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Atomistic simulations of surfactant adsorption kinetics at interfaces[1] EUGENIYA ISKRENOVA, Air Force Research Lab - WPAFB and UES, Inc., SOUMYA PATNAIK, Air Force Research Lab - WPAFB — Heat transfer control and enhancement is an important and challenging problem in a variety of industrial and technological applications including aircraft thermal management. The role of additives in nucleate boiling and phase change in general has long been recognized and studied experimentally and modeled theoretically but in-depth description and atomistic understanding of the multiscale processes involved are still needed for better prediction and control of the heat transfer efficiency. Surfactant additives have been experimentally observed to either enhance or inhibit the boiling heat transfer depending on the surfactant concentration and chemistry and, on a molecular level, their addition leads to dynamic surface tension and changes in interfacial and transfer properties, thus contributing to the complexity of the problem. We present our atomistic modeling study of the interfacial adsorption kinetics of aqueous surfactant (sodium dodecyl sulfate) systems at a range of concentrations at room and boiling temperatures. Classical molecular dynamics and Umbrella Sampling simulations were used to study the surfactant transport properties and estimate the adsorption and desorption rates at liquid-vacuum and liquid-solid interfaces.

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Eugeniya Iskrenova
Air Force Research Lab - WPAFB and UES, Inc.

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