Designing a 3D Printed Catalyst Carrier That Maximizes Reaction Yield

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***Abstract*—A catalyst is a substance that increases a certain chemical reaction rate. However, the currently used catalyst in its normal geometrical form cannot guarantee high single-pass reaction yield. Northern Illinois University's Department of Chemistry and Biochemistry worked with the Department of Industrial and Systems Engineering to optimize the catalyst geometry through design and manufacturing catalyst carriers which is then converted into catalyst. This catalyst carrier has high internal surface area that can facilitate a high reaction yield. Multiple iterations of designs were created in search for an better design that can increase reaction yield but still allowed the carrier to be printed properly and efficiently. These catalyst carriers were then converted to catalysts and their reaction yield was tested.**

Keywords- catalyst carrier, catalyst, surface area, reaction yield.

I. Introduction

Northern Illinois University's Department of Chemistry and Biochemistry required a catalyst that will allow them to have a high single-pass reaction yield when 2 chemicals are reacted. Our team was tasked with designing and 3D printing a catalyst carrier that would be able to facilitate this high reaction yield. The catalyst carrier has to meet specific dimensions that can be seen in Figure 1. The interior mesh was the focus of our design. The team's approach to maximize the reaction yield is to increase the interior surface area of the catalyst carrier while maintaining proper liquid flow through it. A lattice structure was determined to be the best way to implement a high surface area into the catalyst carrier's design. A lattice structure is commonly composed of repetitive cellular unit geometries. These lattice structures can output a high surface area when working with limited space.

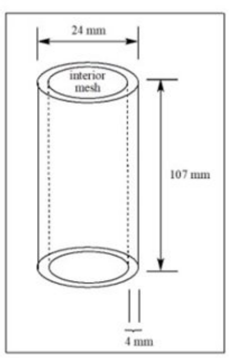

Figure 1. Catalyst Dimensions

The printing method that the team used is an additive manufacturing method known as fused deposition modeling(FDM). Once the catalyst carrier had been 3D printed it is converted into catalyst by treating it with a chemical solution. Once it had been converted, a second chemical solution would be flow through the converted catalyst and the reaction yield would be measured. Reaction yield is the percentage of particles in the solution that completed the reaction.

II. Methodology

The first step to 3D printing the catalyst carrier was to create a design in CAD. The team used Solidworks as our software for this task. The next step would be to import the design into CAM. The team used PrusaSlicer software for this task. This software would allow us to choose printing parameters such as the material used to print, the layer height and the nozzle width. The layer height was .15 *mm*, and the nozzle diameter of the printer was .25 *mm*. This software can than output a G-code which are specific instructions the 3D printer will use to print the catalyst carrier. For this catalyst carrier material, the team used Acrylonitrile Butadiene Styrene(ABS) which is a thermoplastic polymer. This styrene molecule can be sulfonated when treated in sulfonic acid solution, which allows our catalyst carrier printed in ABS to be converted into a polystyrene sulfonate catalyst. The catalyst carrier was then treated in sulfonic acid for several hours and can be seen in Figure 2.

Figure 2. Converted Catalyst

Once the catalyst had been fully converted, chloroform solution was then flowed through it. The amount of chloroform that reacts with the catalyst is our reaction yield. Our first iteration of designs failed in allowing the liquid solution to properly flow through after been converted into catalyst. It was learned that after treated in sulfonic acid, there were slight expansions in the catalyst carrier material, and there is possibly a second time expansion during the catalytic reaction when chloroform solution flows through the catalyst. The initial catalyst carrier was designed with too small feature dimensions, so that after the expansion, this causes difficulties to allow the solution to properly flow through the catalyst carrier. In the second iteration, the team designed experiments to find the expansion ratios of catalyst carrier from as-printed geometry to after converted into a catalyst, and to after reacted with the chloroform. Using the found expansion ratios, an updated design was then created for the second iteration.

III. CAD Designs

The team created six designs in the first iterations of design, the interior mesh of these designs were lattice structures with geometries of circles, squares, hexagons, triangle, and crosses in a linear and circular pattern. The main metric measured in these designs was interior surface area. The surface areas for the designs can be seen below.

Table 1. Surface Area per Design

Design	Surface Area (mm^2)
Circle Design	33,823
Square Design	37,560
Cross (linear) Design	33,547
Cross (circular) Design	30,370
Triangle Design	53,245
Hexagon Design	39,842

An example of our designs can be seen in figure 3, this design was circle design, it was created by making a circle with a diameter of 1.2 *mm* and a spacing of 0.5 *mm.* this circle was then repeated over and over and created the lattice type structure.

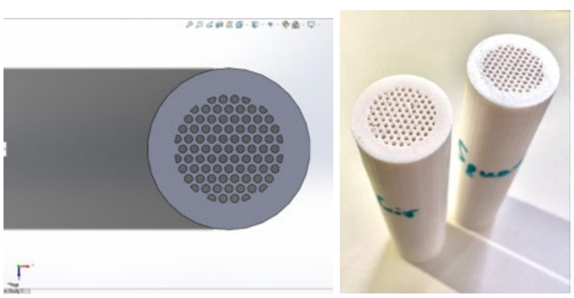

Figure 3. Circle CAD image and 3D Printed design

IV. Expansion Ratio Testing

To find the expansion ratio for our catalyst we printed small catalysts that could print very quickly, and we could measure the dimensions of the catalyst before experimentation and after. These small catalysts or "coupons" were printed on small base and were of two shapes, squares and circles. The squares had three side lengths chosen which consisted of 7, 8 and 9 *mm*. The circle coupons had three diameters chosen which as well consisted of 8, 9, and 10 *mm*. They both had a three wall thicknesses of 0.5, 1, and 1.5 *mm*. A total of 18 coupons were printed and experimented on. An example of a coupon design can be seen in figure 4 below. This circle coupon had a diameter of 10 *mm* and a wall thickness of 0.5 *mm*.

Figure 4. Circle coupon

After the 18 coupons were printed the dimensions of each were measured carefully using a caliper. The dimensions were measure 3 times from different areas of the coupon and then averaged together, this was to ensure that the dimension was correct and the overall variance was reduced. The coupons were then soaked in sulfonic acid and the remeasured. The team found that there was approximately a 1.66% increase in the dimensions. These coupons were then soaked in chloroform, the team found a 2.22% expansion rate. In total the team found a 4% expansion ratio.

V. Results and Conclusion

Using the total expansion ratio and feedback from Northern Illinois University chemistry department the team was able to create a final updated design which can be seen in figure 5. A small lip was added to the end of the design so that the catalyst carrier could be converted easily. This design had a significantly reduced surface area of only 27,233 mm^2. The surface area of the part needed to be reduced for the catalyst carrier to print and experiment successfully. This catalyst carrier had a reaction yield of approximately 20%. The experimentation is ongoing, and the Chemistry department does not expect to finish till late June of 2021.

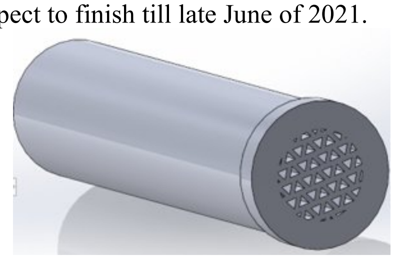

Figure 5 – Final Design

Acknowledgment

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