Actuated Poppet Hydrogen Peroxide Reactor

by
Josef X. Kirkman

Submitted to the Department of Mechanical Engineering
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ABSTRACT

This thesis discusses the design and characteristics of an actuated poppet valve hydrogen peroxide and silver catalyst reactor that can be used to generate compressed gas to use for self-powered robotic systems. The reactor's poppet valve conceals and reveals the silver catalyst to control the reaction. The sealing performance of the valve at working pressures are crucial to the accurate control of the reactor itself. This thesis discusses various design variations of the sealing poppet head and how they can improve performance given various design goals.

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Acknowledgements

I would like to acknowledge Professor Becker, Professor Roche and Sam Gollob for their guidance and mentorship throughout this project.

Biographical Sketch

Josef X. Kirkman, born on December 16th, 2001, in Southern California, is a mechanical engineering student at the Massachusetts Institute of Technology. From a young age, Josef was fascinated by the mechanics of motion and machines, a curiosity that quickly evolved into a passion for robotics. Throughout high school, he dedicated himself to the robotics club, leading his teams to several regional and world wide competitions, earning accolades for innovative design and technical excellence.

This early exposure to practical engineering challenges solidified his desire to pursue a career in this field. Consequently, Josef enrolled at MIT, where he has continued to excel. He has worked on industrial additive manufacturing solutions and pursued product development coursework. His commitment to engineering is not only academic but also personal, as he aims to contribute to advancements that have real-world impact. Josef's journey from a robotics enthusiast to a product design engineer highlights his dedication in the realm of mechanical engineering.

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1. Introduction

A hydrogen peroxide and silver catalyst reactor is a type of chemical reactor that uses hydrogen peroxide (H_2O_2) as a monopropellant and silver as a catalyst to produce a reaction that decomposes the hydrogen peroxide into water (H_2O) and oxygen (O_2). This decomposition releases a significant amount of energy and heat, which can be harnessed for portable robotic systems. Hydrogen peroxide is a powerful oxidizer, and when it comes into contact with a silver catalyst, it rapidly decomposes. The silver acts as a catalyst, meaning it speeds up the reaction without being consumed in the process. Kevin B. Fite discusses the use of hydrogen peroxide as a fuel for a robotic actuator system by using proportional flow control valve with a tapered poppet head and valve body both made of polyetherether-ketone (PEEK) [1]. This allows for volumetric flow rate control of the fuel being injected into the actuator and thus control over the working pressure and position of the actuator.

The volumetric flow rate control studied by Fite enables metered fuel consumption which is crucial for systems where a limited amount of fuel is available for usage. Additionally volumetric flow control provides control over the working pressure of the actuator and thus position control. In this thesis, we will refer to this flow control system as a Fuel to Catalyst (F2C) architecture.

A variation on a F2C architecture is one that controls the reaction by exposing or concealing the fuel from the catalyst, or referred to as Catalyst to Fuel (C2F). This C2F reactor is the type of reactor that was studied in this thesis. One advantage of such C2F reactors is that the fuel is able to stay in contact with the catalyst, instead of flowing past the catalyst, which enables a more complete reaction of the fuel. A C2F reactor can similarly control the working pressure of the system by revealing the catalyst and starting the reaction when the pressure is too low, and by concealing and shutting off the reaction when the pressure is sufficiently high. This controlled operation of the reaction enables metered fuel consumption, as well as control over the working pressure.

2. Mechanical Design

The Design of the hydrogen peroxide reactor included an aluminum frame, clear polycarbonate main body, and a fluoroelastomer o-ring gasket on the poppet shaft. Figure 1 shows an isometric rendering of the design in 3D CAD. The design shows the aluminum frame in teal and orange, the poppet shaft and head in light green, and the off the shelf ⅛" NPT aluminum barb fittings in dark blue. A jam nut, (pictured in red in Figure 1) was included on the poppet head mount to lock it into place on the shaft. Figure 2. shows a cross section view of the poppet head reactor.

One key design criteria for this system was that it must be compatible with hydrogen peroxide. Materials were selected that are chemical resistant and would not significantly degrade over the lifespan of the experimental reactor. For the body and cylinder, aluminum and clear polycarbonate were selected respectively. These were both easy to machine and sufficiently chemically resistant to hydrogen peroxide. The seal between these components were made from a sheet of fluoroelastomer called Viton. The 1/16" Viton sheet was cut into a ring that is undersized on both the outer and inner diameter of the clear polycarbonate tube. This ensures that the gasket, when compressed, has room to expand into the seal and pocket in the body. The Poppet head and shaft, also made from aluminum, included a dynamic sliding o-ring seal and a wear ring for better off axis moment stiffness. The o-ring was also made of Viton to retain appropriate chemical resistance. The wear ring was made of polytetrafluoroethylene (PTFE) due to its low coefficient of friction, and relatively high chemical resistance. Even though PTFE is not as chemically resistant to hydrogen peroxide as the other materials selected, since it is external to the o-ring as seen in Figure 2, it should not be exposed to any significant amounts of hydrogen peroxide.

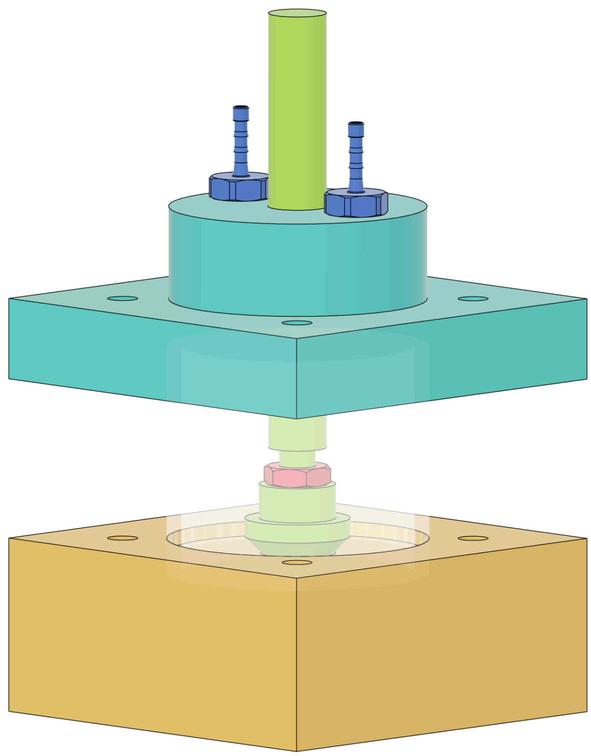


Figure 1. Isometric rendering of CAD design for Poppet Head Reactor. Aluminum body and NPT barbed fittings in teal, blue and yellow. Aluminum poppet head and shaft are in green, with jam nut in red.

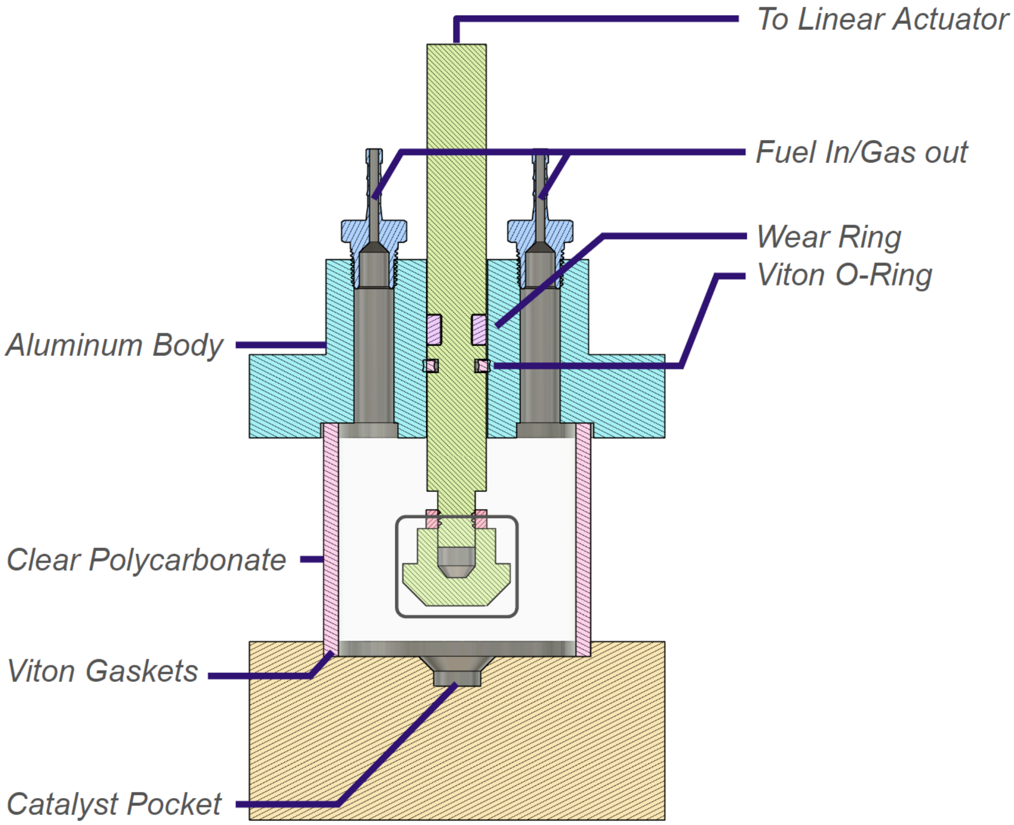


Figure 2. Cross section of Poppet Head Reactor. Viton Gaskets at interface between pink polycarbonate tube and teal and yellow aluminum frame pieces. Poppet shaft in green has a PTFE wear ring with a Viton O-Ring.

3. Poppet Head

The poppet head reactor is a testing platform for control of hydrogen peroxide reduction by using an actuated sealing plunger to control the reaction. The design of the poppet head itself is crucial for the operation of the reaction. The head design controls how much displacement and force are required to seal the reaction thus defining the requirements of the linear actuator that controls it. The opening and closing of the head also define the reaction dynamics of how pressure is built up when opening and closing the valve. Understanding these parameters is key to successful control of the pressure out of the reactor. Additionally, design variations of the poppet head may be able to tune these performance variables for more favorable behavior.

One performance variable of the poppet head behavior that we would desire control over is the sensitivity of the shutoff action. For example, if the reactor is operating at high pressures and thus high sealing forces, a design tradeoff given a fixed actuator power output may result in a high force, very slow actuator. In this case it would be desirable for the poppet head to fully shut off over a very short displacement to increase the possible bandwidths of the poppet valve with the limited actuator speed. This would be realized in a high stiffness poppet head design.

Another performance variable is how the reaction is allowed to continue or not once the poppet is sealed. For example, it may be desirable to allow the reaction to run its course and deplete any remaining fuel in the catalyst pocket without building up a highly pressurized pocket as a pressurized pocket would exert larger than normal forces on the catalyst and poppet actuation, which would demand higher forces out of the actuator. To achieve a complete reaction we may want to design a vent channel in the poppet head that allows excess gas to escape in a controlled manner, even at low pressures. This can be achieved by creating a channel in the rigid poppet head, this locally increases the thickness of the silicone section, and thus lowers the structure stiffness at that region. The region of lower stiffness allows gas to locally leak.

3.1 Poppet Head Construction

The poppet head is designed as a two part overmolding. The design includes a rigid core with a soft overmolding that creates the seal. Figure 3 shows a cross section with the solid core in orange and the overmold in gray. The solid core is intended to be manufactured of aluminum but was 3d printed to enable rapid iteration of poppet head designs. Table 1 shows potential material choices for the overmolding and their relevant mechanical material properties. Five materials are shown here from the Smooth-On Vendor. These five were selected due to their lab availability, and that they represent a wide range of hardnesses. Table 1 includes hardness, 100% Modulus (which is the amount of pressure required to stretch a section of the material by 100% elongation), Max temperature, and cure time. These parameters were used to select Silicone Ecoflex 00-35 FAST for all poppet heads in this thesis, primarily due to its rapid curing time which enables rapid iteration of many poppet head designs. Selecting a different material will significantly affect the results of each measurement, but the overall design considerations and trends should remain consistent over the range of silicone materials.

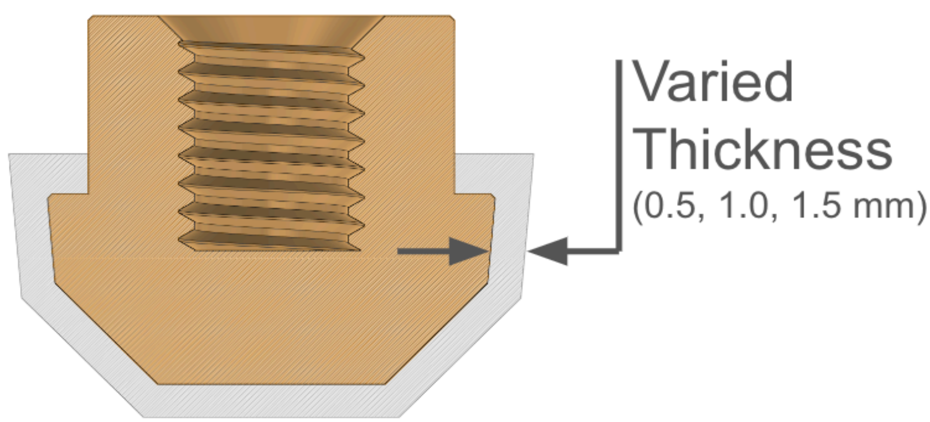


Figure 3. Cross section of Poppet Head. Orange is solid core Poppet Head, gray is silicone overmolding. Silicone overmolding thickness varied is a key parameter in design

Table 1: Poppet Head Materials and Relevant Properties. Five materials selected from Smooth-On Vendor based on lab availability and a representative range of hardnesses.

Properties	**Ecoflex 00-35 FAST**	**Ecoflex 00-20 FAST**	**Ecoflex 00-50**	**Dragonskin 30**	**Simpact 80A**
Hardness	Shore A 00-35	Shore A 00-20	Shore A 00-50	30 A	80 A
100% Modulus [PSI]	10 PSI	8 PSI	12 PSI	86 PSI	1,213 PSI
Max Temperature	450 F	450 F	450 F	450 F	Not listed
Cure time	5 minutes	1 hour	3 hour	16 hours	48 hours

3.2 Poppet Head Manufacture

A custom mold was designed and 3D printed to mold silicone over the poppet head, as described below. Molds were printed on a multi jet printer and fully cleaned of support material, and baked in a 65° C oven for at least 24 hours prior to molding. Once the mold was printed and prepared, the final molding process began with preparing the cavity by spraying it with a mold release agent to facilitate the easy removal of the cured piece. Next, silicone was mixed and poured into the prepared cavity up to the designated fill line. This fill line ensured consistent filling of the mold and that the poppet head was properly encapsulated without excessive overflow. The fill line was the same as the break in the taper geometry for the poppet heads. The silicone was poured evenly to minimize air bubbles. The poppet head was then pressed into the cavity. The alignment channels guided the poppet head into the correct position, ensuring it bottomed out to datum the vertical axis. The alignment channels and bottoming out ensured an even silicone thickness across the entire surface. As the poppet head was inserted, excess silicone was forced out into the overflow region. This design feature helped in preventing voids and ensured that the silicone completely surrounded the poppet head. The silicone was allowed to cure at standard atmospheric pressure and room temperature. Once the cure time recommended by the manufacturer had passed, the silicone was carefully pried away from the cavity to loosen the silicone. This prying was done using a small tool such as a needle or paperclip. The poppet head's internal threads were then used to attach a surface that was drawn against the top of the cavity. This thread drawing aided in the final extraction of the poppet head from the mold by allowing it to be gently pulled out vertically, ensuring the integrity of the molded part.

For the mold design, alignment channels and overflow regions were critical for a successful molding. The cavity was designed with precise alignment channels that served as datum points for the poppet head. An overflow region was incorporated to manage excess silicone during the molding process. This reduced the risk of air bubbles being trapped in the mold. To aid in release from the cavity, its surface should be as smooth and glossy as possible. This can be affected by the printer technology selected for 3D printing the molds. In the case of multi-jet printing, which was used for both the poppet head and molds, design of the mold and orientation on the build plate should ensure that support material is not used on the molding surfaces to get a smoother surface finish. Additionally, a mold release agent helps to prevent the silicone from adhering to the cavity walls.

To further reduce the risk of air bubbles being trapped in the mold, the cavity should be filled prior to the poppet head being inserted. If the silicone was poured afterward, it could flow around the poppet head and trap an air bubble within the mold itself, creating a void. This void defect was seen in Figure 4, an older mold design, where silicone was poured after the poppet was already installed in the mold.

The final molding process components are outlined in Figure 5.

Figure 4. Prior cavity mold design, where silicone was poured after the poppet head was installed, which led to an air bubble causing a void/underflow defect.

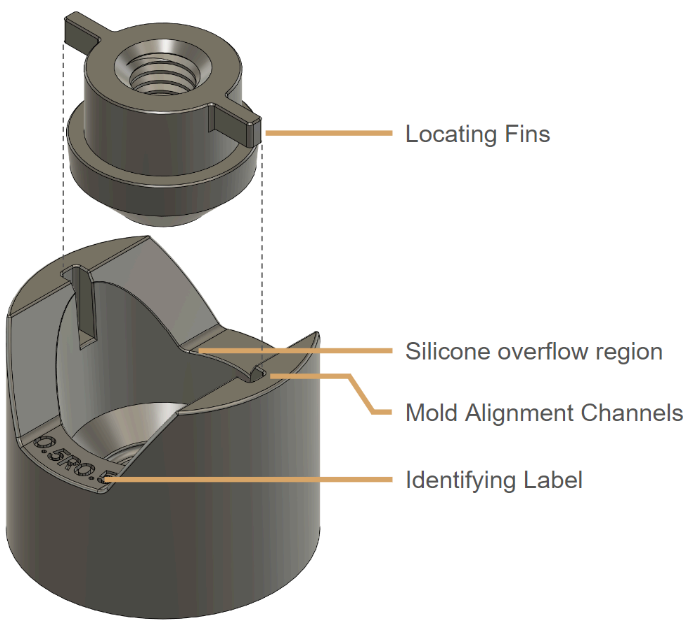
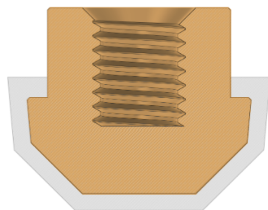
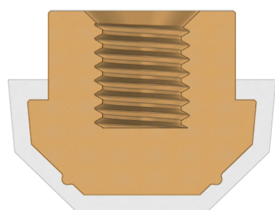
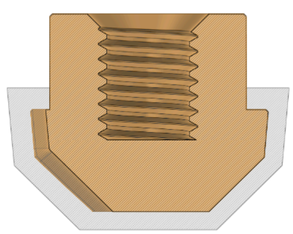
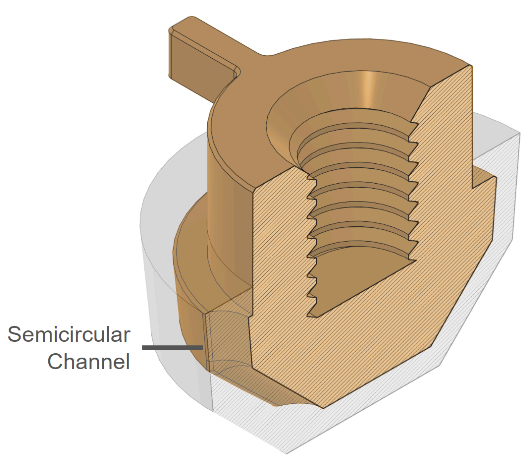


Figure 5. Exploded View of Final Mold Design. Poppet head includes locating fins that seat into tapered mold alignment channels on the cavity. The cavity includes overflow regions and Identifying labels.

3.3 Poppet Head Geometry Design

Table 2 outlines all various poppet head geometries that were tested. These were developed in attempts to improve the consistency of the sealing and to see how they affect performance of sealing.

Table 2. Various Poppet Head Designs and Objectives

Name	Image	Objectives
1. Uniform		Baseline uniform thickness
2. Ridged Head		Ridge creates stress concentration where the primary seal is located
3. Vented Channel	 	Channel in rigid poppet head creates region of lower stiffness for extra O_2 gas to "burp" and escape

Each of the designs outlined in Table 2, show various geometric changes that can be made to the poppet head with the goal of affecting sealing performance variables. Each design is detailed as follows:

Design 1. Uniform Baseline

The baseline uniform poppet head designs were the first design proposed due to its simplicity. As initial tests were conducted the leaking behavior of opening and closing the valve was noticed to be erratic. The origin of leaking was inconsistent radially. Some tests would leak in various locations, or even by pushing through the center of the head ballooning the overmolding up and around the rigid head resulting in separating of the silicone overmold from the poppet head. This behavior of consistent leaking inspired the ridged head and vented channel designs.

Design 2. Ridged Head Design

The ridged head was intended to concentrate the seal of the poppet head to a localized area that could be better controlled as opposed to relying on two surfaces to create the seal. The design also locally thins the silicone to achieve this instead of thinning across the entire section, hereby retaining some structural performance of the thicker poppet head designs.

Design 3. Vented Channel

The objective of the vented channel design was to create a region of lower stiffness in the rigid poppet head, allowing excess O_2 gas to "burp" and escape, even at low pressures. This was intended to control gas escape and prevent the buildup of a highly pressurized pocket. To determine the most effective channel depth for controlling gas escape, two vented channel depths were tested: 0.8 mm and 1.5 mm. The leak tests were conducted at a constant pressure of 30 PSI. Soapy water was applied around the seal, and the compressive sealing force was gradually reduced. When the poppet head began to leak, bubbles formed at the points where gas was escaping.

For the 0.8 mm channel, bubbles appeared randomly around the circumference, similar to other poppet head designs without a dedicated vent channel. In contrast, for the 1.5 mm channel, bubbles formed specifically at the location of the channel. This indicated that a vented channel must be at least 1.5 mm deep to effectively direct the gas out of the channel for silicone overmolding thicknesses ranging from 0.5 mm to 1.5 mm at 30 PSI.

Figure 6 illustrates the alignment of bubble origins with the channel in the 1.5 mm deep channel and 1.5 mm thick silicone overmolding, demonstrating the effectiveness of this design in controlling gas escape.

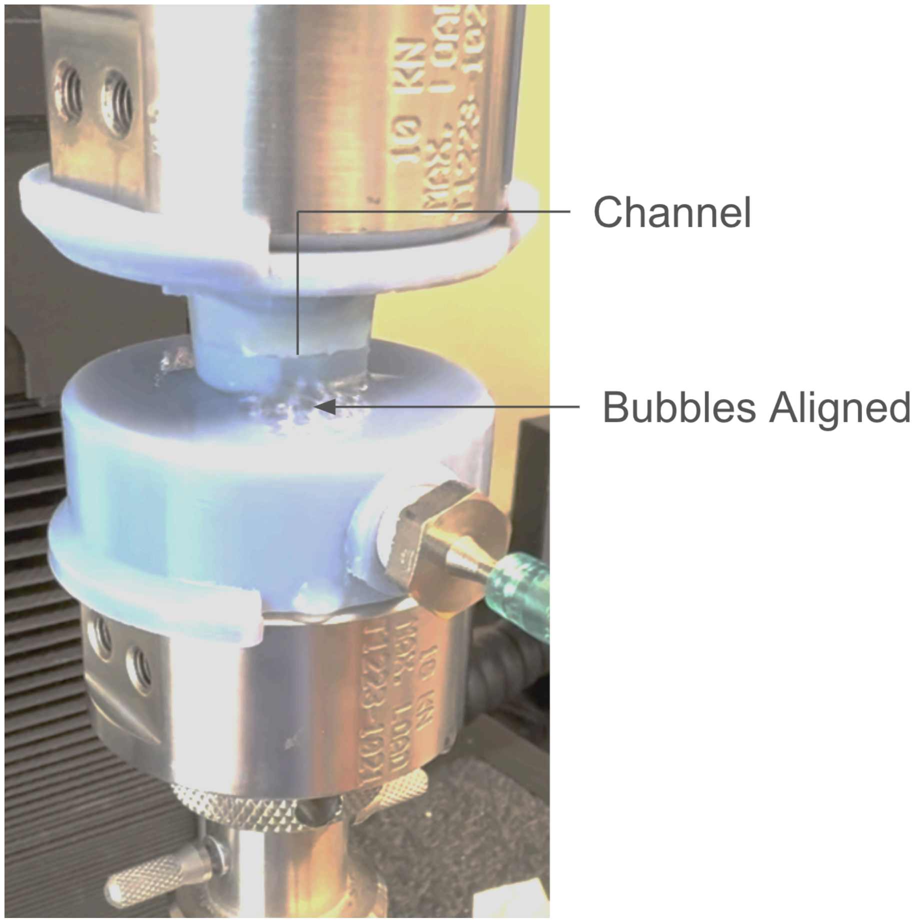


Figure 6. 1.5mm deep Vented Channel Poppet Head in Instron Setup with soapy water surrounding circumference of seal. Bubbles originating inline with the channel demonstrates effectiveness of the design at 30 PSI.

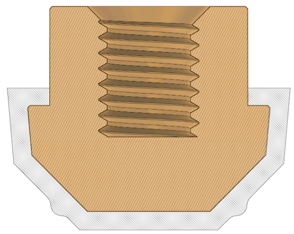
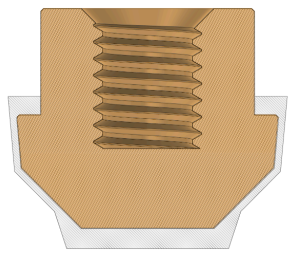
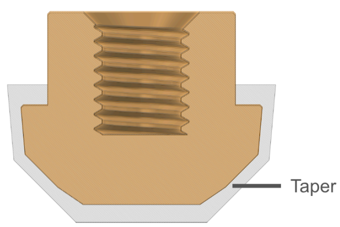
3.4 Exploratory Poppet Head Geometry

Further exploratory poppet heads were designed in order to expand on the design space. Due to time constraints, a full matrix of these designs and thicknesses could not be tested.

Design 4. the silicone ridge is very similar to Design 2, except the ridge is molded into the silicone instead of the rigid head. This will create a thicker section of silicone, instead of a thinner section.

Design 5. And 6 are taper designs but Design 5 has the taper built into the silicone where it gradually decreases in thickness and design 6 has the taper built into the taper head for the silicone to gradually decrease in thickness. The objective for both of these designs is to progressively seal the catalyst away from the fuel while maintaining a thick silicone section at the beginning of contact to allow for sufficient displacement to accommodate surface imperfections or misalignment on the sealing surface.

Table 3. Exploratory Poppet Head Designs and Objectives

Name	Image	Objectives
4. Silicone Ridge		More consistent shutoff at silicone ridge location
5. Silicone Taper		Thicker at the start of the seal, but thinner around the body to allow for large displacement, but a stiffer shutoff
6. Taper Head		Gradually decrease the thickness of silicone as the seal progresses. Progressive seal.

4. Experimental Procedure

The poppet head was loaded into the instron mount and then aligned radially with the air pressure base mount. The instron was lowered until a seal was formed, the air pressure line was opened to 30 PSI and then the instron was manually lowered further until the compressive force read at least 100N. Figure 7. shows the experimental design setup installed in the instron. The instron test was then started, where it moved upwards at a constant rate of 0.05 mm/s. The test was stopped about one second after an audible hissing was heard, or after the instron force dropped below the local minima that was created by the initial leak. The air pressure line was shut off then the procedure repeated for a total of three trials per poppet head design.

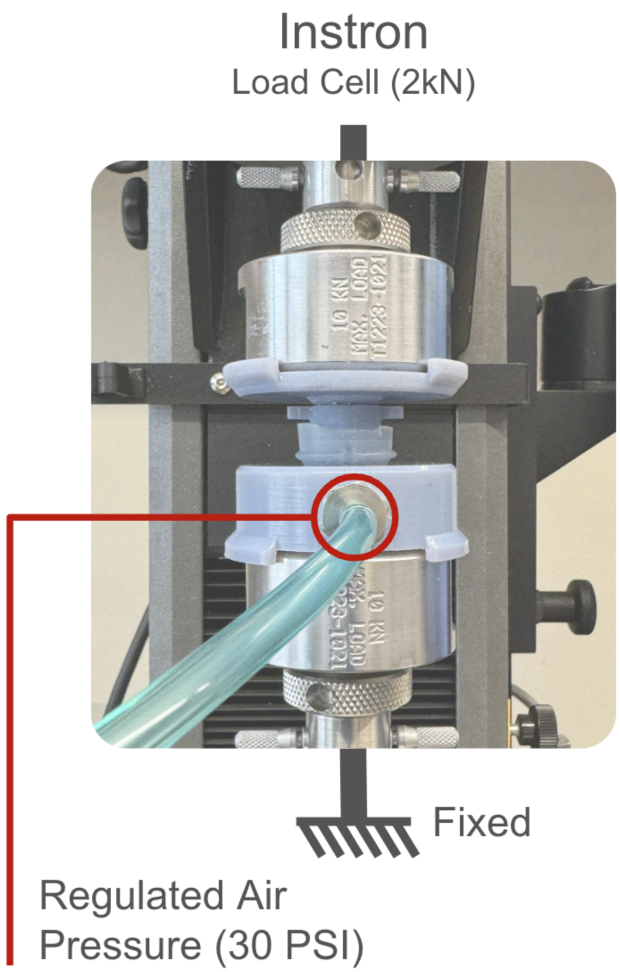
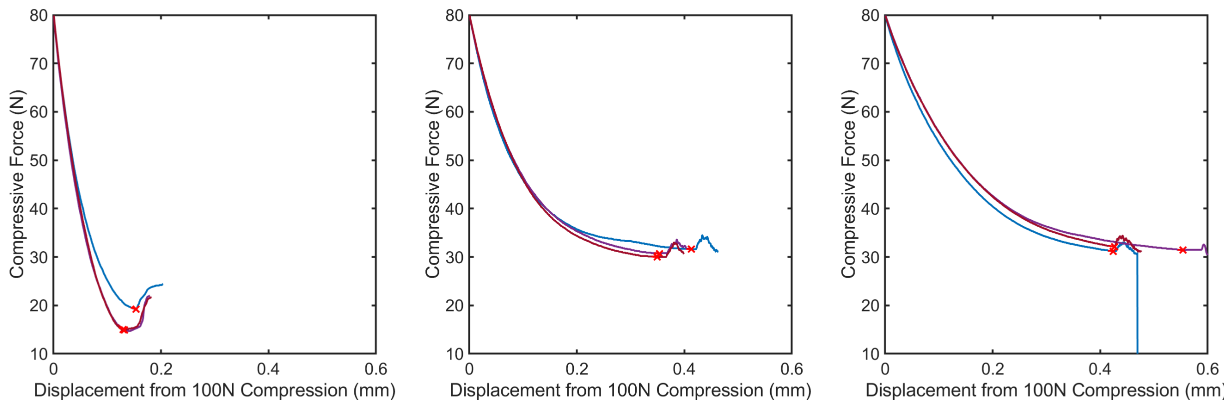


Figure 7. Instron test setup for Poppet Heads. Instron with 2kN load cell installed and air pressure line regulated to 30 PSI

5. Experimental Data Analysis

The raw data of compression force in Newtons vs displacement in mm is post processed to datum position of 0mm to 100 N exactly. This is then plotted as seen in Figure 8. To determine the force required to hold 30 PSI, we must look for a sudden increase in compression force as this correlates to when the air pressure begins to leak, and the instron load cell does bear the force of the compressed air. This is analytically determined by a local minima, as defined as a data point that has a lesser value than its neighboring data points. This value is taken as the force to hold 30 PSI. Then further analysis of the stiffness of this leaking point is determined by taking the average slope of the 20 prior data points (corresponds to 0.01 mm). This analysis is repeated for all 3 trials of the design, and then an average and 95% confidence interval is calculated. Table 3 shows the numerical results for all the poppet head designs. In Figure 8, we can see increasing force as thickness increases and also the smaller magnitude of stiffness as the slope of the point around the red X marker is steeper in a) (0.5 mm) and much shallower in b) and c) (1.0 mm, 1.5 mm).



(a) 0.5 mm **(b) 1.0 mm** **(c) 1.5 mm**

Figure 8: Various plots of Compression Force vs Displacement for Design 1. Uniform silicone thickness. Organized by a) 0.5 mm thickness, b) 1.0 mm thickness and c) 1.5 mm thickness. We can see the increasing force required to hold 30 PSI as the red X marker is at higher force values for increasing thicknesses of silicone.

As seen in Table 4, the regular uniform poppet head shows a positive correlation between holding force and silicone thickness. This is intuitive because as the silicone thickness increases the overall structure becomes less stiff. With a lower stiffness gasket the same working pressure can more easily deform a channel for air to leak, thus the actuator has to press with more compressive force to preload the gasket and maintain a seal.

The correlation between stiffness and silicone thickness is seen across the board with thinner silicones having higher stiffness than thicker silicone sections.

The ridged head in Design 2 shows higher stiffnesses across all thicknesses. This is because the ridge locally thins the silicone section where it actually seals so the poppet is effectively behaving as a thinner section of silicone. The holding force also significantly increases for all thicknesses but appears to reverse the trend of thicker sections requiring higher forces. This reversal of trend is unexpected but could be within the margin of error of the experiment as the 95% confidence intervals of all 3 thicknesses are overlapping.

The channel in Design 3 performed as expected, once the channel is sufficiently large. We see higher required forces, and a similar trend in stiffnesses. The confidence interval for the stiffness between the Uniform and Vent Channel overlap, meaning there is minimal statistically significant difference between the two designs. More samples must be taken to further assess if the vented channel design impacts stiffness.

Table 4: Poppet Head Experiment Design Matrix. Force to Hold 30 PSI listed, as well as Slope stiffness in italics

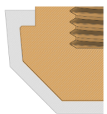
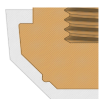
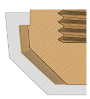
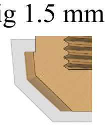
Force (30 PSI) [N] *Stiffness [N/mm]*	**0.5 Thickness**	**1.0 Thickness**	**1.5 Thickness**
1. Uniform 	16.3±2.3 N *stiffness: 60.3±29.1 N/mm*	30.8±0.8 N *stiffness: 9.5±5.2 N/mm*	31.6±0.4 N *stiffness: 12.7±5.2 N/mm*
2. Ridge 	38.7±1.2 N *stiffness: 231.7±46.4 N/mm*	36.1±1.0 N *stiffness: 34.9±5.2 N/mm*	35.3±3.8 N *stiffness: 28.5±18.0 N/mm*
3.1 Vent Channel Small 0.8 mm depth 	36.0±2.2 N *stiffness: 219.0±23.9 N/mm*	33.2±0.6 N *stiffness: 15.9±5.2 N/mm*	31.9±0.3 N *stiffness: 19.0±0.0 N/mm*
3.2 Vent Channel Big 1.5 mm depth 	22.3±1.5 N *stiffness: 120.6±90.6 N/mm*	32.7±0.4 N *stiffness: 25.4±10.4 N/mm*	38.1±0.7 N *stiffness: 15.9±5.2 N/mm*

Table 4. shows the data from additional exploratory poppet head designs.

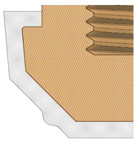
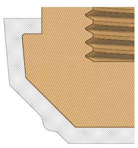
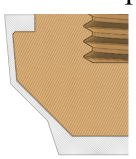
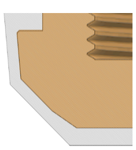
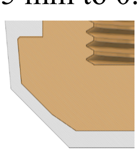
Design 4. The silicone ridge seems to achieve similar holding force as the poppet head ridge (Design 2), but with lower stiffness. This is the expected outcome as the silicone ridge increases the thickness of the silicone section which should reduce the stiffness. This design needs to be explored more as the stiffness for 4.2 is not significantly different from the slope of Design 2. at 1.5 mm silicone thickness. This may be due to the fact that the silicone ridge in Design 4.2 is only 0.2 mm tall whereas it was 0.5 mm tall for Design 4.1.

Design 5 and 6 were intended to create a progressive seal, or a seal that engages sequentially as force is applied. A progressive seal is typically used in applications that require effective fluid containment, so recreating this type of seal may prove beneficial for complete reaction shutoff.

For Design 5, the silicone taper held 30 PSI at a force between a uniform 1.5 thick and 0.5 thick which is intuitive as the taper transitions between those thicknesses. The stiffness however was greater than that of the uniform 1.5 thick silicone poppet. This is the intended behavior as the taper was designed to have a faster and more sensitive shut off action over a uniform design. Additionally the progressive seal seems to have been achieved as the force v displacement curve is very linear, as compared to all the other designs which showed significant nonlinearities. This suggests that as the silicone taper was displaced, more of the material was engaged at a rate that was similar to the nonlinear effect of elastic material compression.

With Design 6, the tapered head designs showed minimal effect. Design 6.1 (taper head with 1.5 mm thick silicone that thins to 1.0 mm thick) has almost identical performance with the uniform 1.5 mm thickness head. Design 6.2 (taper head with 1.5mm thick silicone that thins to 1.0 mm thick) shows increased holding force and slightly increased stiffness as it gradually tapers towards a 0.5 mm thickness. The ineffectiveness of the taper head may be due to the fact that the taper begins at a fixed height away from the tip of the poppet head and this may be too far away from the chamfer in the catalyst pocket to create significant effect. To achieve the progressive seal, moving the beginning of the taper towards the catalyst may increase the effect.

Table 5: Additional Exploratory Poppet Head Design Matrix

Description	**Force (30 PSI) [N]** ***Stiffness [N/mm]***
4.1 Silicone Ridge 0.5 thick 0.5 tall ridge 	avg = 31.5±0.8 N slope = *44.4±22.8 N/mm*
4.2 Silicone Ridge 1.5 thick 0.2 tall ridge 	avg = 37.9±0.5 N *stiffness: 22.2±5.2 N/mm*
5. Silicone Taper 1.5 mm at tip, 0.5 mm after 	avg = 26.4±1.1 N *stiffness: 111.1±123.1 N/mm*
6.1 Taper Head Increase head size by 0.5mm 1.5 mm to 1.0 mm silicone 	avg = 31.9±0.6 N *stiffness: 12.7±5.2 N/mm*
6.2 Taper Head Increase head size by 1.0mm 1.5 mm to 0.5 mm silicone 	avg = 35.5±0.8 N *stiffness: 22.2±5.2 N/mm*

6. Design Conclusions and Recommendations

Thinner silicone sections result in lower forces required to seal and higher stiffness at sealing force. The higher stiffness also means a more displacement sensitive head design. The higher stiffness designs will respond (seal or not sealing) to smaller displacements with higher sensitivity. This can be beneficial for designs with slower moving actuators that desire a quick and clean shutoff of the reaction.

The ridge design successfully increases the stiffness of poppet heads, acting as a more sensitive shutoff control. This can be effective for compensating for an actuator design tradeoff, such as a slower actuator that can provide more force.

There are a few designs that had unintended consequences or risks associated with the geometry. For both the 0.5 mm thick ridged head and 1 mm increase taper head poppet designs, the silicone sheared off right on the ridge line, or taper line, during some of the experiments. The sheared poppet head can be seen in Figure 9. The ridge and taper transition acted as a stress concentration right where the silicone section was the thinnest and thus the silicone would shear off. This could be averted by limiting the compression force the actuator can exert or working at a lower pressure, or by increasing the minimum thickness of silicone at these sections.

Figure 9: 0.5 mm thick ridged poppet head with silicone sheared off after high compression loads. Same effect occurred with 1 mm thick tapered poppet heads.

Notes and Bibliographic References

[1] Design and Energetic Characterization of a Proportional-Injector Monopropellant-Powered Actuator Kevin B. Fite, IEEE