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C1Or2D-03: Vapor-Liquid Interfaces of Cryogenic Fluids in Presence of Non-Condensable Gases: Insights from Molecular Simulations

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Efficient storage of cryogenics fluids (CFs) under microgravity environment requires detailed quantification of interfacial thermodynamics and mass transport. Such mechanistic understanding will provide strategies to mitigate boil-offs in presence of non-condensable (NC) gases and to engineer novel storage approaches. While several continuum models are being employed for this purpose, they lack the resolution to predict the nanoscale phenomena at the vapor-liquid interface and often depend on parameterized description of the interfacial thermodynamics and transport. In this work, we use molecular dynamics (MD) simulations to predict the interfacial transport and thermodynamics of CFs in presence of NC gases with the aim to (i) derive mechanistic understanding of the nanoscale process and (ii) validate the underlying assumptions used in developing the continuum models and quantify properties of interests to develop relevant correlations. These correlations can be typically incorporated into the continuum models thereby integrating critical information across length scales that are necessary for optimizing CF storage. Specifically, we focus on liquid nitrogen (LN2) and liquid oxygen (LO2) as model CFs. Neon was modeled as the NCs gas to predict the CF-NC interactions at the vapor-liquid interface (the Knudsen layer). We show that, the NC gas preferentially adsorb at the Knudsen layer impeding the condensation of the CF, thereby leading to boil-offs. Finally, we also discuss potential molecular descriptors that can be used for tuning the interfacial condensation rates and to mitigate boil-off.

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