EUROPEAN COOPERATION
IN SCIENCE & TECHNOLOGY

SHORT TERM SCIENTIFIC MISSION (STSM) – SCIENTIFIC REPORT

The STSM applicant submits this report for approval to the STSM coordinator

Action number: TD1409 - 41265
STSM title: Mathematical models for moving boundary problems in industry
STSM start and end date: 24/05/2018 to 31/05/2018
Grantee name: Dr. Vincent Cregan

PURPOSE OF THE STSM

The aim of this STSM was to develop mathematical models for two related moving boundary problems from industry, namely:

1) the removal of stains and residues from equipment in the pharmaceutical industry;
2) the contact melting of temperature-dependent phase change materials (PCMs).

The STSM was multi-disciplinary as it bridged the gap between mathematics and industry where the purpose was to understand the interaction between solid-liquid interfaces during the above industrial processes. In this section we describe the problems and the specific goals associated with each.

Problem 1: The removal of residues and stains from equipment surfaces is a critical operation in the pharmaceutical industry. Cleaning is performed during the changeover from the synthesis of one product to another to prevent cross contamination of active product ingredients (APIs). Whilst cleaning has always been a time consuming and costly operation, it has become more troublesome recently with an increasing focus on smaller production volumes. This leads to an increase in product changeovers, and hence more time spent dedicated to cleaning. Consequently, industry is constantly seeking the development of optimal strategies that minimise both the time and resources dedicated to cleaning.

The aim of the STSM was to support the improvement of new cleaning methodologies by developing and analysing an advection-diffusion mathematical model to explain the removal of an API from a surface via a liquid. The model will be validated by comparing the associated solutions to experimental data from a small-scale laboratory cleaning rig constructed by my collaborators in the Pharmaceutical Manufacturing Technology Centre (PMTC) in the University of Limerick (Ireland).

Problem 2: PCMs are substances that absorb and release thermal energy during the processes of melting and freezing, respectively. Due to their desirable properties, PCMs are used in a range of applications including thermal energy storage and the transportation of temperature sensitive materials. Contact melting, a process associated with PCMS, is when a PCM is placed in contact with a warm surface that is maintained above the PCM melt temperature. As the PCM begins to melt, a thin liquid develops between the two surfaces. The weight of the solid acts to squeeze out the liquid, and thus the melt layer remains thin.

The final melt time is a key parameter required by industry. A standard approximation in the existing literature is to assume that PCM material properties do no not vary with temperature. However, this is not always valid, especially for applications subject to large temperature variation.

The goal of the STSM was to reconsider the standard PCM contact melting model and study the effect of temperature-dependent conductivity and viscosity on melting.

DESCRIPTION OF WORK CARRIED OUT DURING THE STSMS

Throughout the STSM I had regular research meetings with Prof. Myers. An initial meeting was used to outline the background to both problems and work-to-date. Daily meetings were arranged to discuss progress and define tasks and goals. In the case of both problems, mathematical modelling techniques were used to describe the underlying physical mechanisms involved. In what follows, I describe the key tasks performed during the STSM.

Problem 1: Prior to the STSM I had formulated part of the model to describe residue removal. The primary task of the STSM was to formulate the full model. The governing equations consist of the Navier-Stokes equations to describe the motion of the liquid over the residue. A two-dimensional advection-diffusion equation is used to explain mass transfer of material from the residue into the liquid. In addition, all of the boundary conditions have now been prescribed. We assume no-slip at the residue-liquid interface, zero shear stress at the liquid free surface and mass conservation at the residue surface.

Next we used a time scale analysis to identify the time scales associated with the physical processes of the problem. The key time scale is the residue removal time scale which is of the order of minutes. This time scale is larger than those pertaining to advection and diffusion. In physical terms, this corresponds to the removal process becoming independent of time after a short, initial, transient period. Using the removal time scale in the nondimensionalisation allowed us to neglect the time dependence in the model.

The next task of nondimensionlisation and the resulting dimensionless model will be discussed in the following section.

Problem 2: As highlighted in the project proposal, I had done considerable research on temperature-dependent contact melting prior to the STSM. My research had led to an extensive outline for a paper on temperature-dependent contact melting. Following Prof. Myers's guidance, I completed my analysis of the problem. In particular, I used the Heat Balance Integral Method (HBIM) to obtain approximate solutions for the temperature of the PCM as melting finishes.

DESCRIPTION OF THE MAIN RESULTS OBTAINED

Problem 1: The main result was the formulation of a reduced, dimensionless model. Rescaling the equations of motions yielded the standard thin film equations, which were solved exactly for the velocity field of the liquid. The advection-diffusion equation was reduced to a two term partial differential equation balancing advection in the direction parallel to the flow with mass diffusion perpendicular to the flow. These reduced equations are much easier to solve than the full model and allow for approximate solutions, and for some parameter regimes, exact solutions.

In addition to the above, there have been several tangible outcomes since the completion of the STSM. Our preliminary results were presented at the Modelling of Cleaning and Decontamination minisymposium at the European Consortium for Mathematics in Industry Conference 2018. This meeting was beneficial as several attendees had useful suggestions on how to advance the model. Future work will be presented at the 2018 summer conference for the UK Fluid Network's Special Interest Group for the Fluid Mechanics of Cleaning and Decontamination. Further, we plan to publish at least two peer-reviewed papers – one on the modelling aspect of the project, the other describing the experiment.

Problem 2:

The solutions obtained from the HBIM were shown to be in excellent agreement with experimental data. This gives us confidence that the model can be used by industry to estimate the PCM final melt time. Moreover, as we included temperature-dependent parameters, the model is particularly suited to applications subject to large temperature variation. The research supported by the STSM has led to the completion of a paper that will be submitted by mid-July 2018.

FUTURE COLLABORATIONS

As the work on problem 1 is ongoing, there is significant scope to collaborate with Prof. Myers in the future. The next step will be to obtain solutions to the model. Since completion of the STSM I have already derived preliminary results. In some simple cases exact solutions to the model can be obtained. In particular, if we ignore the presence of the residue, and impose a fixed concentration at the surface, then the similarity solution method can be used to obtain exact solutions. I have also observed that in the case of the reduced model, the HBIM can be used to find approximate solutions. This is where Prof. Myers's continued involvement with the project will be invaluable as he is a proven expert in applying the HBIM to industrial problems.