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Abstract:

Efficient and cost-effective manufacturing methods are needed for the widespread adoption of
microfluidic devices. This paper focuses on the roller imprinting process, which is a new method
for fabricating microfluidic devices. In this process, a cylindrical roll with raised features on its
surface creates imprints by rolling over a fixed workpiece substrate and mechanically deforming
it. Imprint precision is a function of the imprint roll features, the substrate material, and process
parameters. This paper presents an analysis of the effects of process variables on the imprint
using finite element (FE) simulations of the roller imprinting process.

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PROCEDURAL DESIGN OF IMPRINT ROLLS FOR FLUID PATHWAY FABRICATION

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ABSTRACT

This paper discusses a novel method for designing imprint rolls for the fabrication of fluid pathways. Roller imprint processes have applications in diverse areas including fuel cell manufacturing and microfluidic device fabrication. Robust design methods are required for developing imprint rolls with optimal features. In the method discussed in this paper, the rolls are designed procedurally with the fluid pathway design given as input. The pathways are decomposed into repeating features (or tiles), and the rolls are designed by first modeling a small set of unique tiles and then combining them to model the entire roll. The tiling strategy decreases the complexity of the model, and reduces the time taken for designing the rolls. The modular nature of the tiles also improves the efficiency of post-processing operations like feature identification and optimization, and the generation of toolpaths for machining the roll.

INTRODUCTION

Rapid manufacture of highly complex, precise parts requires a robust and efficient pathway between the design and manufacturing stages. This paper discusses the design of the roller imprinting manufacturing process for the fabrication of fluid pathways. We use procedural methods to rapidly design elements of the manufacturing process for a given fluid pathway design. Manufacturing process design, in this case, is limited to the design of the imprint roll, as the roll geometry plays the strongest

role in the quality of the part. We have developed a system that can fully design an imprint roll for a given pathway geometry. The design system is extensible and can be easily integrated with CAM systems and other post-processors.

There has been growing interest in the fabrication of fluid pathways for various applications, ranging from fuel cell bipolar plates in the macro-scale, to bio-fluidic devices in the micro-scale. These fluid pathways share common fabrication requirements: high form accuracy of cross-sections, controlled roughness in the walls and channels, cost-competitive technology and high throughput processes. Roller imprinting is a suitable candidate for fabricating these parts. In this process a hard cylindrical die (or roll) with raised surface features rolls over a soft workpiece imprinting flow channels onto its surface. Roller imprinting is more suitable than stamping as the stresses applied are significantly smaller and more uniform, resulting in controlled deformation of the workpiece.

The precision of the imprinted features is a function of the features in the imprint roll, the dynamics of the rolling equipment, and the process parameters. Of these, the features in the imprint roll have the most significant effect. Precision is determined by the positional accuracy of the paths, the form error in the path channels, and the profile of the channel surfaces. Optimally designed imprint rolls are those that can create precise features for a given fluid pathway design and workpiece material. To design such a roll, a method is needed to first model the roll from a given set of input parameters. With this model, further analysis can be performed to guarantee precise imprinted path-

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ways. The key challenge lies in developing tools to efficiently model and describe the roll.

This paper discusses a novel method to model imprint rolls which exploits the repetitiveness of features found in fluid pathways. A given family of fluid pathways can be constructed from a small set of repeating units, and this information is used to efficiently describe the roll in a computer model. Apart from the obvious improvements in processing time, this approach aids in the development of more efficient post-processing operations, like machining process planning. Iterative optimal design of the roll is also easy to implement as the features of the roll are parameterized. While the scale of the features on the roll is limited by the manufacturing processes used, the modeling procedure itself is scale-invariant. This paper restricts to looking at rolls with features that can be created using micro-machining processes. Micro-machining processes have been used to create features as small as 20 μm [1]. The next section highlights two application areas for roller imprint processes: bipolar plate fabrication and microfluidic device fabrication.

APPLICATION AREAS
PEM Fuel Cells

PEM (polymer electrolyte membrane) fuel cells are electrochemical devices which generate electricity in the presence of a fuel (Hydrogen) and oxidant (Oxygen) [2]. The "heart" of the cell is the MEA (membrane electrode assembly), which preferentially allows protonic hydrogen to pass through from the anode to the cathode side, while forcing electrons to flow around the cell, generating electricity. The MEA is sandwiched between bipolar (or flow-field) plates which provide it a fuel rich environment. The bipolar plates are so called because they have hydrogen flowing on one side and oxygen on the other, and are used to collect electricity out of the cell as well. Bipolar plates are an important component of the fuel cell stack as they facilitate the diffusion of gases across the MEA. Surface quality and flow field design of the plates is critical in guaranteeing the performance of the cells. Bipolar plates are composed of a network of millimeter-scale flow paths. Figure 1 shows a representative bipolar plate design.

Design of cost-effective and precise process technologies for fuel cell components is very important for the large-scale adoption of fuel cells. The DOE's Fuel Cell Report [4] highlights the importance of manufacturing in achieving widespread use of these devices. The manufacturing processes must guarantee very precise parts, while being flexible enough to allow for quick changes in part design. It is also important that the process is cost-competitive. Currently, machining and stamping operations are being used to manufacture the bipolar plates [5]. Roller imprinting is a capable process for manufacturing these devices. It is also possible to pattern both sides of the bipolar plates simultaneously with this process, leading to a higher throughput.
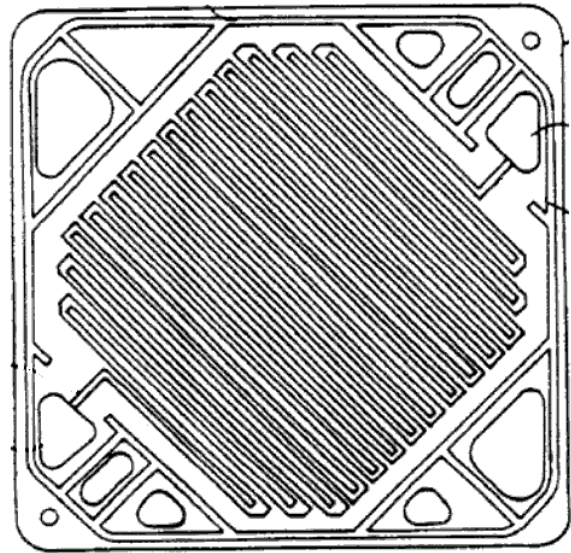

Figure 1. FUEL CELL BIPOLAR PLATE [3]

Microfluidic Devices

Microfluidic devices handle liquids on the nano-liter scale and have chemical, biological, and medical applications [6]. These devices have channels on the order of 10-100 μm with micro- and nano-scale features. Conventionally, silicon and glass were the materials of choice for the substrates of these devices, as they have established fabrication processes developed by the semiconductor industry. Though glass has good properties for use it is expensive to produce, because of this a variety of polymers are currently being developed as substrate materials. Common fabrication methods with polymers include imprinting, hot embossing, injection molding, lithography techniques, and laser photo-ablation [7]. Figure 2 shows microchannels fabricated in PMMA (polymethyl methacrylate) using the LIGA (Lithographie Galvanoformung and Abformung) process. Contact printing methods have also been used in the fabrication of microchannels [8]. Contact printing involves the transfer of features from an elastomeric stamp to a solid substrate by conformal contact. High-resolution features can be printed over a large area with this process.

Although rolls created using micro-machining technology have limited ability to create sub-micron features and three-dimensional features, they can be used in applications where large features need to be created efficiently. They can also be used in hybrid processes, with roller imprinting creating the large features, and a complimentary process creating the smaller features. This approach will decrease the overall fabrication time and cost of the devices.
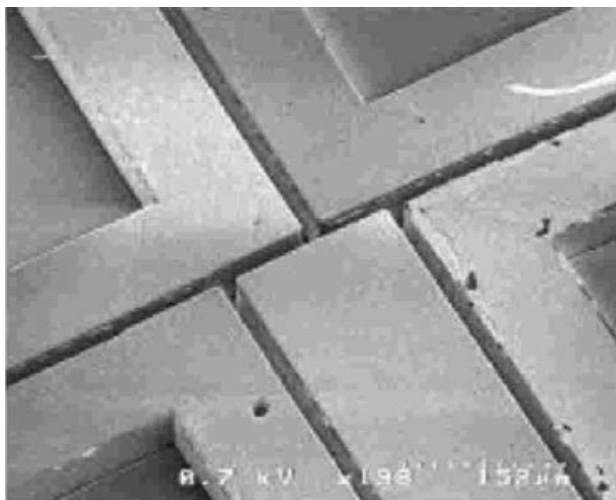
Figure 2.   MICROCHANNELS FABRICATED IN PMMA [7]

MOTIVATION

Design and manufacture of imprint rolls is a complex problem as the rolls have to be customized for a given fluid-pathway design. It is not possible to use a modular roll with replaceable features (much like cutting tool inserts) as this would result in imprecise patterns. The classic approach is manual design in an interactive CAD environment. While this method can be used to produce accurate and optimal rolls, it is dependent on the expertise of the designer, and is not scalable as manual design is labor intensive and expensive. Moreover, in the case of iterative design, manual design will be a bottleneck.

A faster and more reliable option is to automate the design process. Here, two approaches are possible. The simpler method is to take the geometric negative of the fluid pathway to be imprinted and "wrap" this virtually around a solid cylinder by transforming the coordinate system. While this makes the problem seem very easy, it is not entirely feasible as some features such as vertical walls will manifest as undercuts in the cylindrical transform. Also, no guarantees of precision are provided in the imprinted features as the transformations are done blindly. The other method is to individually analyze the features of the pathway and create the roll based on transformations of these features. While this method can be used to generate optimal rolls, designing for complex fluid pathways makes the problem intractable due to the large number of features to be processed.

This paper discusses a procedural method to model the imprint rolls by decomposing the given fluid pathway into a set of repeating features. The repeating features are individually designed and procedurally arrayed to generate the final roll. This method significantly reduces the time between the design and manufacturing of the pathways. Some of the related work in this field is discussed in the next section.

RELATED WORK

Procedural design methods have been used in diverse fields such as in the modeling of cities [9] and in the modeling of botanical systems [10]. Previous research by the authors used procedural methods to design twist drills for use in finite element simulations of drilling [11]. However, there has not been much published work on the development of procedural design tools with applications in manufacturing process planning. Much work has been done in the planning and optimization of individual entities of the manufacturing system, but there is a dearth of research on integrating these together systematically to create design tools for manufacturing. Some of the related work in the application and fabrication of fluid-pathways is discussed here.

Mehta and Cooper extensively reviewed design and manufacturing alternatives for PEM fuel cells, and specifically discussed various processes which can be used to manufacture the bipolar plate [5]. Kumar and Reddy studied the effects of flow field design and path cross-sections on the steady-state and transient performance of PEM cells [12], [13]. Li and Sabir reviewed various flow-field designs for PEM cells from the available literature as well as from patent information [14].

Becker and Locascio presented a review on polymer microfluidic devices and discussed their material properties and fabrication methods [7]. McDonald et al discussed various soft-lithography methods for fabricating patterns in poly(dimethylsiloxane) (PDMS) for various applications [6]. Michel et al also discuss several approaches for high-resolution printing using soft lithography methods [8].

PROCEDURAL DESIGN

Procedural design involves applying a series of design rules on a given set of input parameters to design a part. The design process is largely free of user intervention as the procedural system fully processes the part from the input parameters. For the design of imprint rolls the input parameters are the layout and cross-section of the fluid pathways. The fluid pathway layout is first read and decomposed into a set of unique repeating features, or tiles. The pathway is then described using this set of tiles. The tiles are modeled using the the cross-section of the pathway in the coordinate system of the roll, and are arrayed based on the pathway layout to create the full roll. These process steps are shown in Figure 3. This section discusses in detail the procedural design process, starting with a standard format for describing the fluid pathways.

Reading in the Fluid Pathways

Due to the profusion of CAD packages and standards, the geometry of the fluid pathways can be expressed in a variety of formats. Using converters to read from these varied formats is cumbersome and fraught with issues of numerical imprecision.
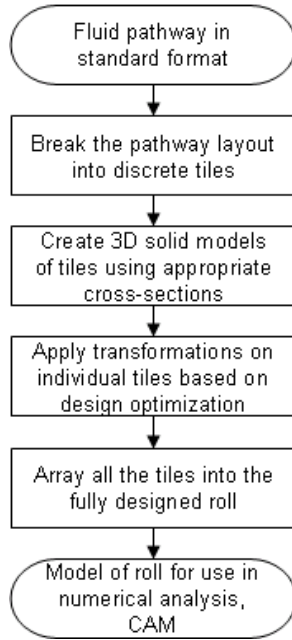
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Figure 3. PROCEDURAL DESIGN PROCESS

Figure 4. EXAMPLES OF FLOW FIELD DESIGNS - (A) SERPENTINE (B) PARALLEL (C) MULTI-PARALLEL (D) DISCONTINUOUS [12]

Fluid pathways, moreover, use only a small set of geometric parameters, and in most cases can be expressed compactly using just a swept-path and a set of sweep cross-sections. The swept path corresponds to the actual pathway, while the swept cross-section corresponds to the geometry of the cross-sections in the pathways. Each fluid pathway family features only a small number of possible cross-sections and pathway designs. For example, the flow fields in many fuel cell bipolar plate designs are orthogonal straight paths with regular spacing, with quadrilateral cross-sections.

We use a simple ASCII-based format to describe the fluid pathways. The fluid pathway file independently describes the swept path and the sweep cross-sections used in the path. The primitives used in describing these entities are customized to the specific pathway family. In the case of the most common fuel cell bipolar plates, the swept-path can be completely described using straight line primitives, and the cross-section can be described using quadrilateral primitives. More complex pathway families can be described using conic-segments and b-spline curves as primitives. The coordinate-system for the format is two-dimensional, and is in the x and y-axes for the pathways, and in x and z for the cross-sections. Figures 4 shows examples of fuel cell flow fields - these flow fields can be fully described using our format. The format also exploits the fact that some features (such as bends in a serpentine flow field) are repetitive, and provides a compact way of describing these repeating patterns.

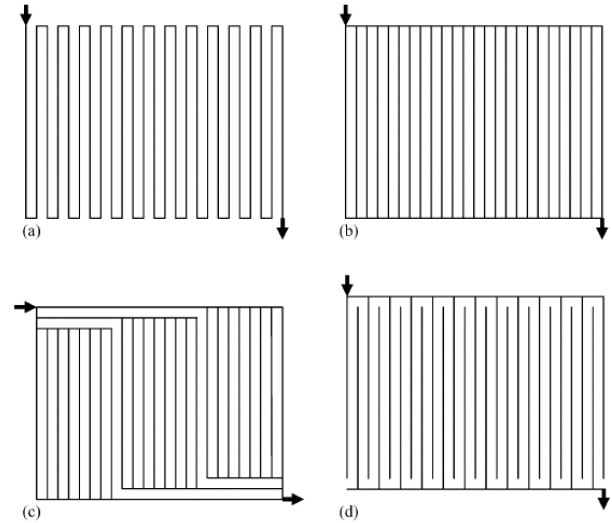The fluid pathway format for the family of bipolar plate designs is made of two sections. The first section describes the arrangement of the flow fields and the second section describes the cross-section of the flow fields. The pathway section is organized into blocks, with each block containing the layout of one continuous pathway and its repeating behavior. The layout is specified as a series of straight line segments with start and end points. The repeat information is specified by the number of times the pattern repeats, and the shift required in the x and y direction after every repeat. By this method very complex designs can be described with few lines of text. Each block also contains a tag specifying the cross-section of its pathway. These cross-section tags correspond to the cross-section description in the second part of the file.

The second part of the file describes the cross-sections. The first line contains how many cross-sections are defined in the file. This is followed by blocks of text which describe the quadrilateral profile of the cross-section by its corner points. Nominally, the mid-point of the cross-section is centered at $(x = 0, z = 0)$. The file also contains a footer area which specifies the maximum bounds of the file in the x and y directions.

Similar formats such as CIF (Caltech Intermediate Form) have been used in circuit design [15]. Using a standard format to describe the pathways greatly simplifies reading the file and decreases processing time for the rolls. Since the input format is standardized, reading in a given file is trivially accomplished. The next step - of processing the pathway layout into discrete units - is discussed in the following section.

Pathway Decomposition

Due to the repeating features present in the fluid pathways, there exists a discrete set of tiles that fully describes a given fam-

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ily of fluid pathways. For the case of bipolar plate flow fields, which are rectilinear pathways with regular spacing, five tiles are adequate for description. Each of these tile types can be oriented in four different ways by rotating about the *z*-axis, and thus (after discarding the symmetry cases) there are a total of 15 possible tiles (see Figure 5). The size of the tiles is determined by the spacing in the fluid pathway. In the case of bipolar plates, as the path spacing is uniform, the tiles are of the same size.
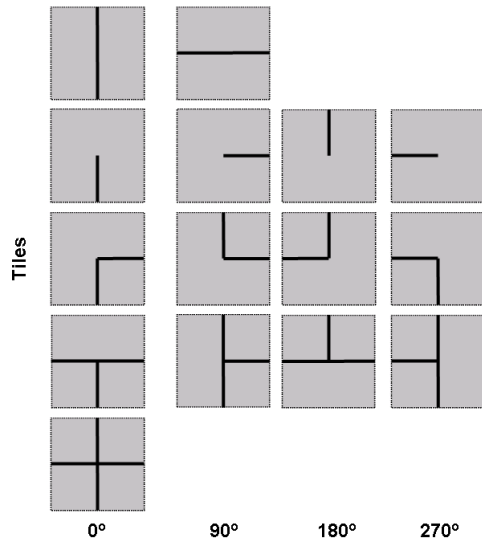

Figure 5.   TILE TYPES FOR BIPOLAR PLATE FLOW FIELDS

The algorithm to decompose the rectilinear pathway family into an array of these 5 tiles, in each of the 4 possible orientations is as follows:

1. Read and store the flow path blocks from the flow-field file with their appropriate cross-sections
2. Calculate the total number of tiles required from bounds of the pathway
3. Enumerate through the tiles, and using the corner vertices of the tiles estimate the flow segments which fall inside each tile
4. From the patterns falling within a tile, set the type and orientation of the tile
5. Assign each tile a cross-section corresponding to the paths that fall within it

Figure 6 shows an example of a pathway design composed of uniformly spaced rectilinear paths with a square cross-section. Figure 7 shows this pattern decomposed into tiles.
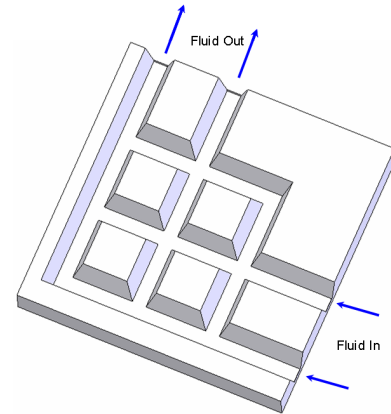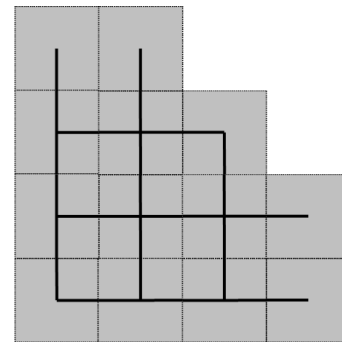

Figure 6.   RECTILINEAR FLUID PATHWAY

Figure 7.   FLUID PATHWAY DECOMPOSED INTO TILES

Creating the Roll

The imprint roll for a given pathway is modeled by first creating a library of the unique tiles in the pathway's family. Since the imprint roll contains the negative of the features in the fluid pathways, the tiles are created with raised features corresponding to the cross-sections in the pathways. Design rules to transform the cross-sections from the pathways to the roll (planar to cylindrical transforms, for example) are applied at this stage. The design rules can also incorporate the changes required in the cross-section from the process parameters of the rolling process. Specific implementation details for creating the tiles are discussed in a following section.

Once the tile library is created, the solid roll is created by instantiating these tiles according to the decomposition of the fluid pathway. Figure 8 shows the solid model of the roll created from the fluid pathway in Figure 6.

ADVANTAGES OF PROCEDURAL DESIGN

This modeling procedure has advantages beyond just decreasing the processing time. Representing the roll as a sum of modular units is useful in design optimization procedures as well
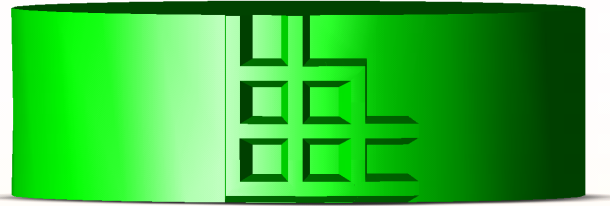
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Figure 8. SOLID MODEL OF ROLL WITH RAISED PATTERNS

as in developing machining toolpaths. Some of the key advantages are discussed in this section.

Feature Recognition

Feature recognition can be used to isolate regions of the roll for targeted optimization. Conventional approaches involve reading and recognizing all the features in the roll and then searching through them for the ones that need to be isolated. Recognizing features on the procedurally generated rolls can be simplified to a matrix search operation, where smaller sub-matrices are searched for inside a larger parent matrix. Instead of searching for features by recognizing geometric parameters, the tiling information is used. Each tile arrayed in the roll is first assigned a unique numerical identifier and the entire roll is represented as a matrix of these values (the position of the tiles in the roll corresponds to the location of their unique identifiers in the matrix). To search for a pattern, the pattern is first represented as a matrix and this matrix is searched inside the roll matrix. If the pattern cannot be represented as a matrix (i.e, if its not rectangular), it can be broken into rectangular sub-matrices, and the sub-matrices are searched in the roll matrix. This is a much faster way of recognizing features without any geometric processing of the roll.

Optimal Design

Optimally designed rolls are those that guarantee precise pathways under a given set of process parameters. The parameters also include the properties of the roll and workpiece materials. To optimize the roll design, specific transformations are applied to the patterns on the roll based on the quality of their imprinted features. The design variables in this optimization problem are the parameters of the geometric features in the individual tiles, and the performance criteria is the precision of the imprinted paths made by the roll composed of these tiles. Using the pattern recognition method described in the previous section, optimal design algorithms can be efficiently applied on the roll. The first step of optimal design is identifying the candidate features to be optimized - this is easily solved using feature recognition. The next step involves applying geometric transformation on these tiles by manipulating its parametrized geometry. Thus

if a tile is flagged to be optimized, the features of that tile are changed on-the-fly by adjusting the design parameters of the tile.

To analyze sections of the roll, tiles of the section can be chosen and a reduced roll can be made with just those features. Sectioning operations are not required to create sub-rolls. Figure 9 shows results from a simplified FEA (finite element analysis) of a rigid roll composed of a small cluster of tiles rolling on a metal workpiece. This was a first-order analysis that did not take into account material hardening effects. The mesh for the roll was also generated using the design tool by combining the meshes of the individual tiles. The analysis was used to visualize the material flow and stress fields in the workpiece during the rolling process. By applying the analysis to rolls with different features, the effect of feature geometry on the workpiece deformation behavior was seen.
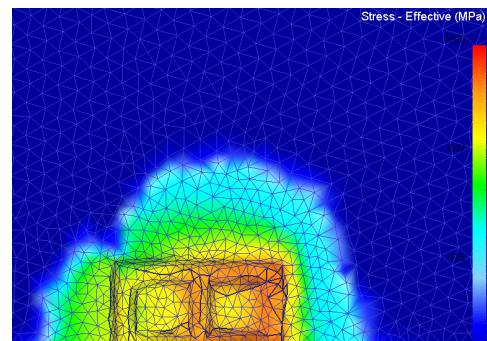

Figure 9. FINITE ELEMENT MODEL OF DEFORMATION IN SS304L FROM ROLLING OF RIGID PATTERNED ROLL

Efficient Machining

Manufacturing process planning is required for the physical realization of the roll. As these models consist of complex features on a cylinder, a cost-effective manufacturing strategy is to use 3-axis end-milling with a rotary indexer. An important consideration at this stage is planning the tool path of the end-milling operation. Having the fewest number of index positions increases the precision of the process, as positional error increases with indexing. This can be framed as an optimization problem whose objective is to minimize the number of index positions required to fully machine the roll. This is a visualization problem akin to those seen in 5-axis machining and injection molding [16], [17], [18], [19]. The conventional way to solve this is to calculate the optimal view locations by applying geometric algorithms. This is a computationally intensive process, but by using the tile-based description of the rolls, a much simpler method can be used.

Instead of explicitly calculating the visible regions of the en-

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tire roll, the visible region of each individual tile is pre-calculated and this can be used to compute the visible regions of the roll. The visible region of a feature is the angular interval it can be indexed and still be machined by a cutting tool positioned directly above its nominal position (see Figure 10). As 3-axis machining is being used, the visible range is two-dimensional. The visible range of each tile is first calculated in its local coordinate system, and then shifted by its nominal angular position in the coordinate system of the roll. After the visible range of each unique tile in all the orientations is calculated, the tiles on the fully designed roll can be "tagged" with these visible ranges. The problem has now been simplified to a search problem and can be applied for different manufacturing considerations.
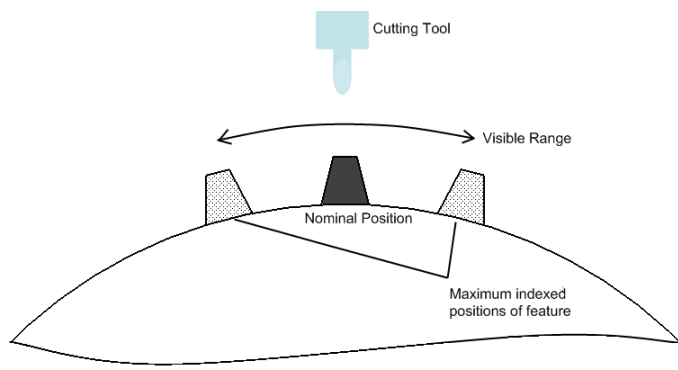

Figure 10. VISIBLE RANGE OF A FEATURE

A simple optimization strategy is to machine axially aligned tiles at the same index position. For this, entire rows of the roll are tagged with the visible range of the least visible tile in it. The machining positions can be calculated using a greedy search to locate the positions which lie in visible regions of the most number of tiles.

As an example, consider the roll in Figure 8. As this roll has only a small number of tiles, there exists one continuous angular region from where all the tiles can be machined. This optimal view region is shown in Figure 11. The figure also shows the visible angular region for each of the tiles; graphically, the optimal view region is the interval where all these intervals overlap.

IMPLEMENTATION

A design tool was developed based on this methodology using C++ and the ACIS solid modeling kernel. The design tool was customized to model rolls for applications in fuel cell bipolar plates. An object-oriented programming environment like C++ was well-suited as the fundamental modeling entity, viz. the tile, could be conveniently encapsulated as a programming object.
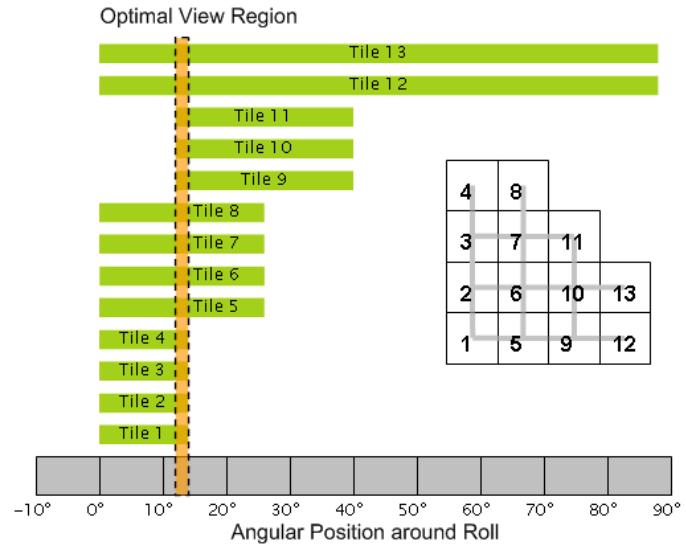

Figure 11. OPTIMAL VIEW REGION OF ROLL

The tool takes in text-files with the flow-field information as input and returns a solid model of the roll as output. The tiles are modeled as solids as well, and are created by sweeping a cross-section along a path. The cross-sections are transformation of those specified in the fluid pathways description, and the paths are from the tile decomposition. The tiles are put together to form the final roll using boolean add operations. Using this design tool, the pattern shown in Figure 12 was processed into a roll. This pattern is representative of the features most commonly seen in PEM fuel cell bipolar plates. The pathway had channels 1mm in width with a trapezoidal cross-section, and the total size of the pattern was 50mm $\times$ 50mm. The roll had a diameter of 6.5 cm. In the modeled roll, some of the features are of the untransformed trapezoidal cross-section while the remaining are of a modified cross-section described using a b-spline curve. The features to be transformed were identified in a post-processing step using the matrix search, and had the cross-sections changed. The two cross-sections used in the roll are shown in Figure 13. The fully designed solid roll can be seen in Figure 14. This roll was then machined using 3-axis endmilling with a rotary indexer; HyperMill was used to generate the toolpaths for machining. The machined roll can be seen in Figure 15. The machined physical roll conformed geometrically to the roll that was procedurally modeled. This validated the procedural process, as the only input given to model this roll was the fluid-pathway design. It also has to be noted that the physical roll is seamless and does not have artifacts from the tiling, such as creases or steps in the features.

While this method is convenient to implement, the boolean operations used to create the roll can behave less than robustly at times, leading to numerical imprecision and error. Also, triangulation and faceting is required for applying machining al-
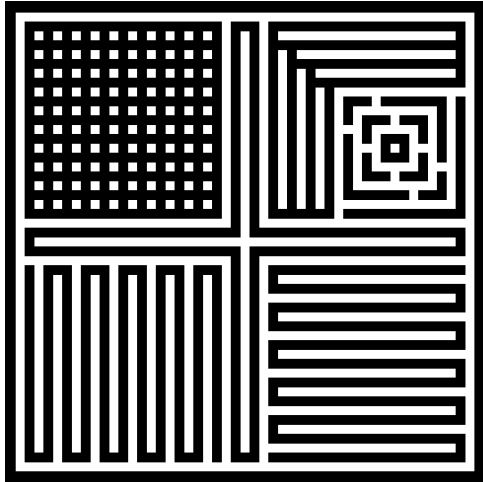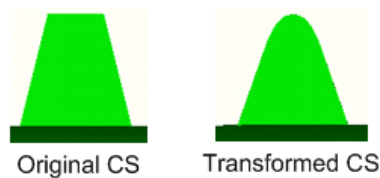
7

Figure 12.   INPUT PATTERN
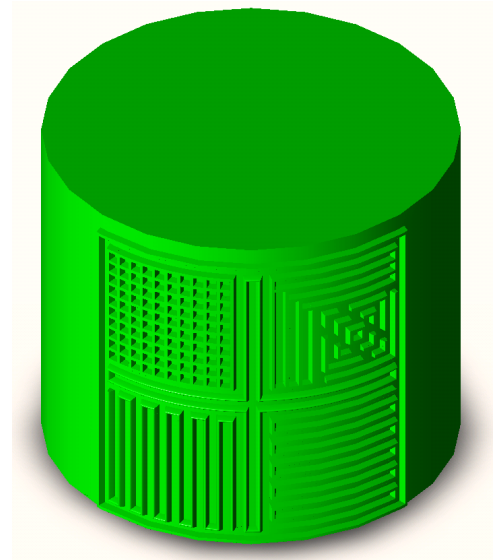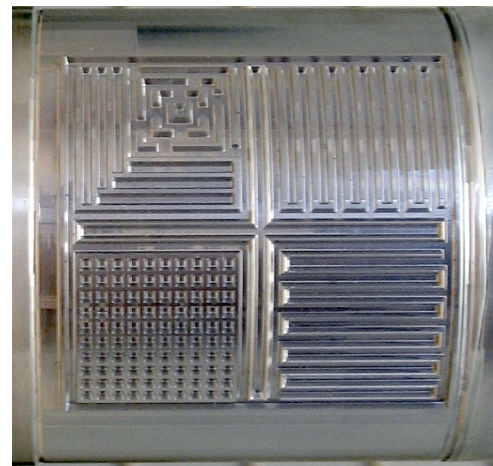

Figure 13.   CROSS-SECTIONS USED

gorithms and to visualize the roll, which leads to further imprecision. We are investigating methods to describe the rolls using b-spline patches to improve the precision in the geometric model.

FUTURE WORK

Future work in this research involves integrating design optimization routines into the procedural design framework. Currently, we are developing numerical methods for the selection of optimal roll features based as a function of process parameters and precision requirements. These numerical methods will serve in establishing a feedback loop to optimize the geometric features of the roll based on the precision of the imprinted pattern. Future work will also address the robustness issues and modeling artifacts in the roll model from using solid-sweeps to design the individual tiles. Also of interest is developing optimization algorithms for the selection of minimal tool-positions for machining the rolls. After the optimal rolls are fully designed and manufactured, the design optimization will be validated by applying the rolls in the fabrication of micro-fluidic and fuel cell pathways, and measuring the precision of these pathways.

Figure 14.   SOLID MODEL OF ROLL

Figure 15.   FULLY MACHINED ROLL

CONCLUSIONS

We have demonstrated in this paper a novel procedural method for designing imprint rolls. This method is scale-invariant and can be applied with other manufacturing processes as well. Procedural methods can also be applied in other areas where the complex features which need to be designed can be expressed as functions of the input parameters.

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