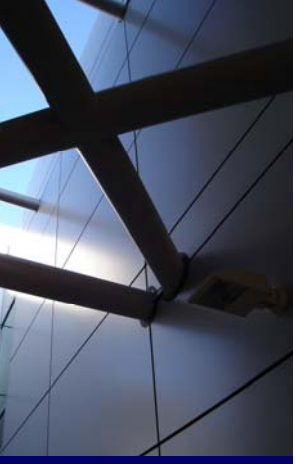

MECHANICAL ENGINEERING
DISSERTATION DEFENSE

*The Department of Mechanical Engineering presents:*

# *The Master's Dissertation Defense of*

# Kairui Xia

## Friday, August 17, 2018,
## 1:00 PM in Bourns Hall A265

### *Modeling & Simulation of a Photocatalytic Microreactor with COMSOL Multiphysics*

Master Master of Science, Graduate Program in Mechanical Engineering

University of California, Riverside, August 2018

Dr. Masaru Rao, Chairperson


Producing enough drinkable water is a great challenge for long-term deep space missions. A small scale photocatalytic microreactors with nano-porous $TiO_2$ coated titanium micropillar arrays is designed to solve the problem. COMSOL Multiphysics is used to simulate several parts of microreactor. The first objective is to model the tree-branched bifurcating inlet and the diamond-shaped inlet, then the flow velocity and pressure drop in these two inlet systems are compared. Based on simulation results, the tree-branched bifurcating inlet can provide more residence time in the microreactor due to lower pressure drop inside the inlet channels which increases the photocatalytic efficiency. However, the extension of channels increases the area this inlet takes up reducing the size of the reactor chamber. The diamond-shaped inlet can increase the volume of water flowing through microreactor due to the uniform flow velocity inside the inlet and outlet channels which enhances the throughput of microreactor. This inlet can be as compact as possible according to its geometry which gives more space to reactor chamber. However, the pressure drop between inlet and outlet increases about 256% compared to the pressure drop of tree-branched bifurcating inlet which reduces the residence time. The second objective is to simulate photons interaction among micropillars and light intensity along the micropillars under UV irradiation, and determine the optimal micropillar heights that can make the microreactor have the best photocatalytic efficiency. According to simulation, the optimal height should be chosen between 50 um and 100 um. For 50 um micropillars, the light intensity reaches 1.42 $mw/cm^2$ where is 10 um away from bottom, and light intensity keeps increasing along the micropillar. For 100 um height micropillar, 50% surface area has low photocatalytic efficiency, but the 100 um micropillar allows more water to flow through microreactor compared to the 50 um micropillar. Combining the advantages of micropillars with these two heights, the height should be chosen between 50 um and 100 um.