Optimization and Modeling of an Energy Harvesting Optical Micropropeller for Microfluidic Applications

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Optimization and Modeling of an Energy Harvesting Micro-propeller for Microfluidic Applications

An honors thesis presented to the College of Nanoscale Science and Engineering University at Albany, State University New York in partial fulfillment of the requirements for graduation from the Honors College.

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Abstract

Geometry for a plasmonically active micro-propeller is designed in Matlab using a Metallic Nano-Particle Boundary Element Method (MNPBEM) toolbox in order to predict its optical response in long wavelengths of electromagnetic radiation. Electric field maps are plotted to determine the feasibility generating torque using the energy harvesting principle. Results indicate electric field lines that would promote rotation and the scattering cross section would cause nano-rods sitting on the propeller to radiate thermal energy. COMSOL modeling is performed to model the evolution natural convection currents as a result of the nano-rod heating which is then optimized to further promote rotation of the micro-propeller.
Acknowledgements

I would like to thank Nicholas Karker for always being available to help and teaching us how to use the optical modeling software. I would also like to thank Tim Kamaldinov for taking the time to introduce me to COMSOL as well as James Castracane and Natalia Tokranova for access to their labs.
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Introduction

Surface plasmon resonance (SPR) is a phenomenon which occurs when a material of a high free electron density interacts with and oscillates in phase with the electric field of electromagnetic radiation. In most cases, SPR is induced by a photon on the surface of a metal nanoparticle where the incident light causes the formation of an oscillating dipole in the particle, causing free electron cloud to oscillate in turn (figure 1). The frequency of this oscillation is dependent on the shape, size, dielectric constant, and other optical constants of the material and the surrounding medium\textsuperscript{1,2,3}. Due to these properties, SPR has been applied to several types of biological and chemical sensors\textsuperscript{4}. Of particular interest, however, is the application of plasmonically active materials to dynamic devices.

The applications of controlled torque on the micrometer length-scale are numerous, from molecular manipulation and propulsion, to mechanical transducers and actuators\textsuperscript{5}. It has been shown by Liu et al. that rotating plasmonic motors are possible by taking advantage of plasmonic materials\textsuperscript{6}. However, like other traditional plasmonic systems, the incorporation of an optical path and light source is required, limiting the application of this technology. To amend this issue, we propose utilizing the thermal energy harvesting principle developed by Karker et al. In their work, it was established that blackbody radiation could be used in the place of incident light on lithographically patterned Au nano-rods to obtain plasmonic responses\textsuperscript{7}. While, this capability would eliminate the need for external light sources, it’s operational range has currently only been shown to be above 300°C. Theoretically, this energy harvesting principle can hold at lower temperatures by tuning the nano-rod to lower frequencies. Doing so would allow for an energy harvesting coupled micropeller to be powered by it’s thermal environment in a more applicable temperature range. Through electric field enhancement and optical scattering, we aim to design an micropropeller that utilizes poynting vectors and natural convection in order to power it’s rotation. In this paper, we determine the necessary geometry to tune the thermal harvesting principle’s operational limit down to 50°C, and model the plasmonic response of an energy harvesting coupled micro-propeller using a Metallic Nano-Particle Boundary Element Method (MNPBEM) toolkit in Matlab. Additionally, we model the natural convection induced by the heat generation at the nano-rods as a proof of concept for the natural convection propelled design.

Specific Aims

To determine whether or not the micro-propeller design presented could rotate under the defined conditions, two physical phenomena had to be modeled: surface plasmon resonance and natural convection. Different modeling software, capable of handling the set of physics involved in each process, was employed to optimize substrate and rod materials as well as dimensions of the propeller.
Aim 1. Model optical properties of the micro-propeller for optimization of rod and substrate material. Provide proof of concept.

Plasmonically active materials are generally characterized by a very dense, polarizable, cloud of electrons. However, because the accuracy of the software is contingent upon the availability of wavelength dependent refractive index and dielectric constant databases, many materials that haven’t been characterized in the deep infrared region could not be modeled. Some of the commonly used and well-characterized plasmonic materials that could be modeled for our purposes include gold, silver, and copper. Determining which of these demonstrates the best scattering cross section at the defined wavelength range will ultimately improve the tendency for rotation in the micro-propeller.

Although the metal nano-rods are the elements which ultimately absorb and scatter the incident thermal energy, the substrate material also plays a role in modifying the energies of the plasmon modes of the nano-rod. Therefore, optimization of the substrate material is also important to the efficiency of the micro-propeller. For these simulations, three different materials were tested: silicon, yttrium-stabilized zirconia, and glass. Finding the types of materials that are most effective may allow physical properties, critical to the success of the propeller, to be identified and optimized in the future.

Silicon was chosen as a metallic substrate for simulation primarily due to its compatibility with lithographic shaping methods established by the integrated chip industry. However, a large point of concern with silicon is that it is not biocompatible nor biostable, which would severely limit this micro-propellers potential as an in vivo bio-MEMS component.

Yttria-stabilized zirconia (YSZ) was chosen as a ceramic substrate for simulation due to its wide use in the Carpenter lab as a material for embedding Au nanoparticles for plasmonic-based sensors. Additionally, YSZ is a desirable material because of its biocompatibility, mechanical strength, chemical stability, and wear resistance. A major drawback of using YSZ is that it is susceptible to corrosion and low temperature hydrothermal degradation (aging).

A fused silica glass substrate, was chosen because of its common use in microfluidic micro-electrical-mechanical systems. Silica-based devices are popular in the creation of microfluidic systems because of their good insulating properties and high resistance to mechanical stress, surface stability, and solvent compatibility. Silica-based microfluidics have been used in biological applications, demonstrating their biocompatibility.

By plotting the electric field lines of the micro-propeller, the direction of the electric field over the rods can be observed. From these electric field lines, inferences can be made about the direction of the angular momentum induced in the pointing vector, a directional energy flux caused by electromagnetic field. This poynting vector can be used to create torque.

Aim 2. Model the natural convection behavior of the micro-propeller for further optimization. Provide proof of concept.
The thermophoretic force generated by the plasmonics of the rod is also essential for rotation as the formation of convective currents around the propeller can further contribute to the rotation of the device. Natural convection is the process of heat transport in which fluid motion is not generated by an external source, but rather from density differences in the fluid caused by temperature gradients. In natural convection, a volume of fluid is heated, causing it to expand by a thermal expansion coefficient and decrease in density. The less dense fluid rises away from the heating element as cooler, denser fluid flows in to replace it. By this process, convection currents are formed. The onset of natural convection is determined by the Rayleigh number:

\[ Ra = \frac{\rho_0 \beta \Delta T g L^3}{\mu} \]

where \( \rho_0 \) is the reference density of the fluid, \( D \) is the thermal diffusivity, and \( \mu \) is the dynamic viscosity of the fluid. For the proposed device, plasmonically excited materials will create the necessary heat generation and temperature gradient to induce thermophoretic and convective forces. Natural convection is more likely to occur, or will occur more rapidly, when there is a large temperature difference. Therefore, in order to use these convective currents to generate torque, temperature gradients must be maximized and localized to opposite sides of both ends of the propeller. To meet this condition, the substrate would optimally have a low thermal conductivity, \( k \), and a high heat capacity, \( C_p \), while the rod material would have a high thermal conductivity and a low heat capacity.

Using the same materials investigated from aim 1, thermal and velocity profiles can be generated for the micro-propeller. These profiles will further illustrate the capability of the propeller to rotate and allow for further optimization of device materials and dimensions.

**Experimental Methods**

**Determination of Metallic Nano-Rod Aspect Ratio**

In order to tune the nano-rod, it was necessary to find the wavelength of light that would be similar to the spectral radiance of the environment at 50°C using plank’s law for modified geometries:

\[ U(\lambda) = \frac{8\pi h v^3}{c^3 \left( \exp \left( \frac{hc}{\lambda kT} \right) - 1 \right)} \]

where \( h \) is Plank’s constant, \( c \) is the speed of light in a vacuum, \( k \) is the Boltzmann constant, \( v \) is the frequency, and \( T \) is the temperature of the heated body. An energy vs. wavelength profile of radiant heat energy at 50°C was found (figure 2). The energy vs. wavelength profile demonstrated a peak position of the broad peak at around 15 µm. Although the broad peak suggests that there is a large wavelength range of spectral radiance that could excite the plasmonic nano-rods, a 15-µm wave was chosen as the theoretical wavelength of the spectral radiance at 50 °C.
Figure 2: Energy vs. Wavelength profile for the spectral radiance at 50°C

The aspect ratio could then be determined from the wavelength and data extrapolation. Karker et al. modeled the longitudinal plasmon peak wavelength as a function of the nano-rod aspect ratio based on experimental samples (Figure 2). The data in the plot was extrapolated out to our target wavelength of 15 µm and the aspect ratio required for absorption was determined to be 1:60. However, the resolution limits of the available electron beam tool is 40 nm, making a 1:60 aspect ratio rod a minimum 2.4 µm in length. A propeller of this length would be severely limited in its scope of application. Therefore, it was necessary to calculate the absorption cross sections of smaller aspect ratios that could still absorb at our target wavelength of 15 µm.

The absorption cross section of the Au nano-rod was calculated from the Lorenz-Mie theory. The absorption cross section is given by:

\[
\sigma_{abs}(\omega) = \frac{V}{3c} (\varepsilon_m)^3 \sum_{i=1}^{3} (Y_i + 1)^2 \frac{\omega \varepsilon_2}{(\varepsilon_1 + Y_i \varepsilon_m)^2 + \varepsilon_2^2}
\]

Where V is the particle volume, c is the speed of light in a vacuum, \(\varepsilon_m\) is the matrix dielectric constant, Yi is the shape factor for the ith axis (which is directly proportional to the aspect ratio), \(\omega\) is the resonant peak frequency, and \(\varepsilon_1\) and \(\varepsilon_2\) and the real and imaginary parts of the dielectric function of the metal, respectively. Plotting the cross section as a function of the resonant peak frequency, it was determined that a 1:20 aspect ratio had a non-zero absorption cross section at around 15 µm and well into longer wavelengths. This indicated that the nano-rods created with a 1:20 aspect ratio, 800 nm in length, would be able to absorb at 50°C.
Simulation of Metallic Nanoparticles using a Boundary Element Method

All modeling of the plasmonic properties of the micro-propeller was performed using a MATLAB MNPBEM toolbox for the simulation of metallic nanoparticles (MNP), using a boundary element method (BEM). Material information regarding the wavelength-dependent refractive index and extinction coefficient was derived of a combination of parameters determined by Rakic et al. and Hagemann et al. This allowed for modeling of the micro-propeller between 1 and 248 µm for gold, silver, and copper.

The model was built using the same MNPBEM toolbox. The substrate that comprised of the body of the micro-propeller was built to be 4 µm long, 200 nm wide, and 100 nm thick. The nano-rods were chosen to have a 40 nm diameter and be 800 nm in length. Two nano-rods were placed on opposite sides of the substrate with one sitting on top of the substrate and one sitting below the substrate (Figure 3).

A spectrum for each plasmonic material was gathered on a YSZ substrate in a water matrix. The scattering cross section of the micro-propeller was gathered for each material from 1000 to 20000 nm. A similar procedure was conducted but modulating the substrate material instead, keeping the rod material the same for each simulation.

The last set of simulations done using the MNPBEM toolbox plotted the field lines of the electric field enhancement of the rod on the substrate. For these simulations, only one rod was modeled on a layer structure to attain a qualitative plot of the electric field enhancement of the rod with a 15-µm wave.

COMSOL Multiphysics Simulation Software and Computational Fluid Dynamics

A qualitative assessment of the heat transfer and fluid dynamics affecting the micro-propeller was performed using COMSOL Multiphysics Simulation Software and the Computational Fluid Dynamics module. Time-dependent simulations were performed to observe the effects of micro-propeller composition and dimensions on thermal diffusion and fluid flow.

Due to limitations regarding the physics modules and toolboxes available for the COMSOL license, the micro-propeller was scaled up to the centimeter length scale. This scaling factor was chosen because the applied boundary conditions and parameters would, when applied to examples from the COMSOL model gallery, successfully replicate the demonstrated results. This
scaling factor combined with the unknown quantity of heat generation due to optical absorption also required assumptions to be made about the nature and amount of heat transfer occurring at the metal nano-rods. For computational simplicity, an overall power output of 0.5 watts over a total rod volume of 2.56 mm$^3$ was applied to all simulations.

To qualify these assumptions, it was necessary to determine the turbulent or laminar nature of the flow regime and verify that our scaling factor does not change the physics applicable to the original micron scaled design of the micro-propeller. To do this, the Grashof number was calculated. The Grashof number for vertical flat plates is given by:

$$Gr = \frac{g \beta \Delta T L^3}{\nu^2},$$

where $\beta$ is the thermal expansion coefficient, $\Delta T$ is the temperature difference, $g$ is gravitational acceleration, $L$ is the characteristic length-scale of convection, and $\nu$ is the kinematic viscosity of the fluid. This dimensionless number is a ratio of buoyancy to viscous forces and is used to determine the tendency of a system towards turbulence. When the Grashof number is above $10^8$ the boundary layer is turbulent. Since the calculation for Grashof number in the micro-scale case and the centimeter-scale case were both below $10^8$, the flow was found to be laminar.$^{24}$

For our purposes, time dependent, non-isothermal, laminar flow was modeled. The propeller was constructed within a rectangular (20 cm x 30 cm x 10cm) volume for the water. Open bounds were applied at the walls for laminar flow while the floor on which the propeller rested was insulated by a non-slip layer of glass. The ceiling of this volume was modeled to be a slip boundary exposed to atmospheric pressure with an external natural convection heat flux term of 2 W/m$^2$. The walls of the fluid volume were placed at a sufficient distance from the propeller to set temperature boundary conditions of fluid infinitely far away at 20°C.

**Results and Discussion**

**Optimizing Rod Material for Surface Plasmon Resonance**

![Figure 5: Scattering cross section of the micro-propeller with gold nano-rods (a), copper nano-rods (b), and silver nano-rods (c) on a YSZ substrate from a wavelength range of 1 to 20 µm.](image)
In order for a 1:20 aspect ratio to be substituted for a 1:60, the rod material needed to have a non-zero scattering cross section at the target spectral radiance wavelength of 15 µm. Simulations The micro-propeller with gold nano-rod (Figure 5a) has a peak at ~8000nm for the x-polarized light and a ~7750nm peak for y-polarized light. At longer wavelengths, the scattering cross section of the micro-propeller exhibits no signal. It will not induce an electric field out at 15 µm and, therefore, the propeller would exhibit no rotation in that environment.

Copper nano-rods give a large peak at around 13 µm that extends much farther into the IR region of the electromagnetic spectrum (Figure 5b). The 1:20 copper nano-rods will be plasmonically enhanced by a 15-µm wave as well as longer wavelengths corresponding to temperatures below 50°C. Based on the modeled spectrum in Figure 5b, copper nano-rods could induce an electric field at these lower temperatures since the scattering cross section is still strong beyond its peak value at 13 µm.

While silver does not have a distinct peak in the mid-IR, it does show promise for electric field enhancement at 15 µm and beyond (Figure 5c). The magnitude of the scattering cross section, which denotes the probability of a scattering even occurring, is higher than the copper spectrum. Additionally, unlike copper, the spectrum beyond 15 µm is not decreasing which indicates that there may be another peak beyond the modeled range. The silver nano-rod micro-propeller has the potential of plasmonic enhancement at 50°C and lower based on Figure 5c, indicating that it would be the best suited rod material for energy-harvesting micro-propeller applications.

Optimizing Substrate Material

Figure 6 shows the scattering cross section of the micro-propeller when the Ag nano-rods are placed onto a Si substrate. The nano-rods demonstrate a notable increase in scattering cross-section at 15µm and beyond. In figure 7a, the field enhancement lines for a single Ag nano-rod on a silicon was plotted for a plane 40 nm above the rod. The field enhancement lines are emanating from the inside end of the nano-rod and point inwards on the outer end of the nano-rod aligned with the edge of the substrate.

A similar analysis was performed for the micro-propeller when the Ag nano-rods are placed onto a YSZ substrate (Figure 5c). The spectra for Si and YSZ are similar in shape, but Si has a much higher scattering cross section. However, the electric field map of a Ag nano-rod on YSZ (Figure 7b) suggests that the intensity of the
electric field generated by a Ag nano-rod on YSZ is larger than that of Si by a factor of 2. This result, combined with the known biological incompatibility and the thermal properties to be discussed made YSZ the preferred material.

![Figure 7: Field enhancement lines for a silver nano-rod on silicon (a) and on YSZ (b). The color bar scale indicates that the field strength for silver on YSZ is greater.](image)

The fused silica glass substrate showed the best optical properties of the three materials. The spectrum for the micro-propeller with a fused silica substrate (Figure 8) is similar in shape to Figure 5c, but the scattering cross section, and therefore the scattering probability, of silver on glass is slightly greater than that of YSZ.

![Figure 8: Scattering cross section of the micro-propeller with Ag nano-rods on a fused silica substrate](image)

The field enhancement on the rod under a glass layer substrate (Figure 9) showed the same field pattern as it did on a Si and YSZ substrate. However, the field intensity was increased by a factor of 4 compared to the field enhancement map on silicon and a factor of 2 when compared to that of YSZ.

In all of the field enhancement plots, the electromagnetic field loops around the nano-rod from one side to the other. Given the electric field direction and the normal direction of the induced magnetic field, a pointing vector can be drawn using $\vec{S} = \vec{E} \times \vec{H}$. When applied to the micro-propeller, an electric field pointing from the middle of the device to the edges, and a magnetic field oriented perpendicularly overtop the nano-rod would result in momentum transfer downwards into the rod. This energy flux density
incurred by the electromagnetic field would be applied over both rods on opposite sides at both ends of the propeller, imparting some torque.

![Figure 9: Field enhancement of a single Ag rod on a fused silica layer 40nm above the surface of the rod with the inside edge of the rod (a), and the right edge of the rod (b).](image)

**Substrate and Rod Material Optimization for Natural Convection**

To maximize the thermal gradients while maintaining distinct thermal nodes, material optimization was required. For the purpose of localized natural convection, three potential substrate materials (quartz glass, yttria-stabilized zirconia, and silicon) and three possible metal rod materials (gold, silver, and copper) were investigated. In the proposed micro-propeller design, the substrate acts as a thermally insulating layer which further promotes the asymmetry of the heat profile. To this end, a substrate material with a low thermal conductivity, $k$, and high heat capacity, $C_p$, were desired. To maximize the temperature gradient for natural convection to occur, a conductive rod material with high thermal conductivity, and low heat capacity, was required. A table of these values can be seen in table 1.

<table>
<thead>
<tr>
<th>Material</th>
<th>Thermal conductivity (W/mK)</th>
<th>Heat capacity at const. volume (J/kgK)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Quartz Glass</td>
<td>1.4</td>
<td>730</td>
</tr>
<tr>
<td>YSZ$^{26-27}$</td>
<td>2.2</td>
<td>400</td>
</tr>
<tr>
<td>Silicon</td>
<td>159</td>
<td>712</td>
</tr>
<tr>
<td>Gold$^{28}$</td>
<td>314</td>
<td>126</td>
</tr>
<tr>
<td>Copper</td>
<td>385</td>
<td>386</td>
</tr>
<tr>
<td>Silver$^{28}$</td>
<td>406</td>
<td>223</td>
</tr>
</tbody>
</table>

*Table 1: Material properties of substrate and rod candidates.*

Simulations were conducted in 2D to observe a cross section down the length of the propeller in order to map thermal profiles of the rod with the substrate. According to the heat transfer simulations, there was only slight differences between the gold, silver, and copper rods in their ability to accumulate thermal energy over the given time range. However, due to the increased scattering cross section of silver at infrared wavelengths, the thermal energy
generations for silver should be greater than copper and gold. Based on the scattering cross sections from the MNBEM toolkit simulations using Matlab and the thermal properties of rod material candidates, it was determined that silver would result in the greatest heat generation and also facilitate the greatest temperature gradient for natural convection.

Heat transfer simulations were also performed to choose the best substrate material among silicon, YSZ, and quartz glass (figure 10). These simulations modeled the thermal evolution of the different materials over 60 seconds with an overall heat generation rate of 0.5 W. Since these models were only used to qualitatively measure the differences in the thermal properties, convective forces and heat flux in the z direction was omitted to allow 2-D simulations and lessen the computational load.

![Thermal profiles of silver on glass (a), silver on YSZ (c), and silver on silicon (e).](image)

*Figure 10: Thermal profiles of silver on glass (a), silver on YSZ (c), and silver on silicon (e). The isothermal profiles of silver on glass (b), silver on YSZ (d), and silver on silicon (f) make the locality of the thermal nodes more apparent.*

In the case of silver on silicon, the relatively high thermal conductivity of silicon doesn’t insulate the heated rods from each other, resulting in a single node of isothermal profiles that envelop the entire micro-propeller (figure 10f). The YSZ substrate is two orders of magnitude less thermally conductive which allows more distinct, thermal notes to form (figure 10d). Finally, quartz glass had both the lowest thermal conductivity and heat capacity which was reflected in the modeled thermal profiles. In figure 1b two distinct thermal nodes can be observed where the temperature at the center of the substrate only rose 2.7°C from the initial condition compared to 4.2°C for YSZ and 53.46°C. From these results, quartz glass was chosen to be the substrate material.

**Fluid Velocity**

In order to observe fluid flow perpendicular to the propeller length, volume forces and buoyancy forces dependent on the depth of the water had to be taken into account. To do this
with minimal computational effort, 2D simulations were performed for cross sections of the propeller, bisecting both the substrate and a metal rod. Initial conditions for laminar flow were initiated by setting depth dependent pressure $P = \rho gh$ throughout the fluid volume. Volume force was applied by setting force in the direction of gravity as $F = -g \times \text{nitf1.rho}$ where nitf1.rho refers to the temperature dependent density of the fluid material. The evolution of the fluid flow was modeled over a span of 45 seconds at 0.5 second intervals. Fluid velocity was probed 2.75 mm away from both sides of the micro-propeller for substrates of varying thickness from 1 mm to 2.5 mm and the. Figure 11a shows a simulation snapshot of a 1 mm thick substrate at $t = 45s$.

Figure 11: Velocity color maps for cross sections of the micro-propeller. The large white rectangles represent the of the substrate and the small squares are the sides of the metal nano-rods. Red arrows represent the direction and relative magnitude of the fluid velocity on both sides of the propeller. Greater velocity difference indicates greater net momentum transfer of the fluid to the propeller face. a.) shows the surface velocity of a 1mm thick propeller. b.) shows the velocity of a 2.5mm thick propeller.

To maximize the generated torque, the differences in fluid velocity on the two sides of the propeller must also be maximized. It was observed that this percent difference in fluid velocity was proportional to the thickness of the substrate as seen in figure 12. This appeared to be primarily caused by the increased insulation across the substrate, more effectively containing the natural convection currents to one side of the propeller.
Figure 12: Percent velocity difference for a rectangular substrate (blue) and for a finned substrate (orange) as a function of substrate thickness. It is worth noting that the fluid velocity on the rod-side of the propeller was consistent for both rectangular and finned substrates, meaning that the net velocity difference was also increasing as a function of substrate thickness.

Over the range of substrate thicknesses tested, the relationship between percent fluid velocity difference and substrate thickness appears to be linear. Based on the observations of the simulations it can be hypothesized that at an infinite substrate thickness, there will be no natural convection on the rod-less side of the propeller, and thus an infinite percent velocity difference. However, one can expect the appearance of an optimum substrate thickness as the fluid velocity has to overcome the inertia of an increasingly massive object. This could be calculated to some degree of usefulness if more accurate boundary conditions could be determined and the correct micro-scale dimensions could be modeled.

It was also found that the cross sectional profile of the micro-propeller substrate could enhance the fluid velocity difference. By adding fins to the top and bottom of the propeller, the percent fluid velocity difference was increased by an average of 9.28% across all thicknesses (figure 12). Qualitatively, this also increases the surface area for the dynamic pressure from the fluid to perpendicularly act upon, increasing the total force contributing to torque (Figure 13). This increase in percent velocity difference is accounted for by a drop in velocity on the rod-less side of the propeller (velocity on the rod-side remains the same) which may be caused by an increase in the insulating volume and the surface area for heat dissipation provided by the fins. However, further investigation is required to determine the real cause of the velocity drop.
Results and Discussion: 3D Model for Velocity Profile

Finally, it was necessary to ensure that fluid velocities down the length of the propeller would not interfere or even cancel each other out. To do this, a full 3D model was built, retaining the initial conditions and boundary conditions from the 2D fluid velocity models. Figure 4 shows a velocity profile along the length of the rod which includes velocity vectors that suggest torque generation.

Due to the computational effort involved in 3D time dependent simulations, only a few simulations were completed. However, based on the 2D simulations, it would be expected that the finned substrate would demonstrate larger velocity differences, implying a greater tendency towards rotation.

Figure 13: Velocity profile of the finned 2.5 mm thick substrate. Fin features increase the fluid velocity difference by about 9.28%.

Figure 14: Color map of the fluid velocity around a 3 mm thick, silver and glass micro-propeller with velocity vectors indicating direction and relative magnitude of fluid flow. The opposite directions of the fluid flow at the two ends of the propeller suggest torque generation and rotation.
**Conclusion**

In this study, the thermal harvesting principle established by Karker et. al. was tuned to an operating temperature of 50°C by extrapolating the necessary aspect ratio of a metal nano-rod. At an aspect ratio of 1:60 was calculated for a nano-rod to be plasmonically active at a wavelength of 15 µm, corresponding to the spectral radiance given off at 50°C. However, to extend functionality, it was found that a 1:20 aspect ratio was sufficient for absorption at the 15 µm wavelength. An MNPBEM toolbox was implemented in Matlab to model the optical response of the micro-propeller to spectral radiance. Using the optical data, the rod and substrate materials were optimized to create the greatest plasmonic enhancement that would lead to the greatest electric field enhancement. It was determined that the best noble metal nano-rod material to use was Ag and the optimal substrate material was fused silica glass. COMSOL was used to provide proof of concept for the formation and utilization of natural convective forces which propel the device. Favorable materials and dimensions for induction of natural convection were determined. It was ultimately found that silver nano-rods on glass resulted in the most conducive conditions for torque generation and rotation.

**Future Work**

More accurate boundary conditions and modeling parameters will allow more telling models to be simulated. Accurate quantitative results will allow researchers to calculate net torque generation that would need to overcome frictional, inertial, and drag forces to rotate. In order for these calculations to be made, the absorption cross section of the micro-propeller would first need to be determined. The absorption cross section would also facilitate calculation of the total extinction cross section, which is composed of absorption and scattering cross sections, and would give the summation over all electric and magnetic multipole oscillations. The end result would be more accurate plasmonic data.

In order for the correct scaling of the device to be modeled, the COMSOL microfluidics module would have to be used. Additionally, a more specific application in mind may allow more relevant assumptions about the boundary conditions to be made. Additionally, the implementation of a deformable mesh geometry available in COMSOL may give insight into the dynamic effects of micro-propeller on the convective currents surrounding it once it has already begun rotating.

Moreover, the size of the device could still be reduced. Other plasmonic materials, such as some metal oxides and plasmonic ceramics, are also potential candidates for implementation into optical micro-propellers. Different geometric features could also be used for absorption of IR radiation. In this study, nano-rods were investigated because of the linear dependence on the peak position vs. aspect ratio determined by Karker et al., but optically induced rotating devices have been made using alternative geometries such as light mills and nanoantennas.
**Individual Contributions**

The MATLAB MNPBEM modeling and analysis was done by Jacqueline Elwood. The COMSOL modeling and analysis was done by Jerry Shih.

**References**


