifying a set of training data and advances in adaptive sampling have improved the usefulness of this training data and the accuracy of the developed model [18, 19]. While these methods provide a reasonable prediction of the feasibility of a candidate design, it provides only an implicit approximation of the feasibility boundary and therefore the precise location of the feasibility boundary is unknown, as represented in Fig. 1. Additionally, if the feasibility boundary is complex, the performance of classification techniques may degrade as designs approach the feasibility boundary. Therefore, while traditional classification techniques such as SVM could be applied to predict mold filling feasibility, they do not satisfy the design criterion of providing an explicit location of the feasibility boundary.

1.4 Proposed Method

This paper presents a new approach for explicitly constructing a moldability-based feasibility boundary for polymer heat exchangers. The proposed method takes inspiration from intelligent design of experiments literature and incorporates ideas from the active learning area to minimize the number of computational experiments needed to construct the feasibility boundary. This study utilizes an approach consisting of the following components:

- Rather than traditional sampling techniques, a method of adaptive design of experiments and sequential sampling is utilized to identify the feasibility boundary across the entire design space, as shown in Fig. 1.
- A design space of *n* variables is constructed with a grid of *n*−1 dimensions and a remaining search variable. At each grid position, the corresponding point on the transition re-

gion is found using adaptive search with the search variable.

- To reduce the number of computationally-expensive simulations required to develop the transition region, a method of feasibility boundary search is applied that uses previously found transition locations and the applied search pattern to predict the next transition locations and refine the search algorithm. These methods are used to efficiently sample the design space to find transition locations across the entire space.
- Using the discovered transition region, a metamodel is applied to predict the transition location for a candidate design. This is used to determine feasibility and is a prediction of the location of the feasibility boundary.

This methodology is well-suited for predicting mold filling of polymer heat exchangers in design exploration or optimization frameworks.

2 APPROACH

This study approaches the goal of developing a metamodel for mold filling of polymer heat exchangers by first developing a general method of adaptive design of experiments for multidimensional classification problems and then applying this method to the issue of mold filling for polymer heat exchangers. An algorithm for constructing an adaptive set of experiments to identify transition locations across the design space from which the transition region can be estimated, entitled the feasibility boundary search (Section 2.1) and transition point search algorithms (Section 2.2), is presented in the following sections and detailed in Fig. 2.



FIGURE 2: Flow diagram for the Feasibility Boundary Search Algorithm for predicting the location of the transition boundary for a candidate design.



FIGURE 3: Overview of Feasibility Boundary Search Algorithm.

2.1 Feasibility Boundary Search Algorithm

Step 1: Initialization. The first step of the feasibility boundary search algorithm is initialization, a primary component of which is spatial partitioning: defining a transition response value for which the design space will be divided into feasible and infeasible subspaces. A transition region is then defined as the boundary between the two subspaces and is the region of interest for this algorithm. While this approach is shared with classification methods, this algorithm uses the defined transition response value to explicitly locate the transition region across the design space, as represented in Fig. 3. As the transition region is identified the partitioning between the feasible and unfeasible subspaces becomes more defined. Additionally, initial values for various search parameters are defined for use in subsequent parts of the algorithm.

Step 2: Construct Design Space for Design of Experiments. With the transition response value defined, the next component of the feasibility boundary search algorithm is constructing the design space in preparation for creating an adaptive design of experiments to identify the transition region. For an experiment with *n* input variables, the design space is separated into a uniform grid of n-1 dimensions using traditional factorial design of experiments techniques, as illustrated in Fig. 3. The remaining input variable is treated as the varying or search dimension and is used to find the transition point at each grid location across the design space. The design problem should be formulated such that the response value has a monotonic relationship with respect to the varying design dimension. This ensures a single transition location at each grid position, a requirement for the method presented in this study, and reduces the complexity of the transition point search method, presented in Section 2.2.

Step 3: Find Seed Transition Point for Feasibility Boundary Search. With the design space defined, the location of the transition region is determined at an initial position in the design space, creating a seed transition point, as demonstrated in Fig. 3. At the first grid location, a full transition point search, described in Section 2.2, is completed with no prior knowledge of the response behavior and using arbitrary values for the necessary search parameters. This seed point and knowledge gained from performing the search is used by the feasibility boundary search component of the algorithm to improve the search efficiency for following locations in the design space.

Step 4: Feasibility Boundary Search. The primary component of the algorithm, a method of adaptive search termed feasibility boundary search, is used to improve the efficiency of the transition location search process at each grid location and therefore further reduce the number of computationally-expensive function evaluations required to define the transition region over the entire design space. By using previously found transition points and the search process used to find them, the feasibility boundary search method predicts the transition location at successive design positions and tunes the transition point search method utilized. In this way, information from the discovered transition region progresses as a frontier to the next grid locations and as the transition region is developed the searching process becomes more efficient. There are two primary components of the feasibility boundary search method: prediction of transition locations and adaptive control of the transition point search method.

Step 4.1: Predict Transition Location. From the seed point, the transition locations at the next grid points are predicted using constant extrapolation, as shown in Fig. 3. The next frontier of grid locations is predicted using linear extrapolation and the following locations are found using quadratic extrapolation. For this study, the maximum number of historical transition points used in the quadratic extrapolation method was set at three in order to reduce the distortion effects of the nonlinear mold filling behavior. As the predicted transition location approaches the actual transition location the search process becomes more efficient and fewer computationally-expensive simulations are required to find the transition location.

Step 4.2: Adaptive Control. The transition point search process utilizes certain control parameters that affect the rate of convergence for the search process, detailed in Section 2.2. As each search process is completed, it is possible to determine the value of the control parameters that would have led to immediate convergence, noted as $k_{p,ideal}$ in Section 2.2. The feasibility boundary search component of the algorithm uses these ideal values to improve the search efficiency of the following locations and in this way improve the overall convergence rate for identifying the transition region.

Step 5: Transition Prediction of a Candidate Design. With the feasibility boundary well defined from the adaptive design of experiments, post-processing and querying methods can be applied to estimate the feasibility of candidate designs. Possible post-processing methods include regression analysis, fitting a metamodel to the transition region, or applying SVM techniques to classify the feasibility subspaces. For a candidate design, the dimensions corresponding to the grid constructed in Step 2 are used with interpolation or other querying techniques to estimate the value of the varying dimension where the transition point occurs. This value is the explicit location of the feasibility boundary for the candidate design and is used to determine feasibility.

2.2 Transition Point Search Algorithm



FIGURE 4: Transition Point Search Algorithm.

At each grid location, the goal is to find the transition location using minimal computationally-expensive function evaluations. For this study a method combining proportional control and interpolation methods, illustrated in Fig. 4, is utilized to perform the search quickly and efficiently.

An initial guess is provided for each point, noted as *z_{initial}*, based on information from previous transition locations, as described in the feasibility boundary search algorithm. The initial guess is evaluated to find the corresponding response value, noted as $f_{initial}$ or f_{prev} , and the error relative to the transition value, f_{goal} , and response function range, f_{range} , is calculated. Proportional control is applied to the calculated error to determine the next evaluation location, znext, using Eqn. 1, with a proportional control constant of k_p . Next, with two known response values, linear interpolation is applied to determine the third evaluation location. Quadratic interpolation is then repeatedly applied until the convergence criterion is met. With the search complete, Eqn. 2 is applied to find the ideal proportional control constant, $k_{p,ideal}$, that would have led to immediate convergence to the found transition location, *z*transition, for use in the feasibility boundary search algorithm.

$$z_{next} = z_{prev} + \left(k_p \frac{f_{prev} - f_{goal}}{f_{range}}\right) z_{prev} \tag{1}$$

$$k_{p,ideal} = \frac{z_{transition} - z_{initial}}{z_{initial}} \cdot \frac{f_{range}}{f_{initial} - f_{goal}}$$
(2)

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FIGURE 5: Plate fin design.

TABLE 1: Problem formulation details.

Design Variables		Min	Max	Grid Spacing
Base Length	L, mm	200	700	100
Base Thickness	H, mm	1	5	Varying
Fin Width	W, mm	1	5	1
Fin Height	F, mm	10	10	Fixed
Fin Spacing	S, mm	3	15	3

(a) Design Dimensions

(b) Material Properties for Selected Material

Material	Resin	Thermal Conductiv- ity, W/m-K	Tensile Strength, MPa
PolyOne NJ-6000 TC Black	PA 12	10	110

For this method, the convergence criterion is defined as the transition value within a certain threshold or a minimum search resolution. The transition threshold is defined as the acceptable error in the calculated transition values and the minimum search resolution is used to ensure convergence and maintain design constraints on dimensional values.

Search constraints include design boundaries, which must be considered due to physical and design limits placed on the varying dimension. If the search extends beyond the design boundaries, the transition location is assumed to be out of bounds due to the monotonic nature of the response function. Since the actual transition location is not known, the transition location is marked at the bound in these instances.

3 PROBLEM FORMULATION

Design Formulation. A plate-fin heat exchanger design, the cross-section of which is detailed in Fig. 5, was chosen for the heat exchanger assembly due to its simple geometry and ability to be stacked in modules. There are five design variables for

this configuration: Base length, L; base thickness, H; fin width, W; fin height, F; and fin spacing, S. Based on exploratory experiments, the design space for the plate-fin heat exchanger is presented in Tab. 1a.

The values for base thickness and fin width were chosen based on injection molding minimum and maximum thickness guidelines. The fin spacing was defined to ensure an adequate number of fins in the heat exchanger and the fin height was fixed at 10mm based on its limited effect on heat transfer performance observed in exploratory experiments. The minimum base length was set to ensure at least approximately 1kW of heat transfer performance based on exploratory experiments and the maximum was set based on injection molding machine constraints.

Material Selection. The material selected for this application is PolyOne NJ-6000 TC Black, a commercially-available carbon-fiber filled Nylon 12. This material was chosen due to its balance of thermal and structural properties, its usefulness for injection molding applications, and the availability of a comprehensive set of material properties provided by the manufacturer for use in mold filling simulation. A selection of material properties for this polymer composite is shown in Tab. 1b.

Simulation Methodology. Moldflow[®], the industryleading finite element analysis tool for injection molding, was utilized to perform the mold filling simulation for this study. Design selections include locating the injection gate in the center of the base plate, using steel mold construction, and utilizing a constant mesh density for all designs. Injection molding machine parameters were chosen using the default selection criteria provided with Moldflow[®] to correspond with industry standards based on overall part size and characteristics. These selections were chosen in such a manner that they reflect standard industry methods and ensure consistent results across the design space.

Feasibility Boundary Search Parameters. For this application, the transition response value is set to 90 ± 1 percent filled for which the design space will be separated into filled and unfilled subspaces. This value was selected based on the assumption that in cases within 10% of fully filled, adjustment of machine parameters, such as melt temperature and injection pressure, and mold design can be utilized to achieve a fully filled part. The response variable threshold is set to ±1 percent filled to ensure that found transition locations are sufficiently close to the transition region.

Table 1a also gives the grid properties selected for this analysis and indicates how the design space was divided according to the second step of the feasibility boundary search algorithm. It is recalled that a requirement of the transition point search process is that the varying dimension and response value should have a monotonic relationship. Base thickness was chosen as the varying dimension in this application due to the perceived relationship that mold filling monotonically increases as base thickness increases. This assumption is a result of the phenomenological relationship that as base thickness increases the flow resistance in



(a) Exploratory Transition Point Search Demonstrating Boundary Termination and Piecewise Mold Filling



(b) Exploratory Transition Point Search with Limited Response Resolution and Piecewise Mold Filling

FIGURE 6: Selective search behaviors.

the mold decreases and the rate of cooling of the flow front decreases as well. These properties increase the flow length of the polymer melt and therefore mold filling increases monotonically with increasing base thickness.

The minimum search resolution is set to 0.002mm for this study in order to ensure sufficient search iterations while not greatly exceeding the limit of typical machining capabilities. Finally, for this study a method of multi-linear interpolation was utilized to predict the transition point of candidate designs based on the discovered transition region. Selective Search Behaviors. Several exploratory searches were performed to verify the performance of the developed transition point search strategy, outlined in Section 2.2. Results from these searches indicate that for this application certain selective search behaviors need to be introduced to ensure search convergence.

Points 1 and 2 in Fig. 6a and points 1, 2, and 4 in Fig. 6b indicate the piecewise nature of mold filling, with a continuous percent filled value for incompletely filled designs and a constant 100% filled value for completely filled designs. This poses difficulties in the employed search method due to undefined results for the interpolation methods when only completely filled values have been discovered. This is remedied with the introduction of selective search behaviors that check the lower design boundary when only 100% filled values have been found and which neglect 100% filled points in interpolation methods.

Figure 6a demonstrates search terminating at a design boundary. Due to the assumed monotonic relationship between the response function and the varying dimension, if the search process reaches a design boundary and the transition point has not been found then the transition point is located beyond the design boundary. The exact transition location cannot be found due to design limitations and while the transition point could be estimated from known response values, for this study the transition point is set at the design bound. Additionally, Fig. 6b demonstrates the limited response resolution of the chosen simulation tool, with small changes in the varying dimension having minimal if no effect on the response value. This phenomenon is resolved with the use of the localized binary search and the minimum search resolution, which serves as a cutoff for the search process beyond which the response function does not respond.

4 RESULTS AND DISCUSSION

The feasibility boundary and transition point search algorithms detailed in the approach section were applied for the given problem formulation in order to identify the transition region and determine the feasibility of candidate designs and the location of the feasibility boundary for finned plate polymer heat exchangers. A set of randomly selected test designs is then used to estimate the accuracy and usefulness of the developed model.

4.1 Transition Region Identification

Over the total design space of 150 grid locations, 715 function evaluations were required to define the transition region with the desired accuracy, with an average of 4.8 search iterations for each transition point. The design boundary was reached for 31 grid locations and the transition point search converged due to reaching the minimum search resolution at 46 grid locations, indicating that the sensitivity of the mold filling simulation as a function of base thickness was dominating for some designs. For comparison, exhaustive search was investigated to evaluate the search efficiency of the developed method. This method represents the more traditional approach to searching across a design space and could be used as an alternative to the developed method to find the transition location across the constructed design space.

Exhaustive search is assumed to use no adaptive sampling techniques and instead the varying dimension is uniformly divided across the design range. In order to achieve the same level of precision as the developed method, the minimum search resolution of 0.002mm should be used to divide the design space from 1 to 5mm, as defined in Tab. 1a. This creates 2,000 design levels for the varying dimension, which, when using the same grid of 150 positions for the remaining variables that was used in the developed method, leads to a total of 300,000 function evaluations for exhaustive search at the same precision as the developed method. Even if the spacing of the varying dimension is relaxed to ten times the minimum search resolution, 0.02mm, the total number of function evaluations required to (imprecisely) define the transition region is 30,000. Therefore, the developed method decreased the number of simulations required by nearly a factor of 420 when compared to the precise exhaustive search method, demonstrating the efficiency of the boundary search and transition point search algorithms in quickly and accurately identifying the transition region across the design space.

4.2 Assessment of Prediction Performance

Due to the unknown nature of the response space, there are no methods to quantitatively measure the accuracy of the developed model. Instead, a significant set of varying test designs is used to develop a qualitative understanding of the developed model. For this study, 50 randomly selected heat exchanger designs were applied to get an understanding of the accuracy of the approach. These designs were selected using randomly chosen values within the design boundaries specified in Tab. 1a.

Of these 50 designs, the developed method successfully classified 100% of them. Of these designs, eight were found to be within 10% of the feasibility boundary, indicating that they were the most difficult to classify and demonstrating the robustness of the developed approach. With the transition points discovered with the application of the developed method, multi-linear interpolation was applied in MATLAB® to determine the transition location for each design and therefore identify the feasibility boundary and classify the feasibility of the design. It was found that application of the developed method consumed 0.0469s of computation time to predict the transition location for all 50 test designs. The average Moldflow[®] simulation time required for each design was found to be approximately 35 minutes on a machine with a 2.83GHz Intel[®] CoreTM 2 Quad Processor and 8GB of RAM. Consequently, completing the simulations for the 50 test designs took nearly 30 hours of computing time. Therefore,

the utilization of the developed method led to a dramatic reduction by a factor of approximately 2.24 million in computation time for predicting the feasibility and explicitly locating the feasibility boundary of candidate designs.

5 CONCLUSION

The complex phenomena inherent in injection molding requires CAE simulation methods for predicting moldability but these methods are too intensive for use in applications where numerous trials are required, such as optimization or design exploration. Additionally, the requirement for minimal wall thickness in polymer heat exchangers necessitates an accurate estimate of the transition from a feasible to an infeasible design. The methods outlined in this study successfully identified the feasibility boundary, fulfilling the design goals and accurately predicting the moldability of finned plate polymer heat exchangers.

This study presents an adaptive design of experiments methodology that uses an adaptive sampling algorithm to explicitly locate the feasibility boundary between the feasible and infeasible subspaces of the design space. The application of traditional statistical metamodeling techniques in which a regular function is fit to a set of experiments was found to be unsuitable due to the complex nonlinear behavior inherent in injection molding. Classification techniques from the field of machine learning were considered but they offer only an implicit prediction of the feasibility boundary and therefore did not fulfill the design requirement of explicitly locating the boundary for use in optimization applications.

While the method utilized in this study was shown to be successful for a number of candidate designs, there are potential limitations and improvements that can be implemented. The use of a uniform grid when constructing the design space can introduce significant error into the constructed metamodel if the spacing is too coarse or important relationships between the design and response spaces are misunderstood. This can potentially be improved with the use of adaptive grid spacing or the introduction of multiple varying dimensions when constructing the design space. The feasibility boundary search process is important for reducing the required number of simulations to construct the transition region and the use of more advanced prediction techniques within the process, such as the application of machine learning methods, could lead to further improving the search efficiency. Finally, complexities inherent in the mold filling simulation, including the piecewise nature of mold filling and the limited response resolution to small changes in input parameters, introduced complications in the search process. The use of more advanced control schemes or search methods could improve the transition point search method and reduce the number of search evaluations needed to find transition points.

The utilized method employed adaptive search to locate points on the transition region while using minimal computationally-expensive simulations and as the transition region was discovered, a feasibility boundary search algorithm was used to improve search efficiency by predicting transition values and tuning search parameters based on previously found transition region information. The applied method was found to significantly reduce the number of required search iterations compared to an exhaustive search method and reduced the amount of computation time to predict the feasibility of 50 test designs from nearly 30 hours for Moldflow[®] simulation to less than 0.05 seconds for the applied method. The proposed method is therefore well-suited for applications such as design exploration and optimization and was successfully utilized to accurately predict the feasibility of candidate polymer heat exchangers designs.

ACKNOWLEDGMENTS

This research was performed as part of the Energy Education and Research Collaboration (EERC) between the University of Maryland and The Petroleum Institute. The authors would like to thank the Abu Dhabi National Oil Company (ADNOC) and its international partners for their generous financial support.

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