NUMERICAL MODELING
OF LIQUID-VAPOR PHASE CHANGE

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(Final Report)

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• We implemented a two- and three-dimensional finite difference/front tracking technique to solve liquid-vapor phase change problems. The mathematical and the numerical features of the method were explained in great detail in our previous reports. Briefly, we used a single formula representation which incorporated jump conditions into the governing equations. The interfacial terms were distributed as singular terms using delta functions so that the governing equations would be the same as conventional conservation equations away from the interface and in the vicinity of the interface they would provide correct jump conditions. We used a fixed staggered grid to discretize these equations and an unstructured grid to explicitly track the front. While in two dimensions the front was simply a connection of small line segments, in three dimensions it was represented by a connection of small triangular elements. The equations were written in conservative forms and during the course of computations we used regriding to control the size of the elements of the unstructured grid. Moreover, we implemented a coalescence algorithm in two dimensions which allowed the merging of different fronts or two segments of the same front when they were sufficiently close. We used our code to study thermocapillary migration of bubbles, burst of bubbles at a free surface, buoyancy-driven interactions of bubbles, evaporation of drops, rapid evaporation of an interface, planar solidification of an undercooled melt, dendritic solidification, and a host of other problems cited in the reference.

• The code was tested against different benchmark problems with known qualitative behavior or analytical solutions. For example, we solved the one dimensional film boiling of a vapor layer beneath a liquid layer using our three-dimensional code. Initially, the liquid and vapor were at T_{sat} (i.e., saturation temperature) and suddenly the lower wall was set to T_w (i.e., wall temperature) which was higher than the saturation temperature. As a result, the vapor film started to grow and interface moved upward. This problem has an analytical solution (See, for example, Alexiades and Solomon, 1993) and it is good for benchmarking. We also compared the results of our numerical simulations with a more challenging problem given by Welch and Wilson (2000). Here, the liquid existed in metastable superheated condition and vapor was at saturation temperature. In contrast to the first case where thermal boundary layer originated from the wall and grew over the time, here, the thermal boundary layer originated at the interface and remained thin during the simulation. The thin thermal layer poses a great deal of difficulty for the numerical computations. In both cases, we were able to get satisfactory results with modest grid resolution (i.e. $1-2$ 1×3 box). In another case, we compared the results of our thermocapillary studies with the available results in the literature (i.e. Young et al. 1959, Chen and Lee 1992, and Nas 1995) and found satisfactory agreement. We did other validation tests for solidification processes and other problems and

the detail can be found in our previous reports.

- We modified our code in several occasions either to make it more robust or to introduce new features. In the original code, we used an iterative scheme based on Newton's method to find the interface velocity. This algorithms was time consuming and later on we replaced it with a non-iterative algorithm which took advantage of some mathematical manipulations to bypass the iterations. In three dimensions, we first started with a point-based algorithm to operate on the front. This algorithm relied on book keeping between the front points and computations of some of the necessary terms such as curvature was difficult and in some cases inaccurate. We later on adopted an element-based technique for the three-dimensional unstructured grid which resulted in a more accurate and robust code.

- We computed various terms for better quantification of the key parameters. Among them was computations of deformation factor in two and three dimensions and implementations of a "cluster multiple labeling algorithm" to quantify the formation of clusters of bubbles in large scale simulations of thermocapillary flows. Again, please refer to our past reports for further detail.

- The mathematical and numerical modeling was modified so that the code can handle interactions of bubbles in unbounded domains. This modification enabled us to follow the long time evolution of bubbles in order to characterize the time-averaged features of the flow. In the original code, this was not possible since the bubbles were confined by the container walls.

- We modified the three-dimensional code to study open surface problems such as film boiling and planar solidification. The code was initially tested against Rayleigh-Taylor instability in a flow without phase change and produced satisfactory results. Later on, (right after grant finished), it was tested against film boiling on a horizontal surface and produced some of the known experimental features such as formation of mushroom in low Jacob numbers and variations of Nusselt number with time in the course of film boiling.

- We did extensive literature survey and numerous computations to gain insight into the problem and improve our methodology. We have already presented and published parts of these studies in various international conferences and journals. We are in the process of finishing up a few articles which we could not complete due to lack of computational resources. We are currently using computational time awarded to us through the university of Michigan to finish some of our two-dimensional simulations. The three-dimensional studies are made possible by an

award from NPACI. The following list shows are past publications, pending ones and the one that will be submitted in the near future.

1) A. Esmaeeli & V. Arpaci. Thermocapillary Migration of Bubbles in Zero-Gravity. Part I-Low Reynolds and Marangoni Number Flows. In Preparation for Submission to J. Fluid Mech.

2) A. Esmaeeli & V. Arpaci. Thermocapillary Migration of Bubbles in Zero-Gravity. Part II-Moderate Reynolds and Marangoni Number Flows. In Preparation for Submission to J. Fluid Mech.

3) A. Esmaeeli & V. Arpaci, A. Chai. Thermocapillary Migration of Bubbles in Microgravity. In Preparation for Submission to Phys. Fluids.

4) A. Esmaeeli& V. Arpaci. Buoyancy-Driven Flow of Interacting Bubbles. In preparation.

5) V. Arpaci and A. Esmaeeli. Radiative Deformation. J. App. phys., 2000, Vol. 87, pp. 3093-3100.

6) V. Arpaci and A. Esmaeeli. On Interface Dynamics. Phys. Fluids, 2000, Vol. 12, pp. 1244-1246.

7) V. Arpaci & A. Esmaeeli. On Scales and Spectra of Interface Dynamics. Submitted to Phys. Rev. E. (October 2000).

8) A. Esmaeeli and V. Arpaci. Thermocapillary-Driven Migration of Bubbles in Shear Flows. Paper Number FEDSM99-7376. Proceedings of 1999 ASME-FED Summer Meeting. July 18-23, San Francisco, CA.

9) A. Esmaeeli and V. Arpaci. Buoyancy-Driven Interactions of Two Bubbles. Paper Number FEDSM99-7088. Proceedings of 1999 ASME-FED Summer Meeting. July 18-23, San Francisco, CA.

10) A. Esmaeeli and V. Arpaci. Numerical Modeling of Three-Dimensional Dendritic Solidification. Paper Number FEDSM98-4983. Proceedings of 1998 ASME-FED Summer Meeting. June 21-25, Washington, D. C.

11) A. Esmaeeli and V. Arpaci. Numerical Modeling of Three-Dimensional Fluid Flow with Phase Change. Fourth Microgravity Fluid Physics Conference, Cleve-

land, OH, Aug. 12-14, 1998 (www.ncmr.org/events/fluids1998.html).

12) A. Esmaeeli and V. Arpacı. Numerical Investigation of Planar Solidification of an Undercooled Liquid. Space Technology & Applications International Forum, Editor: M. El-Genk, Part II (STAIF-97, Albuquerque, New Mexico, 1997), pp. 629-634.

13) A. Esmaeeli, G. Tryggvason, and V. Arpacı. Thermocapillary Migration of Bubbles in Shear Flow. Paper Number FEDSM97-3523, ASME Proceedings of the 1997 ASME (FED) Summer Meeting, June 22-27, 1997, Vancouver, Canada. Editor: Tim O'hern.

14) A. Esmaeeli, V. Arpacı, and A. Chai. Buoyancy-Driven Interactions of Bubbles in Superheated Liquid. Fundamental of Bubbles and Droplets Dynamics Phase Change and Two-Phase Flow. ASME Proceedings of the 32nd National Heat Transfer Conference (Baltimore, Maryland, 1997), Editor: S. G. Kandlikar, C. H. Amon, and D. W. Pepper, HTD-Vol. 342, pp. 97-104.

15) A. Esmaeeli and V. Arpacı. Dynamics of Liquid/Vapor Interface in Zero Gravity. Current Developments in Numerical Simulation of Heat and Mass Transfer. ASME Proceedings of the 32nd National Heat Transfer Conference (Baltimore, Maryland, 1997), Editors: K. Vafai, J. L. Chen, T. R. Chopin, R. Douglas, N. K. Anand, A. F. Emery, and J. A. C. Humphrey, HTD-Vol. 339, pp. 123-129.

16) A. Esmaeeli and V. Arpacı. Dynamics of Bubbles Bursting at a Free Surface. Proceedings of the Second European Symposium on Fluids in Space, Naples, Italy, April 22-26, 1996.

17) A. Esmaeeli, V. Arpacı, and A. Chai. Internal Dynamics of Evaporating Droplets. ASME Proceedings of the 31st National Heat Transfer Conference (Houston, Texas, 1996), Editors: L. Witte and R. Singer, HTD-Vol. 326, pp. 39-45.

18) V. Arpacı and A. Esmaeeli. Kolmogorov Behavior of Interface Dynamics. ASME Proceedings of the 31st National Heat Transfer Conference (Houston, Texas, 1996), Editors: L. Witte and R. Singer, HTD-Vol. 326, pp. 31-37.

19) A. Esmaeeli, G. Tryggvason, and V. Arpacı. Thermal Migration of Bubbles toward a Fluid Interface. AIChE Symposium Series of the 31st National Heat Transfer Conference (Houston, Texas, 1996), Editor: M. El-Genk, Vol. 92, pp. 100-109.

20) A. Esmaeeli and V. Arpacı. An Estimate of Velocity Variances in Low Reynolds Number Bubbly Flows. Submitted to Phys. Fluids (July 1999).

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