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Mentorship for an interdisciplinary numerical and experimental investigation of colloidal transport within evaporating droplets under an electric field

1. Executive Summary

The goal of the proposed work is to develop external mentoring relationships with international renowned experts while furthering an interdisciplinary research collaboration to improve the fundamental understanding of colloidal transport in evaporating droplets in the presence of an electric field. Colloidal transport is typically governed by contact line pinning and the interplay between evaporative and surface tension effects[1–13]. Application of an electric field has the potential to disrupt the interplay between these effects by introducing an electrowetting force at the contact line and an electrophoretic force on charged colloids in a droplet (Fig. 1). The proposed work will isolate the effects of electrowetting and electrophoresis and examine their importance relative to evaporative effects through the development of a mathematical model. The multidisciplinary nature of the team will by leveraged by using experimental data to inform and support the model.

This also proposal seeks to form a mentoring relationship with Dr. Petia Vlahovska, an Associate Professor of Engineering at Brown University, who is an expert in modeling fluidic systems under the influence of electric fields. During her postdoc at the Institute for Mathematics and its Application (IMA), PI Maki worked on modeling evaporating particle-laden droplets focusing on identifying the mechanism causing the formation of a skin of particles during drying[14]. The proposed work requires the inclusion of an electric field, Dr. Vlahovska's area of expertise. PI Maki first met Dr. Vlahovska in 2007 during the Pan-American Advanced Studies Institute on Interfacial Fluid Dynamics: From Theory to Applications, in Mar de Plata, Argentina. Dr. Vlahovska was an invited speaker and PI Maki was a graduate student. The two met again in 2009 at an IMA workshop on complex fluids and flows. We propose to invite Dr. Vlahovska to visit RIT in the fall of 2016. This will allow us to seek her expert advice on modeling

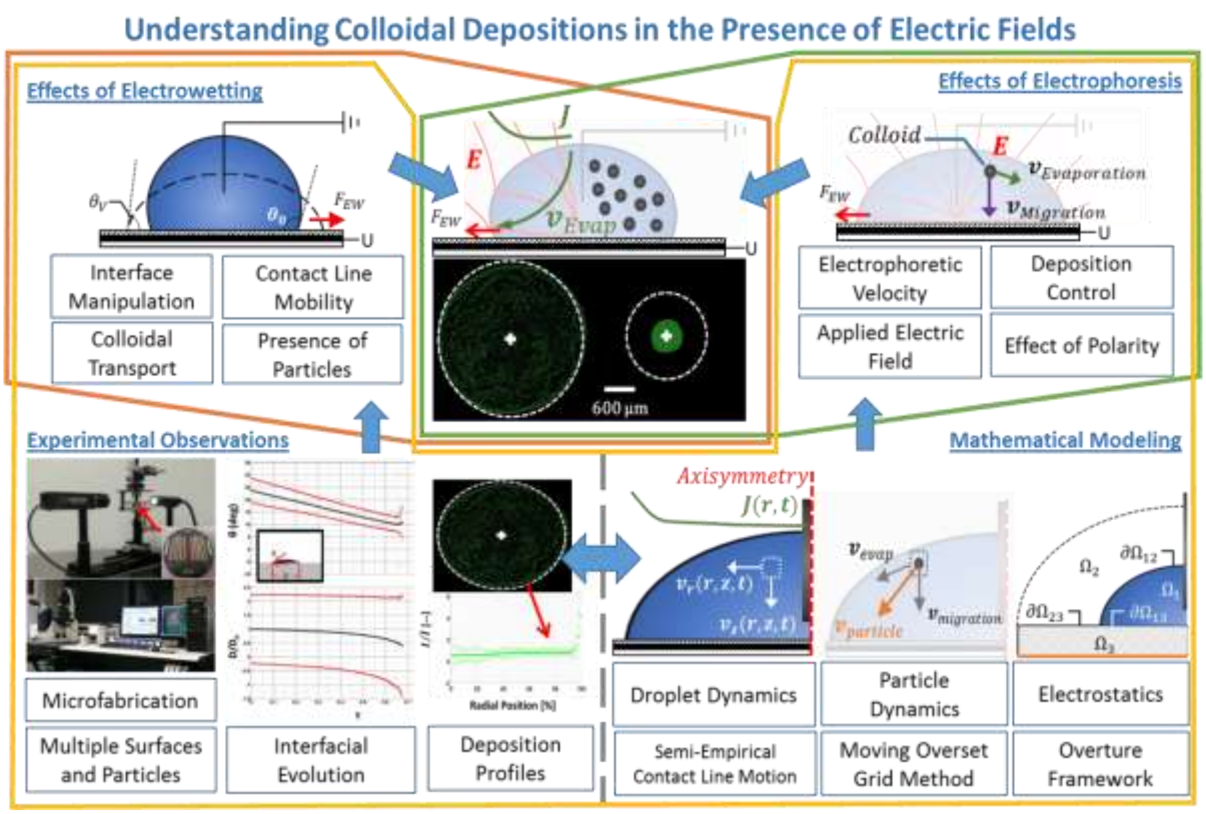

Figure 1 Overview of overall research project. This proposal focuses on implementing the Model above.

electric fields while providing an opportunity to share our current work and explore a potential collaboration. Dr. Vlahovska will also be asked to present a joint organized seminar in COS and KGCOE, bringing visibility to PI Maki and Co-PI Schertzer's interdisciplinary work.

Finally, we propose to present our work at the NTNU International Workshop on New Understanding in Nanoscale/Microscale Phase Change Phenomena in Trondheim, Norway. Participation in this event is by invitation only. PIs Maki and Schertzer were both invited by Dr. Satish Kandlikar (Mechanical Engineering, RIT), who is co-organizing the event. Presenting to an international panel of experts will raise the profile of the research and provide opportunities for external and international collaboration and mentorship. PIs Maki and Schertzer will also be able to build on their joint publication record by writing a book chapter and an invited journal paper together discussing their contributions to the workshop. Co-PI Schertzer will represent the team at this event as PI Maki has an infant at home. Dr. Kandlikar will continue to serve as an internal mentor in all aspects of this opportunity.

2. Detailed Project Description

Hypothesis: *The magnitude and polarity of an applied DC voltage can be used to control colloidal transport in an evaporating droplet through the introduction of an electrowetting force on the contact line and an electrophoretic force on the colloidal material.*

The hypothesis will be tested by developing a mathematical model to identify the underlying mechanism for suppression of the coffee-ring effect observed during DC actuation[15]. Model predications that describe the fundamental underlying mechanisms for colloidal transport in these cases will be tested through comparison with experimental results.

This proposal aims to develop a model that is realistic enough to capture essential behavior of particle dynamics, but simple enough to analyze and solve. Modeling efforts will focus on understanding the interplay of the evaporative-driven flow and the influence of the electrowetting and electrophoretic effects. Experimental results completed in Co-PI Schertzer's lab[16,17] will be used to support and guide the model development. The model is comprised of the three-coupled pieces: (i) droplet dynamics; (ii) particle dynamics; and (iii) electrostatics (Fig. 2). An analytical framework for this model has been developed and is presented in the proposal submitted to NSF by the PIs[18].

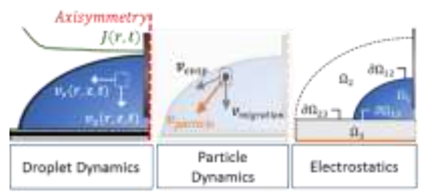

Figure 2 Sketches showing the coupled components of the model.

The droplet dynamics model assumes an axisymmetric droplet of a Newtonian solvent (water) containing colloidal particles with a needle electrode inserted in the center of the droplet. The droplet is small enough that surface tension dominates over gravitational effects and gravitational effects can be neglected. The effects of particles on fluid flow and surface tension are initially ignored, as is the effect of the electric field on fluid flow. Because the droplet is thin, we use lubrication theory to explain the evolution of the droplet interface. Unlike PI Maki's prior work[14], we propose to modify the model to include diffusive-limited evaporation[1-3] and to change the contact line dynamics to better approximate the experimental results. Particle dynamics will be described by a standard convective-diffusion equation[14]. We propose to model electrostatics in the droplet, substrate, and air by solving the Laplace equation for the electrical potential in each domain, and imposing continuity of electrical potentials and current at the boundaries[19]. Using the electrical potentials, we can quantify the electric field and then the magnitude of the electrophoretic and electrowetting effects. Dr. Vlahovska's expertise will inform our modeling choices for the electrophoretic and electrowetting effects[20,21].

3. Project Implementation Plan and Timeline

Over the summer of 2016, a mechanical engineering co-op student (undergraduate) and an applied and computational mathematics master's student will work in a team. The students will modify PI Maki's prior work[14] by (i) changing the evaporation model to be diffusion-limited, (ii) removing the precursor film to match the contact line dynamics of the experiments, and (iii) testing different boundary conditions to match the experimental results. A numerical method based on a moving overset grid method will be implemented in the C++ framework called Overture[22]. The students will be able to modify PI Maki's existing code. We plan to consult Dr. Vlahovska on modeling choices relevant to the implementation of electrophoretic and electrowetting effects. These effects will be added to the model in the fall of 2016 after her visit. First, we will include the electrowetting effects followed by the electrophoretic effect.

The project will be managed by the research team as shown in Table 1.

Table 1: Project Management Plan

Activity	Summer 2016		Fall 2016			Spring 2017		
Initial Derivation of Analytical Model	**Complete**							
Droplet Dynamics model in Overture								
Attend NTNU Workshop								
Invited Seminar: Dr. Vlahovska								
Introduce electrowetting / electrophoretic effects into Overture model ***(Continued by MS student recruited above)***								
Submit Invited Publications								

5. Project Evaluation Plan

The project will be continuously evaluated using the following interactions throughout the timeline:

- weekly planning and project review meetings with students on modeling and experimental teams;
- comparison of experimental results and model predictions;
- solicitation of expert external advice through Petia Vlahovska at Brown Universtiy and the microscale evaporation community at the NTNU Workshop;
- peer review comments from invited publications through NTNU Workshop.

6. Description of Participants Roles

PI Maki will lead the model development. She will advise the requested co-op and master's students supported in this grant. Co-PI Schertzer will lead the experimental team. Experimental details of this research are not included here as they are beyond the scope of this proposal. The experimental team this summer will consist of four undergraduate honors students and one graduate student. Modeling and experimental teams will continue their current practice of meeting weekly to continuously evaluate progress toward the goals of the project.

7. Relevance to Plan of Work

Maki and Schertzer are Research Intensive pre-tenure faculty. Activities proposed here are an excellent opportunity to connect with world renowned researchers and produce high quality publications. The interdisciplinary nature of the proposed research aligns with RIT's new strategic plan and will show a promising growth in future research programs of PI Maki and Co-PI Schertzer in their tenure packages.

The PIs will leverage the mentoring relationships developed here by seeking insight into modeling choices, grant writing, and publication avenues. Relationships with external mentors will also provide the PIs with champions who can support grants and journal articles throughout the review process. Invited publication of high quality manuscripts will lend credibility to external proposals written by the PIs, while providing an opportunity to build their joint publication record.

Preliminary data from the proposed work will be used to support external grant proposals to:

1. *NSF CAREER: Particulate and Multiphase Processes: $500,000 (5 Years) – **New Proposal***
2. *NSF Nanomanufacturing: $300,000 (3 years) – **New Proposal***

3. *Samsung Global Research Outreach*: $99,981 (1 year) – ***New Proposal***
4. NSF Particulate and Multiphase Processes: $300,000 (3 years) – **1st Resubmission**

8. Budget and Justification

Dollar Amount	Budget Item	Description / Justification
$xxxx	MS Summer Salary	Lead (1) development of droplet dynamics model in Overture and (2) compare model predictions to experimental results.
$xxxx *(+$2,000 KGCOE Dean's Match)*	BS Summer Co-Op	Support MS Student activities. *This student is co-funded through the KGCOE Dean's Matching program, which will contribute an additional $2.000.*
$xxx (COS CACM Seminar Match)	Professional Fees	Flight, hotel, and meals for Dr. Vlahovska's 3 day visit to RIT.
$xxx	Domestic Travel	Flight, hotel, and meals for Dr. Maki's 3 day visit to Brown.
$xxxx *(+xxx match from M.E. Dept.)*	International Travel	Registration, flight, hotel and meals for attendance at New Understanding in Nanoscale/Microscale Phase Change Phenomena in Trondheim, Norway. *Round trip flight will fly out of Toronto (~ $750) not Rochester of Buffalo (~ $1,500).*
$13,500	**Total Costs (Includes $3,500 matching Funds from COS and KGCOE)**	
$xxxx	**Total Funding Requested from Connect**	

9. Relevance to AdvanceRIT Goals

The proposed research seeks to *enhance the working environment and support career advancement of women faculty through empowerment, inclusion, and other symbolic aspects of women's professional quality of life*. If awarded, the visibility of PI Maki and Co-PI Schertzer will be raised on RIT's campus through the COS and KGCOE jointly held seminar given by Dr. Vlahovska as well as through the AdvanceRIT's announcements and recognition ceremonies. It will also bring visibility in the scientific community through participation in the NTNU workshop and related invited publications. Finally, the proposed work will show a promising growth in future research programs for the PIs' tenure packages.

10. Broader Impacts

Understanding the role of an applied electric field on colloidal transport may allow for dynamic real-time control of colloidal deposition. Control of this process would benefit applications in medicine (diagnostics, drug screening, biostabilization) and advanced manufacturing of flexible electronics.

The proposed project offers multidisciplinary research opportunities for one MS and one BS student. The PIs support active recruitment of students from groups that are commonly underrepresented in academia. The PIs also engage in activities that promote STEM education for young women and students in low income areas. They also promote STEM education through Imagine RIT.

11. Intellectual Merit

While prior theoretical works describe the electrohydrodynamic flow in non-colloidal droplets in AC and DC electrowetting, few model particle dynamics in an applied DC electric field. The PIs are not aware of any works that systematically identify contributions of electrowetting and electrophoresis to this problem.

A deeper understanding of the effects of electrowetting and electrophoresis on colloidal transport may allow for dynamic control of colloidal deposition. The proposed research presents a systematic multidisciplinary approach to examine these effects. Experimental data will be used to support model results, while detailed model predictions be used to give insight into physical results from experiments.

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