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Interfacial Transport Modeling Through Use of MatLab and Surface Evolver

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Semester Report Benjamin Gaffney
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Abstract: The object of this research semester was to become more familiar with the research area of the Nanoscale Energy and Interfacial Transport (NEIT) lab led by Dr. Damena Agonafer, establish the physical lab and its materials, verify Popov's model using MatLab , and finding the lowest energy state of a steady state meniscus using Surface Evolver. Progress on each of these tasks has been significant, and in the process valuable skills have been developed such as MatLab modeling, coding using c and operating Surface Evolver, collaborating , and holistically analyzing a population of journal articles to understand the subject. Outcomes of this semester include a much deeper understanding on the topic, knowledge in using both MatLab and Surface Evolver, and a lab that is near complete in terms of being set up.

Semester Report
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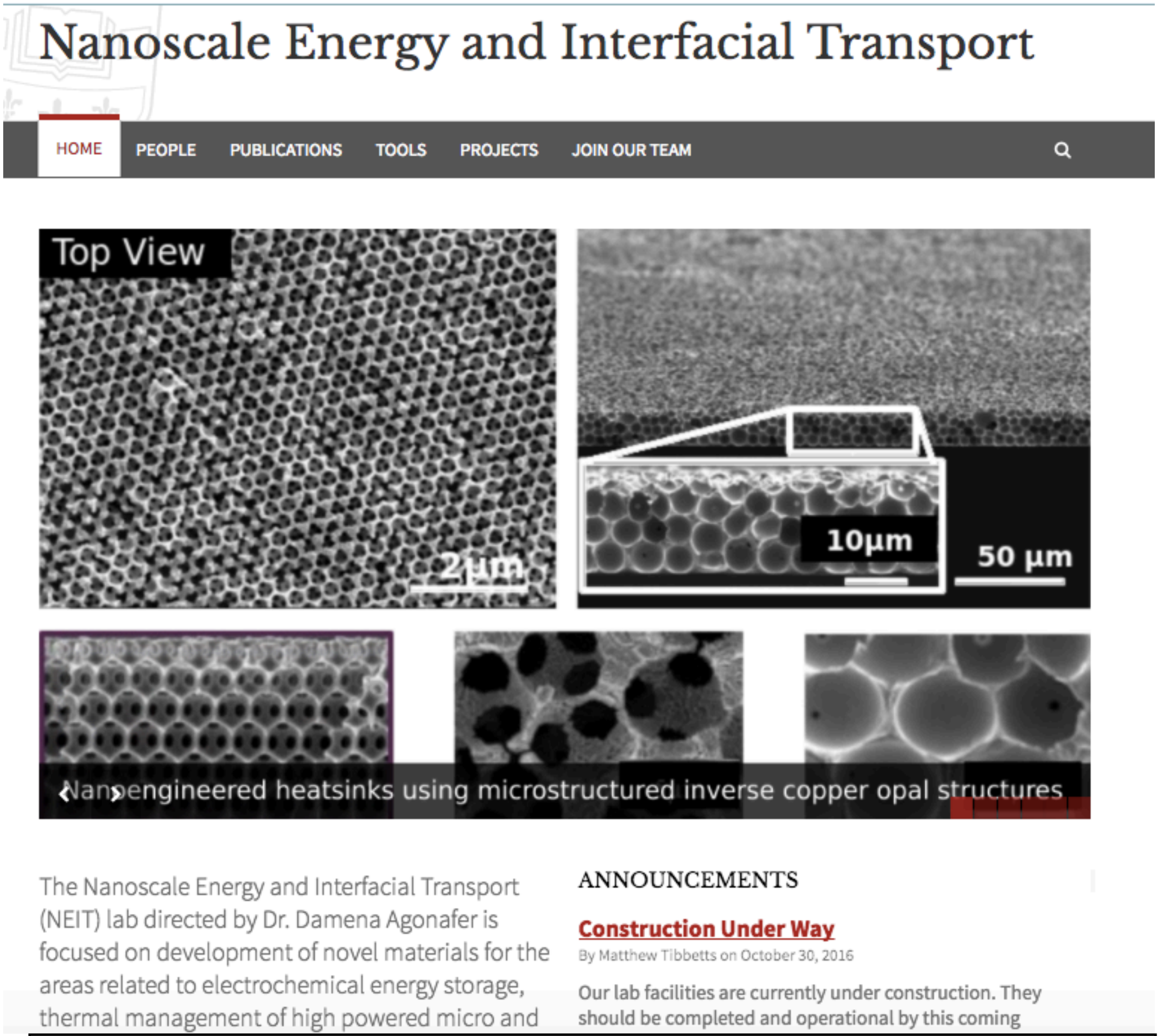
Introduction: This semester the Nanoscale Energy and Interfacial Transport lab, whose Principal Investigator is Dr. Damena Agonafer, began establishing the infrastructure to pursue research into high-heat transfer through liquid cooling, which includes development of microscale porous materials and

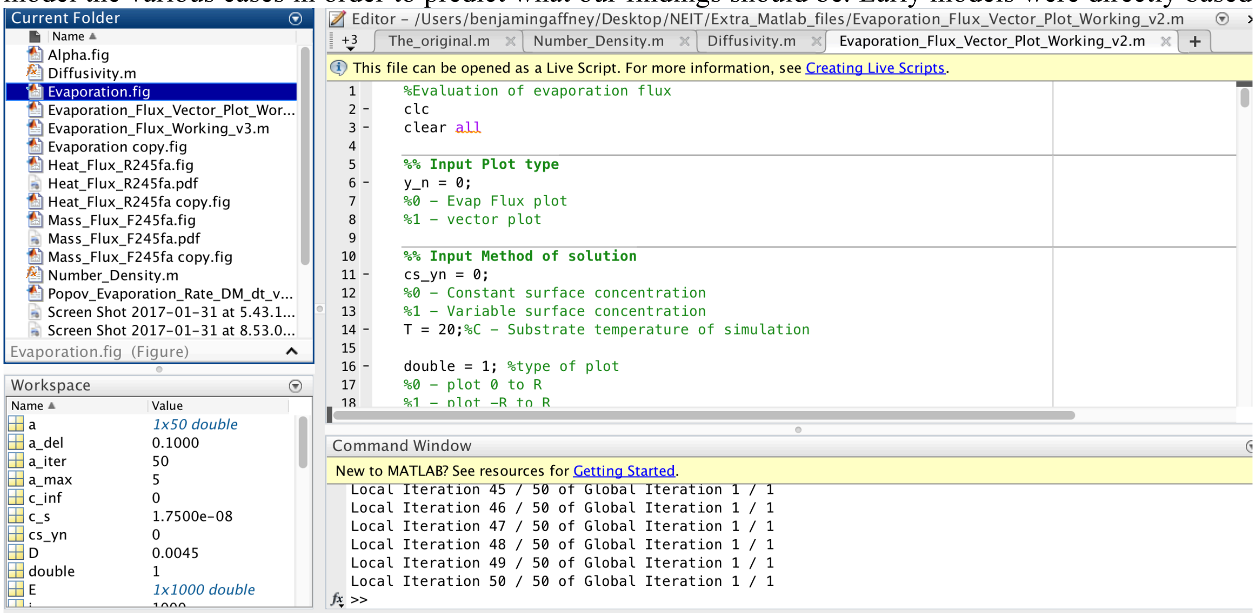


The homepage of the lab website, neitlab.wustl.edu.

nanoscale geometries for optimal pinning and heat transfer.

As a new lab at Washington University, the priority this semester was to get all members familiar with the research material and begin planning experimental methods that would be used in order to purchase new lab equipment and be prepared for when experimentation commences. Dr. Agonafer encouraged the students to pursue their own research online through related journal articles and then relay the new information to the rest of the lab members through summaries and presentations. Each week during lab meetings members would present their findings and Dr. Agonafer answered and asked questions related to concepts that played roles in the larger picture of our project.

The second priority was to become familiar with any tools required for both modeling and experimentation. The goal was to be well prepared for when it came to experimentation and be able to model the various cases in order to predict what our findings should be. Early models were directly based



The Interface of MatLab

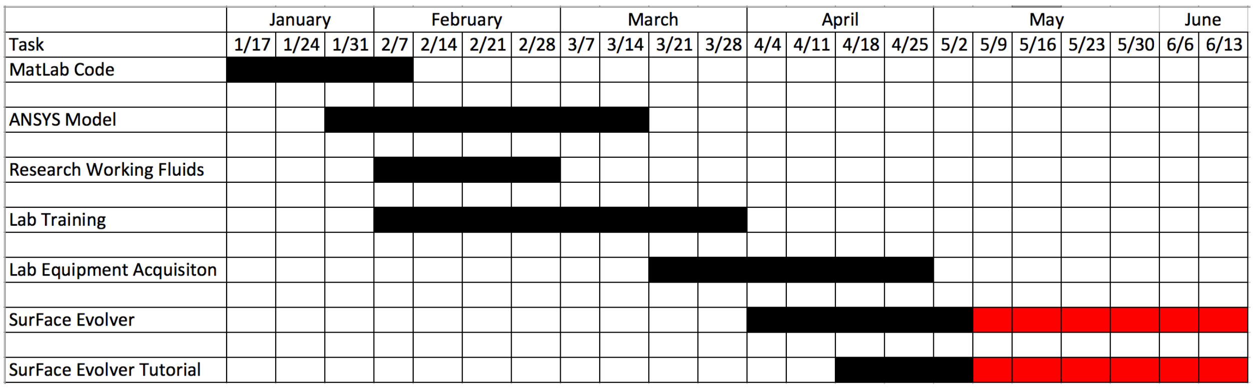
off of research articles, which allowed us to verify our modeling methods against scenarios where we know the outcome.

The work that occupied a majority of time in the first half of the semester was producing the data from the article that was known to be correct. This was the data that would be used to test the numerical model developed by the lab. In order to achieve the Popov Model (the known model against which we tested) and MatLab had to be used. MatLab allowed the use of a code that was previously developed by Dr. Agonafer at Stanford. This code calculated various values involved in Popov's Model, but it had to be adapted in order to produce valuable data that could be compared to the data produced by the numerical model, which was run through the use of ANSYS FLUENT. This verification was part of a deeper goal of developing a numerical model that accounted for more variables than previously developed models.

The second half of the semester was focused on both the use of Surface Evolver and the acquisition of equipment for the lab. Surface Evolver is a program developed to find the lowest energy state of a fluid given certain values such as contact angle and gravity. This tool can prove to be very useful when examining meniscus shape of a droplet that is in steady state. Surface Evolver is based on the coding language of C and its interface is simply a text writer. In order to use Surface Evolver and produce useful data, coding in C must be understood relatively well. Progress for using this program was slow at the start due to the very limited number of tutorials and learning resources related to the program.

To rectify this problem I have been developing a tutorial for the lab throughout the process of learning the program. Along with studying the shapes of droplets general lab equipment had to be taken care of in order to make the lab ready for experimentation come the summer. Simple equipment, such as hand tools, all the way to complicated experimental setups that were designed by the lab had to be ordered. Along with the ordering was the requirement of understanding how the equipment works and learning both how to setup and operate it in the future.

All of this work was in preparation creating a functioning lab that has a strong basis in the simulation side of the research and is prepared to start experimentation of the models created.

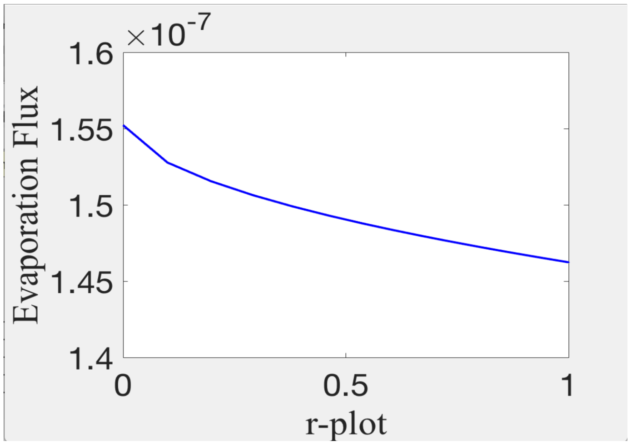


Gantt Chart displaying major tasks of the semester **Note:** red indicates future tasks

Materials and Methods: The primary tools for this semester of research were Surface Evolver and MatLab. These tools proved to be valuable to the creation of a new numerical. MatLab was vital to the verification of the model itself. Before the numerical model could be used in any research it first had to be proved to be a working model that produces correct results. MatLab allowed for the computation of the results against which the numerical model was tested. Other lab members used ANSYS FLUENT to produce the results using the new model. These two results were compared and the model was amended until a working model was created.

Surface Evolver came in later because it is vital to the use of the model. Once the newly developed numerical model was verified, certain characteristics specific to the experimental setup had to be determined. Knowing the materials involved allows for the knowledge of what the fluids working contact angle is. This information can then be used in Surface Evolver to discover what the meniscus shape is. In the implementation of this program gravity was not a factor, because on the scale that our experimental setup is, gravity is not a factor.

Results: Not every goal set at the start of the semester was met, but as the semster went on new goals were created and old ones were determined to be unecessary.



The graph that displays the evaporation flux versus radius obtained form MatLab

Throughout the semester comprehension of the research topics was greatly improved. This was achieved through literature searches that were performed early on in the semester and the collaborative weekly meetings where the all the lab members discuss findings and answer any questions other members may have.

Through tutorials and advice form other lab members proficiency in Surface Evolver and MatLab has greatly improved. The skill level for both these programs will continue to grow as they are used more and more complex models are developed.

Future Directions: Simulations will be run using ANSYS FLUENT that utilize the new numerical model, which is implemented through the use of a UDF (User Defined Function). This program will be used to run various simulations based of different geometries and the information found from the use of Surface Evolver. Surface Evolver will be used to crate a wide range of non-wetting surfaces in order to predict the meniscus shape of the droplets.

These meniscus shapes will then be imported to ANSYS FLUENT, which will be able to simulate our results. These geometries that are simulated will then be implemented in a lab setting where an actual experimental setup is used and the properties such as contact angle and meniscus shape can be observed. The new equipment that was ascertained this semester will be used to examine the properties of the experimental geometries and droplets.