Sabbatical Leave Report for Fall Semester 2007

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Summary

I spent my sabbatical leave for the Fall 2007 Semester in the Laboratory of Food Process Engineering (LMVT) at the Swiss Federal Institute of Technology Zurich (ETH Zurich). The main research topic of my sabbatical leave was in the area of dispersing processes for emulsions and polymer blends. The main goals of my sabbatical leave were to develop and/or adapt computational algorithms for the investigation of droplet deformation in dispersing devices, as well as to maintain and expand my research collaboration with LMVT.

Four objectives related to scholarly activity and professional development were cited in my Sabbatical Leave Research Program. As described below, these objectives have been largely met.

Accomplishments

- **Objective 1:** *Adaptation and/or development of computational algorithms to compute drop deformation in complex flow fields and drop detachment in flow fields*

  Two types of industrially-relevant dispersing devices were considered: a multi-toothed annular gap device and a rotating membrane annular gap device.

  Under the operating conditions of interest for our study, the flow field in the multi-toothed device is a highly complex mixture of transient shear and elongational flow, containing stagnation points and separating streamlines. The focus in the rotating membrane device was the detachment behavior of droplets from the membrane into the flow field.

  We decided to take different computational approaches for these applications.

  To study droplet deformation and breakup in the multi-toothed annular gap device, a computational algorithm was adapted that couples (1) a finite element calculation of the flow field in this device, (2) numerical particle tracking techniques to determine particle paths and the history of strain rates along these paths, and (3) a boundary integral method to calculate the deformation of a droplet as it traverses its particle path through the flow field. Parts (1) and (3) were already developed before my sabbatical, so the focus was on part (2). The three-part algorithm was then applied to study the deformation and breakup behavior of droplets in the multi-toothed device. (See Objective 2 below.)

  To study drop detachment in the membrane device, we decided to develop an algorithm that couples a finite element calculation of the flow field with a level set method to track the interface. The level set method will allow us more flexibility in the future to consider topological changes and to study non-Newtonian fluid systems. During my sabbatical, I have developed an accurate level set algorithm for computing the evolution of an interface, along with its normal vectors and local curvature, in a given, fixed velocity field. Currently, I am working on the coupling of this level set algorithm with the finite element flow solver to compute droplet formation, deformation and detachment in the rotating membrane device.

- **Objective 2:** *Computational and experimental investigation of drop deformation and breakup in industrially-relevant dispersing devices*

  The algorithm described above for the multi-toothed device has been used to predict the deformation and breakup behavior of droplets in this device. Experiments had already been performed at ETH before my sabbatical. Comparisons between experimental and numerical results generally showed good agreement, in terms of the path that a droplet traverses through the flow field and its deformation. The simulations were useful in examining the details of the flow field and in quantifying the amount of elongational to shear flow effects experienced by a drop. Moreover, the simulations were able to confirm some proposed conclusions drawn from the experimental data, such as the usefulness of a limiting time-averaged apparent shear rate along particle paths in characterizing drop deformation behavior.

  A paper on this study was submitted for publication to *Chemical Engineering Science*.

  Since the algorithm for the rotating membrane device was not completed during my sabbatical (as it was developed from scratch), no relevant simulations were performed during that time. However, I and scientists in LMVT discussed and designed the complementary experiments to be performed at ETH Zurich.

- **Objective 3:** *Maintain and expand my research collaboration with LMVT*
  Objective 4: *Formulate joint research projects and proposals and identify joint funding opportunities*

  Both these objectives were met. Specifically, several new research projects for joint collaboration were discussed and formulated. These include: (1) a biomedical application concerning the transport of material through deformable tubes or channels, serving as models of the esophagus or intestines; (2) a microfluidic application involving droplet deformation in microchannels; (3) the effect of interfacial properties, particularly surface elasticity, on droplet deformation in flow fields; and (4) development of novel numerical methods to solve complex thermodynamic models of multiphase flow, involving different length and time scales.

  Several potential sources of joint funding were discussed, the most promising of which is the Nestlé Corporation. I had discussions with a research group at Nestlé Research Center in Vers-chez-les-Blanc (Switzerland) who expressed interest in my simulations of surfactant-covered droplets. A feasibility study was formulated for their particular application.

Talks and Presentations

I have given the following talks, seminars and colloquia during my sabbatical leave.

- K. Feigl, "Introduction to Computational Fluid Dynamics and FLUENT," Wildhaus Seminar Series, Laboratory of Food Process Engineering, Swiss Federal Institute of Technology Zurich (ETH Zurich), September 12, 2007.
- K. Feigl, "Numerical calculation of non-Newtonian flows: Methods and applications," Lecture Series on Computational and Experimental Investigations of Non-Newtonian Fluids, Swiss Federal Institute of Technology Zurich (ETH Zurich), October 8-22, 2007.
- K. Feigl, "Behavior of liquid droplets in flow fields," Invited speaker, Colloquium of the Institute of Food Science and Nutrition (ILW), Swiss Federal Institute of Technology Zurich (ETH Zurich), October 30, 2007.

- K. Feigl, "Droplet deformation behavior in flows: Numerical and experimental results," Keynote lecture at the Annual Meeting of the Swiss Group of Rheology (SGR), Nestlé Research Center, Vers-chez-les-Blanc, Switzerland, November 1, 2007.

Publications

The following paper has been submitted for publication during my sabbatical leave.

- R.D. Egholm, K. Feigl, P. Fischer, P. Szabo, *Experimental and numerical analysis of droplet deformation in a complex flow generated by a rotor-stator device*, Submitted to Chemical Engineering Science, 2007.

Additional Activities

- **Professional Visit:** Visited Nestlé Research Center, Vers-chez-les-Blanc, Switzerland, November 9, 2007. Held discussions with the Food Stucturation Group and identified research project for future collaboration.
- **Refereeing/Reviewing:** Reviewed paper for *Polymer Engineering Science*; Reviewed research proposal for the *Petroleum Research Fund*.
- Held discussions with visiting scientists and local scientists at ETH Zurich.
- Attending colloquia and seminars at ETH Zurich.