Modeling of Electrolytic Membranes for Large Area Planar Solid Oxide Fuel Cells

THESIS

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A planar solid oxide fuel cell is characterized by a thin ceramic electrolyte sandwiched between porous electrodes, along with seals and current collectors. To perform as a good oxide ion conductor, the electrolyte needs to be very thin. However, a thin electrolyte is highly prone to damage during production, assembly, and subsequent operation. To be both electrochemically efficient and mechanically robust, NexTech Materials Ltd has developed an innovative electrolyte, the FlexCell™, for use in electrolyte-supported SOFCs. This electrolyte design has a honeycomb structure that supports thin, “active areas” thus providing good electro-chemical efficiency as well as mechanical robustness.

To optimize the FlexCell and understand its mechanical limits, a combination of experiments and finite element modeling are performed. The out-of-plane dimensions are much smaller than the in-plane dimensions, and hence a two-scale approach is required for optimizing the geometrical design of the FlexCell. At the large-scale, the whole electrolytic membrane is modeled with equivalent properties, whereas at the small-scale, the repeating pattern of the honeycomb structure is studied.

Nextech’s goal to commercially produce ultra large FlexCells of the order of 700 to 1200 cm² depends largely on its mechanical performance. The aim of this work is to suggest ways to geometrically alter the design so that the mechanical
membrane performs well under mechanical and thermal loading. By performing finite element simulations on the large area *FlexCell*, design parameters which influence its mechanical robustness are identified. Results of this analyses show the areas of high stresses. The stresses can be mapped to the small-scale to study small-scale failure. Since it is not known if optimal geometries scale with membrane size, a more methodical approach is undertaken to ensure that the thin active areas have adequate support in thermally varying environments.
“I can do all things through Him who strengthens me” – Philippians 4:13

I am grateful for God’s provision of joys, challenges, peace and grace for growth, and this work is dedicated to Him.
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Above all, I am most thankful to God for bringing me this far in this academic endeavor and in life.
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CHAPTER 1

INTRODUCTION

1.1 FUEL CELL

A fuel cell is an electrochemical device that has two reactants flowing along the positive and negative electrodes on either side of an oxide ion conducting electrolyte [1]. Fuel cells have a cathode, electrolyte and anode sandwich assembly. Chemical reactions occur at interfaces producing various benign by-products and delivering electrical energy to an external load. Figure 1.1 gives a schematic representation of the functioning of a solid oxide fuel cell. Fuel cells are different from batteries in the way that they have an external source of energy which needs to be replenished. Although a fuel cell is a thermodynamically open system like a combustion engine, unlike a combustion engine, fuel cells are more efficient and much cleaner way to produce energy without releasing harmful nitrogen based byproducts into the atmosphere.
1.1.1 TYPES OF FUEL CELLS

Though the basic operating principles are the same, there are several different types of fuel cells, each having characteristic materials, operating temperatures, reactants and geometry [2]. The most common types of fuel cells are as follows:

- Alkaline fuel cells (AFC)
- Phosphoric acid fuel cells (PAFC)
- Polymer electrolyte membrane (PEM) fuel cell
- High temperature fuel cells
  - Solid Oxide Fuel Cell (SOFC)
  - Molten carbonate fuel cell (MCFC)
1.2 SOLID OXIDE FUEL CELL

A solid oxide fuel cell is characterized by a solid, dense ceramic electrolyte that is sandwiched between two porous electrodes. At the anode, the fuel undergoes oxidation and the released electrons are carried through the load circuit. These electrons are accepted on the cathode side by the oxidant which is thusly reduced. Upon reduction, the oxide ion flows through the electrolytic membrane. This electron and oxide ion flow is responsible for the flow of electric current.

Figure 1.1 shows the operation of a SOFC and the reactions that take place within the cell are summarized in Table 1.

Table 1.1: Chemical reaction occurring within the fuel cell

<table>
<thead>
<tr>
<th>Place of occurrence</th>
<th>Reaction</th>
</tr>
</thead>
<tbody>
<tr>
<td>Anode</td>
<td>( \text{H}_2 + \text{O}^{2-} \rightarrow \text{H}_2\text{O} + 2\ e^- )</td>
</tr>
<tr>
<td>Cathode</td>
<td>( \text{CO} + \text{O}^{2-} \rightarrow \text{CO}_2 + 2\ e^- )</td>
</tr>
<tr>
<td>Overall</td>
<td>( \text{O}_2 + 4\ e^- \rightarrow 2\ \text{O}^{2-} )</td>
</tr>
<tr>
<td>Overall</td>
<td>( \text{H}_2 + \text{CO} + \text{O}_2 \rightarrow \text{H}_2\text{O} + \text{CO}_2 + \Delta E )</td>
</tr>
</tbody>
</table>
1.2.1 MATERIAL COMPONENTS FOR SOFCs

The most commonly used SOFC electrolyte material is the oxide ion conducting Yttria stabilized Zirconia (YSZ) [3]. This solid impermeable ceramic allows for the exchange of oxide ions without diffusion of fuel across it. Scandia stabilized Zirconia (ScSZ) is as an alternative to YSZ because of lower operating temperature and higher ion conductivity [4]. The anode is a porous cermet type structure made of nickel or noble metals and YSZ so that they are stable at high temperatures and are electrically conducting [5]. The cathode is usually Sr-doped lanthanum manganite which offers good conductivity and electro-catalytic activity [6]. The interconnects which provide electrical contact between cells in a stack require that they are impermeable, electrically conducting and stable in both oxidizing and reducing atmospheres [7].

1.2.2 GEOMETRY OF THE SOFC

A planar SOFC is flat, sandwich-type SOFC described earlier. Another geometric variation is the tubular design where one of the reactants is passed through the inside of the tube and the other is passed along the outside of the tube. Though the tubular design is very helpful in sealing the fluids from mixing, it is expensive to manufacture. Furthermore, planar designs are capable of higher power densities than tubular design.

1.2.3 SUPPORT TYPES

The SOFC “support type” refers to the component of the SOFC which provides the major part of the structural support. SOFCs are either electrolyte-supported or anode-supported. Anode-supported SOFCs are susceptible to breakage due to the redox reactions and thermal cycling and are more challenging to seal. Electrolyte-supported cells require thicker electrolytes and higher operating temperatures. Nonetheless, the
increase in fuel flexibility, including less sensitivity to sulfur contamination and ease of sealing makes electrolyte-supported SOFCs very attractive. As will be described in this work, a novel method for providing thin, electro-chemically active regions together with thicker support regions enables electrolyte-supported cells to be both electro-chemically active and provide sufficient mechanical support.

SOFCs afford high power density, internal reforming, fuel interchangeability and the possibility of high efficiency through combined power application. Equally important, exclusive of providing the necessary hydrogen fuel, SOFCs provide electricity with no harmful byproducts. It is critical new sources of clean energy are developed quickly. The advantages of SOFCs are such that they may play an important role in world’s evolving energy portfolio. To be successful, the cost of SOFCs must be further reduced and the reliability and durability of SOFCs must be increased. Reliability and durability of SOFCs requires better understanding of materials, manufacturing, assembly and operation.
2.1. WHAT IS A *FLEXCELL*™?

An innovative design concept incorporating both efficient energy production and mechanical support architecture for a planar electrolyte-supported SOFC has been developed by NexTech Materials Ltd. The *FlexCell*™ membrane is manufactured by tape casting thin layers of green tape which are stacked on top of each other and then sintered together. The green tape can be easily cut out to form out-of-plane features. For the *FlexCell*, several continuous tapes are first laid down, followed by layers with perforations. In the end, the electrolyte membrane consists of “active” regions that are approximately 40 micron thick surrounded by a “support” mesh and frame that is approximately 200 microns thick. The active areas allow for effective oxide ion exchange while the support mesh provides the necessary mechanical support.
A standard FlexCell design for a 110 cm² cell is shown in Figure 2.1; it consists of a support layer that is perforated with hexagonal cut-outs and is surrounded by a dense peripheral frame. As seen in the figure, the active area is so thin that it is translucent. The proven advantages of using the FlexCell design in fuel cell stacks are the unique combination of mechanical strength with electrochemical efficiency along with fuel flexibility, reliability, and scalability [8].

2.2 CHALLENGES IN DESIGNING A FLEXCELL

For the desired higher power densities, larger cells must be produced. The goal is to produce FlexCells which are in the order of 400-1000 cm². In this case, the ratio of the length to its thickness is as high as 1000:1. Hence, as the dimensions of the cell get bigger, there is a greater need to provide sufficient mechanical robustness at the
manufacturing, assembling, and operating stages. The dimensions of the hexagonal perforations, outer frame, and potential mid-cell ribs could play a key role in providing the required mechanical robustness. Models are required to optimize design variables.

Finite element analysis is employed to identify design parameters that could be altered to improve the geometric design of FlexCell membranes. The out-of-plane dimensions of the cell are very much smaller compared to its in-plane dimensions.

As seen in Figure 2.2, a two scale approach is followed because of the mismatch between the in-plane and out-of-plane dimensions. Initially, experimental techniques are used to determine the mechanical properties of the material. At the small-scale, the perforation pattern is examined as a repeating unit cell. At the large-scale, the whole membrane is analyzed by making use of data provided by the small-scale analysis.

Figure 2.2: Illustration of the two scale approach for FlexCell modeling
2.3. DESIGN PARAMETERS AT THE LARGE-SCALE

Figure 2.3 represents the geometry of a large area *FlexCell* and is characterized by an outer frame, horizontal and vertical support ribs, and four active membrane areas made up of a combination of large and small cutouts. At the large-scale, the following factors are taken into consideration for optimizing the electrolyte support architecture:

- Distribution of cutout patterns
- Addition of support only regions (cross ribs)
  - Rib thickness
  - Rib width
  - Rib number and placement
- Width of the outer frame
- Fillet placement and radius
The goal of this research is to define the optimal geometry of the large area FlexCell (400 cm$^2$) by studying the design parameters described earlier and to be able to apply them to refine the geometric design of ultra-large area FlexCells (700 cm$^2$). It is not known if the optimal geometry of a large area cell is also optimal for ultra-large sized FlexCells. Hence, numerical analysis of the various design parameters is needed to ensure that the thin, active areas are sufficiently supported as the overall size of the electrolytic membrane becomes larger. At the same time the amount of thin, active area must remain as large as possible in order to have highly efficient and hence commercially viable SOFCs.
CHAPTER 3

MATERIAL PROPERTY MEASUREMENT AND EXPERIMENTAL VALIDATION

3.1. MOTIVATION

In order to develop effective finite element models, it is necessary to know the geometry, have accurate material properties, and to be able to appropriately define loading and boundary conditions. Thus the first step in this research is to make experimental measurements on bulk electrolyte material and perform finite element analyses at the small-scale to find the equivalent stiffness of various cutout patterns. It is also desirable to experimentally validate the stiffness of the material used. Four-point bend experiments were conducted to experimentally validate the effective mechanical properties obtained through the small-scale simulations.
3.2. OBTAINING MATERIAL PROPERTY DATA

As mentioned previously, the work done at the small-scale level helps in determining the bulk equivalent properties.

3.2.1 EXPERIMENTAL MEASUREMENT OF MATERIAL PROPERTIES

The material property for the electrolytic material was determined using a sonic resonance technique. The experimental apparatus can be mounted inside a furnace (Figure 3.1) so that high temperature material properties can also be obtained. As shown in Figure 3.2, a rectangular bar specimen is suspended by from two strings inside the furnace, which are connected to two transducers which are in turn connected to an arbitrary waveform generator and oscilloscope. This sample is made to vibrate through a range of frequencies through one string and the amplitude of the vibration is sensed with the other string. The amplitude of vibration increases as the excitation frequency

Figure 3.1: Experimental set-up for measuring flexural and torsional moduli by the sonic resonance technique
approaches the fundamental flexural and torsional modes of vibration. These resonant modes are dependent on the specimen geometry and material properties. Thus the following equations can be used to determine the Young’s Modulus and shear modulus [9]:

\[
E = 0.9465 \left( \frac{mf_f^2}{b} \right) \left( \frac{L^3}{t^3} \right) \left( 1 + 6.585 \left( \frac{t}{L} \right)^2 \right)
\]

(1)

\[
G = \frac{4Lmf_i^2}{bt} \left[ \frac{b/t + t/b}{4(t/b) - 2.52(t/b)^2 + 0.21(t/b)^6} \right]
\]

(2)

where \(E\) = Young’s Modulus (Pa); \(G\) = Shear Modulus (Pa); \(m\) = mass of the bar (g); \(b\) = width of the bar (mm); \(L\) = length of the bar (mm); \(t\) = thickness of the bar (mm); \(f_f\) = fundamental resonant frequency of the bar in flexure (Hz); \(f_t\) = fundamental resonant frequency of the bar in torsion (Hz).

Figure 3.2: Representation of specimen positioned for measurement of resonant frequencies using thread suspension [9]
Keeping in mind the operating temperatures for a solid oxide fuel cell, the experiment was performed for temperatures up to 800° C and the results are plotted as shown in Figure 3.3. The Poisson’s ratio ($\nu$) is assumed to be constant at 0.3 and hence it is not necessary to include shear modulus data in the material model.

![Figure 3.3: Plot of Young's Modulus of YSZ for varying temperatures determined using resonance technique](image)

3.2.2 POPULATING THE MODEL WITH EQUIVALENT PROPERTIES

Since the membrane area is made up of a repeating pattern of cutouts, as shown in Figure 3.4, a representative area is chosen so that it be repeated in all directions to represent the entire active membrane. On this area, periodic boundary conditions are applied and simulations are performed. Percent active area (%AA) is a new metric proposed to indicate what portion of the unit cell is thinned by the cutout pattern and is given by Eqn (3). The %AA should correlate with the overall electro-chemical efficiency of the fuel cell [10].
A finite element model of repeating unit cells with different cutout geometries of interest are subjected to a known displacement along the boundaries and the equivalent stress and strain is obtained. From these equivalent stress and strain values, the equivalent stiffness ($E_{eq}$) of the material for a given small-scale geometry is obtained. Also since there is a possibility of using different materials for the electrolyte, it is advantageous to normalize $%E_{eq}$ so that equivalent stiffness can be applied to any linearly elastic material for a given $%AA$. The equivalent stiffness is normalized by

$$%E_{eq} = \frac{t_s + f(%AA)t_m}{t_s + t_m} \times (100\%) \quad (4)$$

where $t_m = $ thickness of electrolyte layer (microns); $t_s = $ thickness of support layer (microns); $%AA = $ percent active area, and, $f$ is a function of $%AA$, determined by a curve fit.
The \( E_{eq} \) results are plotted against \( AA \) in Figure 3.5. Though cutout geometries like hexagons and circles of different sizes were analyzed, it is important to note that the \( E_{eq} \) is a function of \( AA \) rather than the shape of the cutout pattern.

With equivalent stiffness results, it is possible to model the *FlexCell* in the large-scale. Also, since the material is linearly elastic, even if the stiffness changes at elevated temperatures, the normalized \( E_{eq} \) will not change. Initial simulations on the large area *FlexCell* use these equivalent properties as the input for creating material models.

The \( AA \) and \( E_{eq} \) for the specific types of cutout geometry that are of interest are obtained from Figure 3.5 and tabulated in Table 3.1. As can be seen, the model
without any cutouts is used as the normalization reference and the other cutout geometries have a lower \(\%E_{eq}\) in comparison. These values are helpful in creating material models for modeling the patterned active membrane at the large-scale.

Table 3.1: \(\%E_{eq}\) and \%AA of specific cutout geometries

<table>
<thead>
<tr>
<th>TYPE</th>
<th>% Active Area (%AA)</th>
<th>% Equivalent Stiffness (%E_{eq})</th>
</tr>
</thead>
<tbody>
<tr>
<td>NO CUTOUT</td>
<td>0</td>
<td>100</td>
</tr>
<tr>
<td>SMALL CIRCLE</td>
<td>36</td>
<td>55</td>
</tr>
<tr>
<td>SMALL HEX</td>
<td>39</td>
<td>52</td>
</tr>
<tr>
<td>BIG CIRCLE</td>
<td>53</td>
<td>42</td>
</tr>
<tr>
<td>BIG HEX</td>
<td>57</td>
<td>39</td>
</tr>
</tbody>
</table>

3.3 FOUR POINT BEND EXPERIMENTS

Apart from conducting four point bend experiments to validate the effective mechanical properties obtained through the small-scale simulations, the experiments are also helpful to

- determine failure initiation and identify breakage pattern
- check the non linear trend of the electrolyte material during cyclic loading

3.3.1 SAMPLES

The specimens prepared for this study are made of YSZ. As shown in Figure 3.6, the overall dimensions are approximately 140 mm in length and patterns are cut in the center of the specimen. Samples were prepared with a) constant thickness – no pattern, b)
large hexagons, c) small hexagons, and d) large circles. Samples have standard NexTech thicknesses – approximately 200 microns in the support areas and 40 microns in the active regions.

The width and thickness of the FlexCell strips were measured using a vernier caliper and micrometer, respectively and are tabulated in Table 3.2. It is interesting to note that the geometry differs among the sample types, but are the same within a given type of cutout geometry. This indicates that thickness can vary significantly from batch to batch.

Table 3.2: Width and thickness measurement of the thin FlexCell strips

<table>
<thead>
<tr>
<th>SAMPLE</th>
<th>MEASURED VALUES</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>WIDTH (mm)</td>
</tr>
<tr>
<td>UNPATTERNED</td>
<td>21.13</td>
</tr>
<tr>
<td>SMALL CIRCLE</td>
<td>23.52</td>
</tr>
<tr>
<td>SMALL HEX</td>
<td>23.52</td>
</tr>
<tr>
<td>BIG HEX</td>
<td>23.53</td>
</tr>
</tbody>
</table>

Figure 3.6: CAD drawing of a test specimen having big hexagonal cutouts.
3.3.2 EXPERIMENTAL SET UP

The experiments are conducted using an 800L load frame from TestResources as shown in Figure 3.7. The upper moving part of the fixture is connected to the load cell. The lower half of the fixture is stationary and is fixed to the base of the frame. The load frame is displacement controlled and crosshead movement and load data are recorded for subsequent analyses. The sample is placed on the rollers and acoustic emission (AE) sensors are placed on the sides of roller supports. The acoustic emission controller records the occurrence of acoustic events which will help in the interpretation of occurrence of damage. The AE threshold is set to 40 dB.
Figure 3.7: Four point bend experiment setup
3.3.3 FINITE ELEMENT SIMULATIONS TO IDENTIFY KEY VARIABLES

A series of simple 2D simulations were done in ANSYS™ to help understand the effect that some of the test variables could have on experimental results. SHELL181 elements were used to model the test specimen. SHELL181 is a 2D element available in ANSYS where the thickness is given as a real constant. Hence, the model is designed in the xy-plane as per what is shown in Figure 3.6 and the thickness along the z-direction is given as a constant. The material properties are obtained from the resonance experiments and small-scale equivalent stiffness models.

The mesh is shown in Figure 3.8. The boundary conditions are such that the specimen cannot translate in the x- and y-directions, and it can rotate along the y-direction. To simulate the effect of a roller, the load is applied as an evenly distributed load along the width at equal distances from the middle of the sample.

Figure 3.8: Meshed model with boundary conditions and loading to represent 4-point bending in ANSYS
By varying the distance ‘a’ between the support and load rollers, and results show that a change in the spacing even by 1 mm significantly alters the trend of the load-displacement curve. This requires for greater control over fixture adjustments. Also, by having this distance constant, the moment and hence the stress do not change, but by fixing the load span on the patterned region, simulations show that the specimen undergoes more deflection as it is of less stiffness.

Based on these results, it was decided to have a support span of 90 mm and a load span of 30 mm so that it is loaded in the patterned region. The sample was marked as per these specifications and loaded symmetrically as shown in Figure 3.9. The displacement of the load rollers, load applied and the occurrence of acoustic emission events are recorded.

Figure 3.9: Illustration of loading geometry for the thin strip sample
3.4. DISCUSSION AND RESULTS

Figure 3.10 shows how a thin strip specimen undergoes deflection under load. The specimen was set up such that the load rollers are in the weaker patterned region. As seen from the curvature of the specimen, it has the characteristics of pure bending. It was also surprising to note that though the specimen is very thin, it is elastic and can deflect more than what was expected. The following sections provide a detailed study of the behavior exhibited by these thin strips.

Figure 3.10: Deflection of the thin strip specimen under load
3.4.1 VALIDATION OF RESONANCE EXPERIMENT AND SMALL-SCALE SIMULATION

The load and displacement data recorded by the load frame controller are converted to stress and strain values to calculate the stiffness of the various patterned samples. By incorporating the theory of pure bending [11], Ponraj et al. formulated relationships for calculating the stress and strain of a ceramic specimen that is deformed elastically [12].

\[
\sigma = \frac{3(L-a)F}{2bh^2} \tag{5}
\]

\[
\varepsilon = \frac{6hx}{(L-a)(L+2a)} \tag{6}
\]

where \(L\) = the total gage section (mm); \(a\) = distance between support and load roller (mm); \(F\) = the load; \(b\) = width of the specimen (mm); \(h\) = height of the specimen; \(x\) = the deflection at the load points. The load and displacement data from the experiments are fed into equations (5) and (6) and plotted in Figure 3.11.
Figure 3.11 indicates that a sample with no cutout pattern (0% AA) is much stiffer as compared to the samples with cutouts. It also validates the fact that the stiffness of the samples with small cutout patterns (hexagons and circles) is not a function of the geometry of the cut out patterns; rather it is a function of the % AA as already determined by the simulations done on the repeating unit cell. Also, the sample with big hexagons (57% AA) cut in the active membrane has the lowest slope and hence the lowest stiffness. The Young’s modulus is calculated by measuring the slope of the curve at 0.02% strain i.e., in the region before the stress-strain curve begins to have a non-linear trend. The results are tabulated in Table 3.3.
Table 3.3: Comparison of Young's modulus obtained by different methods

<table>
<thead>
<tr>
<th>TYPE</th>
<th>Equivalent Stiffness (%E)</th>
<th>Young’s Modulus (GPa)</th>
<th>% Deviation</th>
</tr>
</thead>
<tbody>
<tr>
<td>NO PATTERN</td>
<td>100</td>
<td>204.6</td>
<td>201</td>
</tr>
<tr>
<td>SMALL CIRCLE</td>
<td>55</td>
<td>111.65</td>
<td>113.5</td>
</tr>
<tr>
<td>SMALL HEX</td>
<td>52</td>
<td>106.35</td>
<td>103.4</td>
</tr>
<tr>
<td>BIG HEX</td>
<td>39</td>
<td>79.58</td>
<td>83.5</td>
</tr>
</tbody>
</table>

It can be concluded that the stiffness of the electrolyte material is a strong inverse function of % AA and is independent of the geometry of the cut out patterns. The values show that there is a close match between the values obtained by the resonance technique and four point bend experiments. The results obtained from the bend test experiment were better than expected because the calculations are based on cross-head displacement rather than the conventional mid-point displacement.

3.4.2 STUDYING BREAKAGE PATTERN IN THIN STRIP SAMPLE

Since the specimen with big hexagonal cutouts is the weakest, the sample is loaded up to breakage and studied. Figure 3.12 shows the load vs. displacement plot for thin FlexCell strip with big hexagonal cutout pattern (57% AA) in the center of the specimen. It also shows the number of hits that are recorded by the AE sensor. Looking at Figure 3.12, there are a higher number of hits that occur in very quick succession within 0.42 seconds just to sample failure.
The hit number, position of the crosshead, duration for which the hit occurs and the energy of the hit are tabulated in Table 3.4. The AE energy is calculated by the system and is the square the AE signal integrated over time. The AE hit that occurs at crosshead deflection = 2.1 mm has a hit duration of only 4.8 μs, where as the other hits that occur when deflection is around 14.1 mm have higher hit durations. Hence it is assumed that this first AE hit is not an indication of specimen breakage or non-linear behavior. The hit with the longest duration is the 2\textsuperscript{nd} hit that occurs at 14.13 mm. Also the energy recorded at this hit is 68000 μVs where as for all the other 19 hits, it is comparatively less. It is assumed that this 2\textsuperscript{nd} hit is first, catastrophic thru-crack. The hits that succeed the 2\textsuperscript{nd} AE hit have an average hit duration and energy of 1706.2 μs and 114.8 μVs respectively. The hits numbered from 12 to 20 are low energy hits though the average duration is 485.66 μs. The tabulated load data indicates that the specimen fails at 0.88 N. The data scatter ranging from 0.82 to 0.91 N is due to machine noise. The broken sample (Figure 3.13) shows how the thin hexagonal regions break away from the rest of the sample.
Figure 3.12: Load, Hits vs. crosshead displacement plot for sample with big hexagonal cutout pattern

Figure 3.13: Broken test specimen with big hexagonal cutout pattern
Table 3.4: AE sensor and load data for specimen with big hexagonal cutout pattern

<table>
<thead>
<tr>
<th>Hit No.</th>
<th>Crosshead position (mm)</th>
<th>Duration (μs)</th>
<th>Energy (μVs)</th>
<th>Load (N)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>2.11</td>
<td>4.8</td>
<td>2.6</td>
<td>0.05</td>
</tr>
<tr>
<td>2</td>
<td>14.13</td>
<td>96051.2</td>
<td>68000</td>
<td>0.88</td>
</tr>
<tr>
<td>3</td>
<td>14.14</td>
<td>3</td>
<td>10</td>
<td>0.88</td>
</tr>
<tr>
<td>4</td>
<td>14.14</td>
<td>2012</td>
<td>120</td>
<td>0.85</td>
</tr>
<tr>
<td>5</td>
<td>14.14</td>
<td>6998.4</td>
<td>580</td>
<td>0.82</td>
</tr>
<tr>
<td>6</td>
<td>14.14</td>
<td>0.6</td>
<td>8.8</td>
<td>0.85</td>
</tr>
<tr>
<td>7</td>
<td>14.14</td>
<td>4780.8</td>
<td>340</td>
<td>0.85</td>
</tr>
<tr>
<td>8</td>
<td>14.14</td>
<td>1431.6</td>
<td>61</td>
<td>0.82</td>
</tr>
<tr>
<td>9</td>
<td>14.14</td>
<td>2330.4</td>
<td>210</td>
<td>0.91</td>
</tr>
<tr>
<td>10</td>
<td>14.14</td>
<td>4502.4</td>
<td>210</td>
<td>0.88</td>
</tr>
<tr>
<td>11</td>
<td>14.14</td>
<td>4281.6</td>
<td>250</td>
<td>0.83</td>
</tr>
<tr>
<td>12</td>
<td>14.14</td>
<td>480.6</td>
<td>29</td>
<td>0.85</td>
</tr>
<tr>
<td>13</td>
<td>14.15</td>
<td>1088.8</td>
<td>66</td>
<td>0.85</td>
</tr>
<tr>
<td>14</td>
<td>14.15</td>
<td>445.6</td>
<td>28</td>
<td>0.85</td>
</tr>
<tr>
<td>15</td>
<td>14.15</td>
<td>1172</td>
<td>52</td>
<td>0.88</td>
</tr>
<tr>
<td>16</td>
<td>14.15</td>
<td>137.6</td>
<td>17</td>
<td>0.93</td>
</tr>
<tr>
<td>17</td>
<td>14.15</td>
<td>311.8</td>
<td>18</td>
<td>0.88</td>
</tr>
<tr>
<td>18</td>
<td>14.15</td>
<td>71.2</td>
<td>13</td>
<td>0.88</td>
</tr>
<tr>
<td>19</td>
<td>14.15</td>
<td>305.6</td>
<td>26</td>
<td>0.82</td>
</tr>
<tr>
<td>20</td>
<td>14.15</td>
<td>357.8</td>
<td>27</td>
<td>0.88</td>
</tr>
</tbody>
</table>
3.4.3 NON-LINEAR BEHAVIOR OF THIN STRIPS

A loading-unloading sequence is performed twice on the test specimen to check for plastic behavior of the material. For a thin strip specimen with no cutout patterns, the sample is loaded up to about 1.6 N which corresponds to a 13.5 mm cross-head displacement. Then the sample is unloaded until the rollers lose contact with the sample. This sequence is performed again without any change in the setup. A similar procedure is repeated for thin strip specimen with small circular cutout pattern. This sample is loaded up to approximately 1.3 N. The limits set upon loading or cross head displacement depends on the stiffness of the specimen. Since the patterned sample is considerably weaker than the sample with no cutouts, a lower load is applied on the specimen.

Figure 3.14 and Figure 3.15 represent the stress vs. strain plots for two different types of samples. The following observations can be made from the plots:

- The difference in the loading and unloading curves during a particular run occurs when the sample is loaded into the plastic range [13].
- The area between the loading and unloading curve gives the amount of energy dissipated in the sample. Comparing the two figures, the energy released by the specimen with no cutout pattern is higher since it is stiffer.
- There seems to be some non-linear behavior when the strain exceeds 0.06% in Figure 3.15.
- Since the specimen is loaded cyclically, it exhibits some characteristics of hysteresis. In Figure 3.14, during the second run, when the sample is unloaded, the load reaches 0 N though the crosshead does not get back to its original
position. A similar trend is observed in Figure 3.15 also. There is a small amount of residual strain. Apart from loading the sample up to its plastic range, this non-linear behavior in the sample could also be due to roller slippage, actuator losses, etc.
Figure 3.14: Plot of stress vs. strain (loading-unloading sequence performed twice) for sample with small circular cutout patterns

Figure 3.15: Plot of stress vs. strain (loading-unloading sequence performed twice) for sample with no cutout patterns
3.5 CONCLUSION

The work done at the small-scale examined the repeating nature of the cutout patterns found in the active membrane, and this eliminates the need to consider the cutout geometry while developing large-scale models. To get bulk material properties, the resonance technique was used and the stiffness of the material over a range of temperatures is obtained. These experimental results were further validated by four point bend experiments and comparing the results, there is a deviation of only about 1% which is a very good measure. Different types of cutout geometry, quantified by %AA were studied by modeling repeating unit cells and a normalized %E_{eq} for a given %AA and thickness is obtained. This helps in developing material models even if the electrolyte material is changed or high temperature studies are done, since the material is linearly elastic. Failure and non-linear behavior of the thin strip specimens were also studied. The material is highly elastic, but when the failure stress is reached, breakage occurs instantaneously.
CHAPTER 4

OPTIMIZATION OF LARGE AREA FLEXCELLS

4.1 INTRODUCTION

The aim of performing this modeling effort is to determine the most optimal design which is mechanically robust and does not compromise electrochemical efficiency. Simulations were performed to better understand how, under fixed loading conditions, changes to key geometric properties altered the maximum principal stress and maximum displacements. The results obtained for improving the mechanical robustness of the large area FlexCell will be used as a basis for refining the design of the ultra-large area FlexCell.

4.2 SELECTION OF ELEMENT TYPE IN ANSYS

The finite element analysis was done using ANSYS™ finite element software. As there is a significant mismatch between the in-plane and out-of-plane dimensions of the FlexCell, a prohibitively large number of elements would be required if 3D solid elements were used to model the entire membrane. The 3D solid elements were used for the small-scale unit cell model, which provided equivalent stiffnesses for different honeycomb mesh patterns. Having appropriate representative materials properties and
since plane stress conditions ($\sigma_z = \tau_{yz} = \tau_{xz} = 0$) can be assumed for a thin membrane, shell elements were used for modeling the whole *FlexCell* membrane.

### 4.2.1 COMPARATIVE STUDY BETWEEN SHELL AND SOLID ELEMENTS

A comparative study has been done to validate the use of shell elements over solid elements. Simple cantilever beams with load acting on their free ends were modeled in ANSYS using 3D solid brick elements (SOLID185) and quadrilateral shell elements (SHELL181) taken from the ANSYS program library [14]. SHELL181 is a 4-noded element with six degrees of freedom (translations and rotations in the x, y, and z-directions), and is suited for non-linear applications. It also works well for distributed pressure simulations. It was found that the results of the solid and shell element models were comparable with each other and also to beam theory. Also, simulation results for both shell and solid element models with spatially varying material properties and with varying thicknesses were comparable. Hence, it was decided that quadrilateral shell were appropriate for modeling entire *FlexCell* membrane.

### 4.3 FLEXCELL SIMULATIONS

#### 4.3.1 DEVELOPING THE FINITE ELEMENT MODEL

Figure 4.1 and Figure 4.2 show the CAD drawing of the *FlexCell* and the corresponding finite element model developed in ANSYS using shell elements. The honeycomb-type pattern in the *FlexCell* is made up a combination of bigger hexagonal (width=4.57 mm, spacing= 1.43 mm) cutouts in the middle and smaller hexagonal cutouts (width= 3.79 mm, spacing= 2.21 mm). The hexagonal geometry is shown in Figure 4.3. The bigger cutouts are arranged in the form of a bigger hexagon which is
surrounded by the smaller cutouts. Also, it has already been presented in Section 3.4.2 that though the bigger hexagonal cutouts have a higher %AA, they are weaker. Hence the smaller hexagonal cutouts are made in the active membrane to provide better support. This active membrane is supported by vertical and horizontal cross ribs and a frame around the edges of the membrane. To develop material models for this finite element analysis, equivalent properties obtained from the small-scale model are used. The different colors in the FEA model in Figure 4.2 show the different regions where the elements are assigned different material properties and thickness. The element edge length is set as 0.5 and the total number of elements is around 155000.

Figure 4.1: CAD drawing of a large area FlexCell
Figure 4.2: Model of FlexCell developed in ANSYS showing the areas with different material properties

Figure 4.3: Representation of big and small hexagonal cutout pattern (dimensions are in mm)
For ease of discussion, the different models are identified by the width of their horizontal and vertical support ribs. For example, the standard model is a 13.5-13.5 model, which means that the width of both the horizontal and vertical cross ribs is 13.5 mm. A 5-10 model has a 5 mm wide horizontal cross rib and 10 mm wide vertical cross rib. The support rib configurations considered here are 0-0, 5-10, 10-10, 13.5-13.5, 10-20.

4.3.2 DEFINING LOADING AND BOUNDARY CONDITIONS

Appropriate mechanical boundary conditions for an operating fuel cell are difficult to define. Since the FlexCell is arranged one above the other in a stack, it was decided to apply normal pressure with all of or part of the frame being clamped. A normal pressure of 1 kPa was applied on the FlexCell. While this is not a perfect representation of the actual loading of a FlexCell, it is assumed to be appropriate to study the principal stresses and out-of-plane displacement for the different membrane geometries under this type of pressure loading.

Figure 4.4 shows one type of pressure loading that is analyzed. The entire frame area is clamped with all six degrees of freedom are arrested), and a normal pressure of 1 kPa is applied to the active area and cross ribs. The red lines in the figure indicate that pressure acts on those regions. Figure 4.5 shows the second type of pressure loading under study where normal pressure is applied on a 5mm overlap section of the frame area in addition to the conditions described earlier.
Figure 4.4: ANSYS plot of the 13.5-13.5 FlexCell with pressure applied normally on the active areas and cross ribs and with the entire frame clamped.
4.3.3 RESULTS AND DISCUSSION

The main objective of this phase of the present work is to understand which geometric parameters reduce the principal stresses and out-of-plane deflection. Figure 4.6 shows stress contour plots of the deflected *FlexCell* membrane for a standard, 13.5-13.5 cross-rib configuration whose loading and boundary conditions are depicted in Figure 4.4. The areas of stress concentration are near the region of clamping where the cross-rib meets with the outer frame. Hence we need to analyze how this stress can be reduced. In parallel, we also look at out-of-plane deflection and how it can be reduced. The main studies involve five different cross-rib configurations, two different clamping conditions, two different support rib thicknesses, and three different cutout geometry arrangements.
4.3.3.1 Cross-rib configurations

Figure 4.7 and Figure 4.8 show the trend of the 1st principal stress ($S_1$) and out-of-plane displacement ($u_z$) against different cross-rib configurations of *FlexCell* membranes experiencing normal pressure on the active and cross rib areas and entire frame is clamped (Figure 4.4). Table 4.1 gives the percentage of area occupied by the active membrane and cross-ribs. The percent membrane area is an indirect metric used for %AA since this is the area available for cutouts. The 0-0 model has the highest available membrane area. The 13.5-13.5 and 10-20 models have almost the same amount of membrane area.
Table 4.1: Values of percent membrane area for varying cross-rib configuration

<table>
<thead>
<tr>
<th>Model</th>
<th>% Membrane Area</th>
<th>% Cross-rib area</th>
</tr>
</thead>
<tbody>
<tr>
<td>0-0</td>
<td>73.4</td>
<td>0</td>
</tr>
<tr>
<td>5-10</td>
<td>67.7</td>
<td>5.7</td>
</tr>
<tr>
<td>10-10</td>
<td>65.4</td>
<td>7.9</td>
</tr>
<tr>
<td>13.5-13.5</td>
<td>62.8</td>
<td>10.6</td>
</tr>
<tr>
<td>10-20</td>
<td>62.5</td>
<td>10.9</td>
</tr>
</tbody>
</table>

Figure 4.7: Plot of 1st principal stress (MPa) for FlexCell models having different cross rib configurations experiencing normal pressure on the active and cross rib areas
Though it seems that the stress experienced by the model with no cross-ribs (0-0) is very low and hence questions the need for cross rib support, it is seen that the membrane experiences significant deflection. As the rib area is increased, the stress and deflection reduce. As expected and as shown, the cross ribs impact the out-of-plane displacement to a significant level. Also, since stress concentration occurs near the vertical cross-rib – frame interface, the width of this rib plays a crucial role. Comparing the standard 13.5-13.5 model with the 10-20 model, there is a decrease in $S_1$ and $u_2$. Thus the width of the shorter vertical rib is more critical in reducing the stresses and deflection than the width of the horizontal rib which is longer in comparison. The width to which it can be increased depends on how much the area of the active membrane can be compromised for mechanical robustness. For the models considered here, a FlexCell
membrane with a 10 mm horizontal support rib and 20 mm vertical support rib serves the purpose.

4.3.3.2 Frame area clamping

When reducing the amount of the frame being clamped, the total normal force acting on the FlexCell area is slightly higher than the previous case of loading and hence an increase in both the stress and deflection values as compared to the results presented in Section 4.3.3.1 but the trend exhibited in Figure 4.10 and Figure 4.9 are almost the same. While the results for the 0-0 model in both the loading cases do not vary much with only an increase in maximum $S_1$ of about 2%, for the other configurations, it is much higher. The results further emphasize the importance of a wider vertical rib compared to the horizontal rib.
Figure 4.9: Plot of out-of-plane displacement for *FlexCell* models having different cross rib configurations experiencing pressure normally on the active area, cross ribs and 5mm overlap section of the frame area.

Figure 4.10: Plot of 1st principal stress for *FlexCell* models having different cross rib configurations experiencing pressure normally on the active area, cross ribs and 5mm overlap section of the frame area.
4.3.3.3 Thickness of support ribs

The FlexCell’s frame is manufactured to a thickness of 275 microns. In the active membrane, the thickness of the support mesh is 195 microns and patterns are cut into it. Now, the thickness of the cross rib has to be standardized so that there is mechanical robustness, cost efficiency, and ease of manufacturing. The loading conditions are those prescribed in the previous section and a FlexCell model having the standard combination of big and small hexagonal patterns is analyzed. A set of simulations are conducted to compare the effect of thickness and the results corresponding to the more significant cross-rib configurations are presented in Figure 4.11 and Figure 4.12.

![Figure 4.11: Plot of 1st principal stress vs. thickness for varying support rib configurations](image-url)
As expected, the maximum principal stress and out-of-plane displacement are much lower when the thickness of the support ribs is 275 microns. For the 10-20 cross-rib configuration, the 1st principal stress and displacement reduced by 14.1% and 29% respectively, when the thickness is increased from 195 to 275 microns. There is clearly a significant loss in mechanical robustness associated with cross rib thickness reduction. Without experimental evidence, it is not known how thin the cross ribs can be made. Thinner cross ribs might save material cost and possibly simplify sealing and/or connections between electrodes, electrolytes, and/or interconnects, but from a mechanical strength perspective, it is better to opt for a design where the thickness of both the frame and the cross ribs are the same.

Figure 4.12: Plot of out-of-plane displacement vs. thickness for varying support rib configurations
4.3.3.4 Arrangement of cutout geometries

In Figure 4.7 and Figure 4.8, for cross-rib configurations other than 0-0, the trend between the cutout distributions is the same. For the 0-0 FlexCell configuration, the design with a mixture of big and small hexagonal cutout patterns has a higher stress value than the design with only big hexagonal cutouts though the active membrane is at a higher stiffness. This is because when the support ribs are removed, the model is designed in such a way that the four regions with big hexagonal cutout pattern are joined together. It is difficult to design a model which could be compared on par with the models having cross ribs. Since the membrane with big hexagonal cutouts is less stiff, load is transferred to the cross ribs, and therefore stresses at the cross rib – frame intersection are higher. The FlexCell with small hexagonal cutouts have the lowest stress concentrations at the cross rib – frame intersection. But, the %AA of the smaller hexagonal pattern is lesser by 18% compared to the bigger pattern which reduces the electrochemical efficiency of the FlexCell to a great extent. Hence, the strategic arrangement of the cutout patterns is very important.

A study almost identical to what was presented was done with circular cutout geometries instead of hexagons in the active membrane of the FlexCell and the results are marginally better for circular patterns. This is to be expected since the equivalent stiffness is slightly higher. At the same time, the %AA goes down. The main benefits to changing cut out patterns would most likely appear as stress reductions at the small scale. The large scale analysis uses equivalent stiffness, and therefore the cut-out geometries are studied in the context of equivalent stiffness.
4.4 CHANGING THE DESIGN OF THE FLEXCELL

The results described in Section 4.3.3 bring to light the key variables which affect mechanical robustness and electrochemical efficiency. The width of the shorter, vertical rib is more critical than that of the longer, horizontal rib since it greatly reduces stress concentrations. Since out-of-plane displacement and stress scale linearly with cross-rib thickness, the thicker the better. Also, the electrochemical efficiency has an inverse relationship with stiffness and so to design a FlexCell which is both mechanically robust and electrochemically effective, the arrangement of the cutout patterns is crucial. These key factors are useful in redesigning the large area FlexCell to improve the mechanical robustness of the same.

Based on the suggestions, the design of the large area FlexCell is changed accordingly and the corresponding CAD drawing is shown in Figure 4.13. The FlexCell has been redesigned in such a way to increase the size of the active membrane, thereby enhancing its electrochemical efficiency. A few comparisons can be made to the older design:

- The overall size and shape of the electrolytic membrane remains the same. The percentage of area occupied by the active membrane has been increased from 61.7% to 67.4%. This is done by reducing the width of the frame to 12.8 mm along its length and to 12 mm along the width
- The width of the shorter vertical rib is greater than the horizontal rib. The width of the cross ribs has been reduced, the vertical cross rib’s width being 7.7 mm and the horizontal rib’s width is 6.4 mm
- The thickness of the cross ribs is increased to 275 microns.
- The arrangement of the differently sized hexagonal cutout geometries is changed in such a way that the smaller hexagonal cutouts are fewer in number and placed around the periphery of the four individual active membranes so that there is a smoother transition and reduction in stress concentration.

The changes that have been made have struck a balance between the design suggestions put forth in the previous section and the need to increase the % AA for increased efficiency. This design is further analyzed to see how the its mechanical robustness can be further increased without affecting the membrane area.

Figure 4.13: CAD drawing of modified large area *FlexCell*
4.5 ANALYSIS ON REDESIGNED LARGE AREA FLEXCELL MODEL

4.5.1 DEVELOPING THE ANSYS MODEL

A finite element model similar to what was developed in Section 4.3.1 is recreated with the following changes:

- The material models developed for this set of finite element simulation use actual material properties instead of the equivalent properties
- There is less number of small hexagonal cutouts. Hence, altering the fillet radii of individual active membranes reflects on number of smaller cutouts.

The boundary conditions for the redesigned large area FlexCell were altered to more realistically simulate clamping and sealing conditions in a NexTech SOFC stack. In planar SOFCs, seals are placed along the circumference of each cell to prevent mixing of gases during operation [15,16]. Hence, the electrolytic membrane is clamped along its edges 5mm from the outside (Figure 4.14) instead of clamping the entire frame region as discussed earlier. For the initial structural studies, the loading remained a 1 kPa loading on the membrane area, cross ribs, and unclamped portion of the frame area. As will be discussed in Sec. 4.6.2, for analyzing the performance of the cell under thermal load, temperature gradients are set up.
4.5.2 DESIGN PARAMETERS UNDER STUDY

As has been discussed, the %AA must remain at high levels to produce cells with adequate electrochemical efficiency. NexTech’s revised FlexCell design had a %AA of 67.4%. With the need to maintain this %AA or increase it, we proceed to analyze what parameters that could be varied to make the membrane mechanically more robust. The following parameters are studied:

- Frame width
- Cross rib width
- Fillet radius of individual active membrane areas

These parameters are varied systematically to see how the stresses and deflection are reduced.
4.6 RESULTS AND DISCUSSION

4.6.1 STRUCTURAL ANALYSIS

4.6.1.1 Frame width and cross ribs

The width of the frame is 15.6 mm along the length of the FlexCell and 17.4 mm along the width. The width of the FlexCell frame is varied to see how it affects the stress and displacement. The size of the active membrane is not changed but is spatially moved horizontally, vertically or diagonally. An illustration for moving the active membrane horizontally is shown in Figure 4.15 (a) where the arrows show the direction of movement and in (b) it is seen that this movement leads to an increase in vertical rib width and decrease in frame width along the FlexCell’s width. So, a reduction in frame width leads to an increase in the width of both the horizontal and vertical cross ribs.

Figure 4.15: (a) ANSYS Model of revised standard FlexCell depicting the direction in which active membrane is moved (b) ANSYS model depicting the change in geometry
The results are tabulated in Table 4.2. Compared to the work done previously, the %AA is maintained constant and the membrane area is moved around spatially to see how the design affects the mechanical robustness. When the frame width is reduced along the width and hence an increase in the width of the vertical cross rib, the stress decreases. This result again concurs with the simulations done with the old design of the large area FlexCell. But decreasing the frame width along the length of the cell increases the stress. The maximum stresses occur in the region where the vertical cross rib is joined to the outer frame (Figure 4.16). Hence the support frame needs to be wide enough to prevent high stresses and reduce deflection. When the frame width is decreased on all sides (the active membrane areas are moved diagonally), both the stresses and out-of-plane deflection are reduced.

Table 4.2: Values of 1st principal stress and displacement for reduction in frame width

<table>
<thead>
<tr>
<th>Standard Model</th>
<th>Reduction in frame width along</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Width (mm)</td>
</tr>
<tr>
<td>S1 (MPa)</td>
<td>221.06</td>
</tr>
<tr>
<td>u2 (mm)</td>
<td>8.95</td>
</tr>
</tbody>
</table>
Figure 4.16: Contour plot representing the distribution of 1st principal stress of redesigned large area FlexCell
4.6.1.2 Fillet radius

One way of reducing the stress concentrations near the region where the vertical cross rib is attached to the frame is by increasing the membrane area fillet radii close to the vertical ribs. In other words, the arrangement of the small hexagonal cutouts is altered so that the cross-ribs have a smoother transition and additional mechanical support. The fillet radius is varied from 5 to 10 mm and the results are plotted in Figure 4.17. For a fillet radius of 7.5 mm, the stress is at a minimum value of 206.7 MPa, and then gradually increases. This is because the stress concentrations shift from the filleted corners to the region where the *FlexCell* is clamped, and hence this increase becomes unrealistic. So, the optimum radius of 10 mm is chosen. For such an alteration, the displacement improves by only 0.57% and hence is not discussed.

Figure 4.17: Plot of 1st principal stress (MPa) vs. fillet radius near vertical cross rib (mm)
4.6.2 THERMAL ANALYSIS

SOFCs operate at temperatures on the order of 850 °C and reactants flow across membranes causing significant thermal gradients from the initial reactant gas temperatures and from the exothermic reactions that occur. The mechanical performance is influenced by thermal gradients because ceramics typically have low thermal conductivity which leads to very high stresses and ultimately, to failure.

Figure 4.18 summarizes the different thermal states of an SOFC. It is separated into three major phases, namely the startup, operation, and shut down. During the startup stage, a cell that is at ambient temperature (25 °C) is heated up to 850 °C to make the cell ionically active. The cell is then clamped/sealed securely. If components are not bonded to each other, no stresses are developed during this startup phase. During operation, as the two different fuels pass on either side of the non-permeable electrolyte in the same directions (co-flow), a temperature gradient of 200 °C is set up. During the shutdown phase, the clamped fuel cell is cooled from this elevated temperature to ambient temperature. During shutdown, components that are bonded to other components with different thermal expansion coefficients will experience high stresses and most likely fail.

To perform a thermal-mechanical finite element simulation, ANSYS uses coupled field analysis which is a combination of two or more individual types of engineering analyses. The results of one type of analysis are dependent on the other. For coupled thermal-structural analysis (Figure 4.19), the thermal analysis is done first, the results of which are coupled along with the structural analysis conditions and solved. For the thermal analysis, SHELL57, a 4-noded shell element with temperature as its degree of freedom is used. After the thermal gradient is analyzed, the element type is switched to
SHELL181, the 4-noded shell element used in previous simulations. Temperature dependent data such as thermal conductivity and thermal coefficient of expansion are obtained from [17] and [18], respectively.

![Figure 4.18: Thermal cycling in a FlexCell; grayed hash mark indicate clamping](image)

**Figure 4.18:** Thermal cycling in a *FlexCell*; grayed hash mark indicate clamping

![Figure 4.19: Thermal-structural coupled field analysis in ANSYS](image)

**Figure 4.19:** Thermal-structural coupled field analysis in ANSYS
Because of the thermal gradients, the behavior of the *FlexCell* during its operation is of interest. The temperature of the *FlexCell* is raised and clamped during the startup phase. To set the temperature gradient, it is assumed that the fuels are made to flow on either side of the electrolyte in a co-flow manner. The fuels enter one side of the cell at 650 °C and by the time they reach the other end, the reactants are heated up and hence the temperature is raised to 850 °C. Upon solving, contour plots of the temperature gradient and 1st principal stress ($S_1$) are obtained and shown in Figure 4.20 and Figure 4.21, respectively. The displaced structure is also seen and there is more expansion near the hotter end and hence the interior of the *FlexCell* is displaced towards the cooler end. Due to uneven expansion and imposed clamping conditions, stress concentrations are developed around the filleted edges near the cooler end. Table 4.3 tabulates the results that have been obtained from this simulation, and comparing the stress values to the structural analysis done earlier, it is seen that the stress values are almost triple the values from the structural analysis.

<table>
<thead>
<tr>
<th>Description</th>
<th>Values</th>
<th>Units</th>
</tr>
</thead>
<tbody>
<tr>
<td>$S_x$</td>
<td>626.39</td>
<td>MPa</td>
</tr>
<tr>
<td>$S_y$</td>
<td>643.02</td>
<td>MPa</td>
</tr>
<tr>
<td>$S_1$</td>
<td>770.24</td>
<td>MPa</td>
</tr>
<tr>
<td>$U_x$</td>
<td>0.0664</td>
<td>mm</td>
</tr>
<tr>
<td>$U_y$</td>
<td>-0.157 to 0.157</td>
<td>mm</td>
</tr>
</tbody>
</table>
Figure 4.20: Body temperature contour plot (in Kelvin) of large area *FlexCell* having a
temperature gradient from co-flow reactants

Figure 4.21: Principal stress contour plot of large area *FlexCell* having temperature
gradient from co-flow reactants
4.7 CONCLUSION

The main motive of performing these sets of finite element simulations on the large area FlexCell was to identify the parameters which are crucial in enhancing mechanical robustness. Shell elements have been used to model the thin membrane and distributed pressure with clamped edged conditions was imposed on the meshed model. The set of simulations gave valuable information about regions of stress concentration and changes were made to the shorter vertical rib, rib thickness and cutout geometry arrangement. The redesigned FlexCell has both electrochemical efficiency and mechanical strength. On identification of these design factors, the next step is to apply them to the ultra-large area FlexCell so that its design can be refined.
CHAPTER 5

INCORPORATING DESIGN CHANGES IN ULTRA-LARGE AREA FLEXCELLS

5.1 INTRODUCTION

As the FlexCell area is increased, it becomes more susceptible to mechanical damage with respect to manufacturing, stack assembly, and operation. The design needs to be optimized for sufficient mechanical robustness and electrochemical efficiency. It is unlikely that dimensions of the large area FlexCells (400 cm²) can be simply scaled up to ultra-large area FlexCells (700 cm²). In particular, it is expected that multiple support ribs will be needed. The work described in the previous chapters on the large area FlexCells enables us to identify the areas of concern for ultra-large FlexCells. Simulations will be used to investigate key geometric parameters relevant for optimization of ultra-large area FlexCells.

5.2 DESIGN VARIABLES AND FINITE ELEMENT MODEL

Figure 5.1 provides a CAD drawing of NexTech’s standard ultra-large area FlexCell design. The FlexCell consists of 3 vertical and horizontal ribs which result in 16 separated “active membrane areas.” As compared to the smaller area FlexCell, this model
has additional side ribs, thinner frame support, and a larger number of individualized membrane areas.

As per the specifications provided and based on simulations done on the smaller *FlexCell*, the following aspects of the design will be left unchanged:

- Thickness
- % Active Area
- Overall shape

Therefore, the design parameters that could be varied are as follows:

- Horizontal and vertical frame width
- Side rib width
- Fillet radius of active area

Figure 5.1: CAD drawing of an ultra-large area *FlexCell*
Figure 5.2 shows a rendering of the full size FEA model in ANSYS. In this standard design configuration, the number of shell elements used is around 0.25 million. The hatched area in the figure also shows how the FlexCell is clamped from the outside up to 5 mm. A normal pressure of 1 kPa is applied on the unclamped area. In this model, the active membrane area is about 67.8% of the total area of the ultra-large FlexCell. Additional models are constructed by varying the design parameters listed in the previous paragraph.
5.3 RESULTS AND DISCUSSION

The design shown in Figure 5.2 is kept as the basis of comparison for the results discussed in the following sections. Each of the parameters listed in Section 5.2 are varied one at a time and the geometric design is refined by incorporating changes that most improve mechanical robustness.

5.3.1 FRAME WIDTH

As stated earlier, clamping on the FlexCell for the purpose of sealing is done around the circumference of the cell for a width of 5 mm. However, it is required that there is some space for the gas sealant to expand during operation. Hence, it is set that the minimum frame width should be 7 mm. The frame width along the FlexCell’s length is varied from 7 mm to 12 mm in 1 mm increments, and the frame width along its width is varied from 7 mm to 12.81 mm, in 1 mm increments. A comparison is done to see how the FlexCell behaves for changing only the frame width length-wise, width-wise, or both. To keep active membrane area the same, reducing the frame width implies an increase in the cross rib width.

Figure 5.3 gives a plot of the 1st principal stress versus frame width. As can be seen, reducing the frame width along the breadth decreases the stresses considerably which can be better explained from the contour plot shown in Figure 5.5. Because of the loading imposed on the FlexCell, there is a larger stress concentration at the region where the vertical cross rib joins with the frame. Hence, the shorter vertical cross rib should be able to reduce this concentration and strengthen the FlexCell. Figure 5.3 also shows that reducing the frame width along its length increases the stress by more than 100 MPa. This is because there needs to be a wider frame region to minimize the stress.
concentration at the place where the central vertical cross rib connects with the outer frame.

The results presented in Figure 5.4 are a comparison of the out of plane displacement and for varying frame width. Reducing the frame width along the length produces an effect contrary to what is desired. Additional frame support is needed along the length of the cell. However, by reducing the width of the vertical frame from 12.81 mm to 7 mm, the displacement comes down to 21.63 mm. This is the result of increasing vertical rib widths. Reducing the width of the frame along both its length and breadth also reduces the displacement, but the main factor contributing to reduced displacement is the increase in the width of the central, vertical cross-rib. It is to be noted that in all the above cases, the % Active area has been maintained constant. In conclusion, it is decided to reduce the frame width along the breadth of the FlexCell for improved mechanical performance.
Figure 5.3: Plot of 1st principal stress (MPa) vs. Frame width (mm) for varying arrangements.

Figure 5.4: Plot of out-of-plane displacement (mm) vs. Frame width (mm) for varying arrangements.
5.3.2 FILLET RADIUS

As shown in Figure 5.5, there are high stresses around the sharp corners created by the individual active membrane areas of the *FlexCell*. Hence, simulations are performed to see how the fillet radius changes the stresses. There are two factors that come into play. It is important that the % AA is not drastically altered. To simplify the process, only the most critical fillets are changed. The most critical fillets are the ones closer to the central vertical cross rib.

Figure 5.5: Contour plot depicting 1st principal stress experienced by the large area *FlexCell* for vertical central rib width= 17.61 mm, vertical frame width=8 mm
Figure 5.6 shows how both the stress and out-of-plane displacement reduce when the radii of the four filleted corners closer to the central vertical cross rib are increased. However, for a fillet radius greater than 15 mm, there is a slight increase in the 1st principal stress although the displacement shows a decreasing trend. This behavior can be better explained by the user defined contour plots of a quarter symmetry model in Figure 5.7 whose contour range is from 250-410 MPa. For radii of 5 or 15 mm, the stress concentration is at the filleted corner, whereas for radii of 20 mm, the stress concentration moves towards the frame due to the clamping imposed on the FlexCell. Since the main motivation is to reduce the stress concentration around the filleted corner, the increase in stress values can be ignored because it is due to the assumed boundary conditions. Hence, the fillet radius is set at 20 mm and a model incorporating this change is shown in Figure 5.8.

Figure 5.6: Plot of principal stress (MPa), out-of-plane displacement (mm) vs. fillet radius (mm)
Figure 5.7: Contour plot depicting the 1st principal stress over the range 250-410 MPa for quarter models where fillet radius is (a) 5 mm, (b) 15 mm, (c) 20 mm

Figure 5.8: Large area FlexCell model with fillet radius=15 mm near the central vertical cross rib.
5.3.3 SIDE RIBS

The third parameter that could be varied without changing the %AA is the width of the non-central rib (side rib). Figure 5.9 shows the trend for principal stress and out-of-plane displacement for the standard model where the frame width along the width of the FlexCell is not reduced. By maintaining that frame width constant and reducing the width of the side rib, the width of the central vertical rib is increased. The plot shows that by decreasing the width by 3.5 mm from the standard 8 mm, the stress and displacement are reduced by 4% and 3.4% respectively. This seems to indicate that reducing the width of the vertical side rib and thereby increasing the width of the vertical central rib is advantageous.

As seen in Figure 5.10, results are plotted for the vertical side rib width starting from 4.5 mm up to 11 mm, at which point the width of all the vertical ribs are about the same (vertical central rib width=11.59 mm, vertical side rib width=11 mm). By varying the side rib width from 4.5 to 11 mm, the out of plane displacement is decreased by 5.8%. However, the 1st principal stress is at a maximum on either ends of the range, but reaches a minimum when the width is maintained at approximately 7 mm. A similar procedure is repeated for determining the width of the horizontal side ribs also. Hence, to obtain an optimal result, the side rib width is reduced by only 1 mm as compared to standard design.
Figure 5.9: Plot of principal stress (MPa), out-of-plane displacement (mm) vs. width of vertical side rib for a constant frame width=12.81 mm

Figure 5.10: Plot of principal stress (MPa), out-of-plane displacement (mm) vs. width of vertical side rib for vertical frame width=8 mm
5.3.4 COMBINING THE CHANGES

Table 5.1: Comparison between principal stress and out-of-plane displacement for models having progressive design changes

<table>
<thead>
<tr>
<th>Standard design</th>
<th>+Reduced vertical frame width (=8 mm)</th>
<th>+ Increased fillet radius along central vertical rib (=20 mm)</th>
<th>+ Increased fillet radius along central horizontal rib (=10 mm)</th>
<th>+ Reduced side rib width Vertical (=7 mm)</th>
<th>+ Reduced side rib width Horizontal (=5 mm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>$S_1$</td>
<td>409.33</td>
<td>372.742</td>
<td>372.74</td>
<td>374.98</td>
<td>375.06</td>
</tr>
</tbody>
</table>

The next step is to incorporate the changes made to the individual parameters into the FlexCell. The results are presented as a comparison between the standard design and progressively refined designs for out-of-plane displacement and 1$^{\text{st}}$ principal stress in Table 5.1. Changes in central and side rib widths, frame widths, and fillet radii are done step by step and tabulated. As was presented in Section 5.5.1, reducing the width of the frame along the length has adverse effects as compared to reducing the width along the FlexCell’s width. Small changes are made to the fillet radii along both the ribs and also the width of the horizontal side rib is reduced by 1 mm to enhance support.

Hence, the final model has a reduced frame width of 8 mm along its width, 4 individual active membrane areas along the central vertical rib having a fillet radius of 20 mm on one corner, 4 individual membrane areas along the central horizontal rib having a fillet radius equaling 10 mm at the corner where there are high stresses, vertical central rib width equals 19.6 mm, and the horizontal and vertical side ribs are reduced by 1 mm.
each respectively. An ANSYS plot of the modified *FlexCell* design is shown in Figure 5.11. This rendering was used to develop a CAD drawing.

Figure 5.11: An ANSYS rendering of the modified *FlexCell* design
5.3.5 EFFECTS DUE TO TEMPERATURE

The thermal cycle experienced by a *FlexCell* has been presented in Section 4.4 and illustrated again in Figure 5.12. In a similar fashion to what was done for the large area *FlexCell* FEA model, a set of simulations was established to examine the behavior of this ultra-large area *FlexCell*. For the operating cycle, a temperature gradient of 200 °C is set up to simulate co-flow of reactants on either side of the electrolytic membrane at an elevated temperature of 850 °C. The frame region is clamped along the outer 5 mm of the frame.

Figure 5.13 shows the temperature gradient (in degree Kelvin) in a deformed model that is formed during the operating cycle for the standard ultra-large area *FlexCell* design. As expected, there is more expansion at the hotter end of the *FlexCell* and because of this, the whole membrane is displaced towards the cooler end. Hence there is displacement in both the x- and y- directions. Since there is uneven expansion, the membrane also experiences shear stresses ($\tau_{xy}$).

![Figure 5.12: Thermal cycle of a *FlexCell*](image-url)
The results presented in Table 5.2 are for a set of simulations done on the ultra-large area *FlexCell* having a thermal gradient. The geometric parameters for the different models correspond with those in Table 5.1 (structural loading). From the table, it can be seen that while reducing the frame width and removing areas of stress concentration by increasing fillet radii along the ribs is also effective for thermal loading. Reducing the width of the peripheral rib leads to slightly increased stresses and displacements. This increase in stresses and displacements may be attributed to the fact that there is now in plane displacement and hence cross rib support should be more evenly distributed across the cell. For a *FlexCell* model whose frame width along the width is reduced to 8 mm, and the fillet radii along the central vertical and horizontal cross ribs are increased to 20

Figure 5.13: Contour plot of the temperature gradient formed in the *FlexCell* model
mm and 10 mm respectively, the y-displacement is reduced by 3.86%, 1st principal stress is reduced by 2.74% and the shear stress ($\tau_{xy}$) is decreased by 9.72%.

Table 5.2: Comparison between principal, shear stress and in-plane displacement for thermal models having various progressive design changes

<table>
<thead>
<tr>
<th></th>
<th>Standard design</th>
<th>+Reduced vertical frame width (=8 mm)</th>
<th>+ Increased fillet radius along central vertical rib (=20 mm)</th>
<th>+ Reduced peripheral rib width Horizontal rib (=10 mm)</th>
<th>+ Reduced peripheral rib width Vertical rib (=7 mm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>$U_y$</td>
<td>0.0114</td>
<td>0.01104</td>
<td>0.01097</td>
<td>0.01096</td>
<td>0.01106</td>
</tr>
<tr>
<td>$S_1$</td>
<td>700.44</td>
<td>691.63</td>
<td>692.15</td>
<td>681.22</td>
<td>692.23</td>
</tr>
<tr>
<td>$\tau_{xy}$</td>
<td>225.86</td>
<td>204.32</td>
<td>199.4</td>
<td>203.9</td>
<td>200.9</td>
</tr>
</tbody>
</table>

For the modified design just described, Figure 5.14 and Figure 5.15 show the 1st principal stress ($S_1$) and XY-shear stress ($\tau_{xy}$) contour plots, respectively. As can be seen in Figure 5.14 the principal stress increases as we move from left to right, but there are regions of stress concentration around the filleted region. A similar observation is made in the XY-shear stress contour plot also. These stress concentrations exist because thermal strains are highest in these areas.
Figure 5.14 Contour plot of 1st principal stress formed in *FlexCell* model

Figure 5.15: Contour plot of the shear stress along xy plane ($\tau_{xy}$) formed in the *FlexCell* model
To eliminate the stress concentrations near the edges under thermal loading, the fillet radii of the active area regions near the corners of the *FlexCell* are increased. The plot in Figure 5.16 shows how, as the fillet radius is increased, there is a decrease in both the 1st principal stress and XY-shear stress. The shear stress dips more when the fillet radius is increased to about 8 mm and then almost reaches a steady value of 178 MPa. Whereas the 1st principal stress value decreases almost linearly for up to 15 mm radius, and beyond radius=16 mm, the change is very gradual. Comparing Figure 5.14 and Figure 5.17, we can see that the areas of stress concentration around the corners have been eliminated. Hence, this change is also incorporated into the design. By doing so, the 1st principal stress and out of plane displacement are reduced by 11.6% and 10.52%, respectively.

![Figure 5.16: Plot of 1st Principal stress (MPa), XY-shear stress (MPa) for varying fillet radii (mm)](image-url)
Figure 5.17: Contour plot of the 1st principal stress formed in the *FlexCell* model where the fillets around the corners are widened
5.4 CONCLUSION

Design variables that were identified by optimizing the large area *FlexCell* were used to refine the ultra-large area *FlexCell*. The finite element model was simulated for both structural and thermal loading by varying these parameters one by one, and specific values have been obtained for the central and side rib widths, vertical frame width and fillet radii of individual membrane areas. Combining all the changes suggested in Section 5.5, the modified 700 cm² *FlexCell* membrane is presented in Figure 5.18. Using this model, a CAD drawing is also generated. Compared to the standard model, the area occupied by the active membrane is reduced only by 1.24%. The maximum 1st principal stress and out-of-plane displacement have been reduced by 11.6% and 10.5%, respectively. Hence the goal of maintaining an almost constant %AA has been achieved so that electrochemical efficiency is not affected, while at the same time, mechanical robustness for both structural and thermal loads is improved.
Figure 5.18: An ANSYS rendering of the modified *FlexCell* design
CHAPTER 6

SUMMARY AND FUTURE WORK

6.1 CONCLUSION

To optimize the NexTech Materials Ltd FlexCell™, an electrolyte used for electrolyte supported solid oxide fuel cells, a two scale approach has been followed. Defining an optimal geometry for an ultra-large area FlexCell involves identification of design parameters which will help in strengthening the FlexCell and methodically analyzing the parameters such that the active membrane is adequately supported as the overall size is increased. Because of the computational difficulty involved in modeling a membrane whose in-plane and out-of-plane dimensions vary by a ratio of almost 1000:1, a two-scale approach is employed for modeling FlexCell electrolytes.

At the small scale, material models have been developed by performing finite element simulations on a representative unit cell. The equivalent material model that is developed has a reduced stiffness which changes according to the thickness and %AA. The representative unit cell uses bulk materials properties which were measured with an ASTM resonance technique at temperatures up to 800 °C. At the large scale, entire membranes are simulated with shell elements having the appropriate representative
stiffnesses for the different regions of the membrane. Experiments with *FlexCell* strips in a four point bend test setup validated the equivalent stiffness models and the large-scale shell element models.

A set of finite element simulations on the large area *FlexCell* have been presented. The results of these simulations help identify the design factors crucial for optimization. The important design factors considered are the inclusion of additional cross rib support, frame geometry and distribution of cutout patterns. The boundary conditions for these first simulations involved a clamped frame and uniform pressure on the cell. From the initial simulations on the large area *FlexCell*, the importance of the shorter vertical rib and that out-of-plane displacement scales linearly with cross rib thickness becomes evident. The strategic arrangement of cutout patterns is also important primarily because of the need to maintain high active area. Though stresses and deflection reduce for a *FlexCell* design with a 10 mm horizontal rib and 20 mm vertical rib composed of smaller hexagonal cutouts, when compared to a design with all bigger hexagonal cutouts, the %AA of the whole membrane decreases from 35.6% to 24.41%. Optimization of the mechanical robustness of *FlexCell* membranes is primarily a tradeoff between the %AA and mechanical strength.

In the new large area *FlexCell* design, the area occupied by the active membrane of the *FlexCell* has been increased from 61.66% to 67.41%, thereby increasing its electrochemical efficiency. This %AA is kept constant and minor changes to the cross-ribs and frame are studied. Also, a study of the effects of thermal gradients on the *FlexCell* while it is operating at high temperatures has been presented.
Designing 700 cm² ultra-large area *FlexCells* is not merely a case of scaling up from the large area model discussed above. The ultra-large area cells are more susceptible to mechanical damage and so the number of support ribs has been increased from 2 to 6. With the goal of maintaining constant %AA, a systematic study of the following dimensional changes is made: central and side cross ribs, vertical frame width, and fillet radii of individual membrane areas. Figure 6.1 represents a CAD drawing of the optimized ultra-large area *FlexCell*. A slight decrease in %AA is due to increasing the fillet radii. For this decrease in membrane area of only 1.24%, the stresses and out-of-plane deflection are decreased by 8.37% and 9.04%, respectively.

Coupled thermal structural analysis has also been done to improve the *FlexCell’s* design when a thermal gradient develops across its length. By using the improved cell design, the areas of stress concentration due to thermal loads have been identified and addressed. Compared to the standard design under thermal gradient loading, the refined geometrical design of the ultra-large area *FlexCell* reduces the 1st principal stress and out-of-plane displacement by 11.6% and 10.52%, respectively.

As NexTech proceeds in its current path of scaling up the size of the electrolyte-supported planar SOFCs to 700cm² and larger, this research will help in addressing issues related to mechanical robustness of the *FlexCell* since it is very critical to the successful commercialization of the SOFCs.
Figure 6.1: CAD drawing of the modified ultra-large area *FlexCell*
6.2 FUTURE WORK

6.2.1 IMPROVED BOUNDARY CONDITIONS AND COUPLED ANALYSIS

The actual boundary conditions in an operating solid oxide fuel cell are difficult to simulate. Further work is needed to identify appropriate mechanical and thermal conditions. While performing coupled thermal-structural analysis, other types of flow pattern such as cross flow, counter flow could also be investigated. The startup and shutdown phases of a thermal cycle of a fuel cell are of particular interest because the risk of cell failure is higher as the temperature range is bigger.

6.2.2 MAPPING RESULTS TO SMALL-SCALE MODEL

Loading conditions for finite element analysis on the repeating unit cell can be applied more realistically by providing the results obtained from the large-scale finite element analysis and also from four point bend experiment sample breakage results.

6.2.3 MODELING THERMAL CYCLING OF A STACK

Once the geometry of the FlexCell is set by taking into consideration the failure limits at the small and large-scales, the focus can shift to incorporate other SOFC layers such as glass seals, electrodes and interconnects. The finite element analysis takes on a multiphysics approach. The final motive will be to simulate the performance of the electrolyte in the context of a full stack.


14. Release 11.0 Documentation for ANSYS, Element Library


