Abstract Submitted
for the MAR13 Meeting of
The American Physical Society

Atomistic simulations of surfactant adsorption kinetics[1] EUGENIYA ISKRENOVA, Propulsion Directorate, Air Force Research Laboratory, Wright Patterson Air Force Base, OH 45433, USA and UES, Inc., Dayton, OH 45432, USA, SOUMYA PATNAIK, Propulsion Directorate, Air Force Research Laboratory, Wright Patterson Air Force Base, OH 45433, USA — Enhancing heat transfer is an important and challenging problem in a variety of industrial and technological applications including aircraft thermal management. Nucleate pool boiling is recognized as one of the most efficient methods to enhance heat transfer. Describing the plethora of multi-physics phenomena involved in nucleate pool boiling requires developing a multiscale model aimed at not only advancing our understanding but also at providing insights into the mechanisms for control and prediction of heat transfer in boiling. Adding surfactants to boiling water has been experimentally observed to enhance or inhibit the heat transfer depending on the surfactant concentration and chemistry. On a molecular level, addition of surfactants leads to the development of dynamic surface tension and changes in interfacial and transfer properties, thus contributing to the complexity of the multiscale model. We present an atomistic modeling study of the interfacial adsorption kinetics of aqueous surfactant systems at a range of concentrations at room and boiling temperature. Large scale classical molecular dynamics simulations were used to study the surfactant kinetics and estimate the adsorption and desorption rates at liquid-solid and liquid-vacuum interfaces.

[1]The authors acknowledge the funding from AFOSR Thermal Science Program and AFRL DSRC for computer time and resources.

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Date submitted: 29 Oct 2012 Electronic form version 1.4