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Assessment of Open-Source simulation in cryogenic LNG re-liquefaction

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The cryogenic re-liquefaction of Boil-Off Gas (BOG) is a critical step in LNG infrastructure, where methane vaporized due to unavoidable heat ingress must be recovered to mitigate energy losses and reduce greenhouse gas emissions. Methane's high global warming potential—over 80 times greater than that of CO_2 over a 20-year horizon—makes its release particularly concerning from both environmental and regulatory standpoints. Consequently, efficient BOG re-liquefaction systems are essential for improving the sustainability and economic performance of LNG operations. This study evaluates the applicability of DWSIM, an open-source process simulator, for modeling and optimizing cryogenic refrigeration cycles dedicated to BOG re-liquefaction. Two classical cycle configurations, Claude and Kapitza, were implemented using operational parameters extracted from the reference study by Moon et al. (2007). The Coefficient of Performance (COP) was used as the primary indicator for thermodynamic efficiency and model fidelity. Simulation results demonstrated excellent agreement with published data: the Kapitza cycle yielded a COP of 0.180, closely matching the reported value of 0.195, while the Claude cycle produced a COP of 0.170, in comparison with the literature value of 0.180. These results confirm the reliability of DWSIM in reproducing complex cryogenic processes under realistic operating conditions. Following the validation phase, a comprehensive process optimization strategy was applied. A Design of Experiments (DOE) framework based on Latin Hypercube Sampling (LHS) was employed to systematically explore the input variable space. The resulting dataset was used to train a Multi-Layer Perceptron (MLP) model capable of approximating the system's behavior across a wide range of conditions. Subsequently, a multi-objective optimization routine was performed on the trained surrogate model to identify optimal operating points that balance performance and energy consumption. This integrated methodology—combining open-source simulation, statistical design, and machine learning—provides a robust and scalable framework for process analysis and improvement in cryogenic engineering. The approach is particularly valuable for research institutions and small-to-medium enterprises (SMEs), where access to commercial simulators may be limited. Additionally, the flexibility and transparency of open-source tools like DWSIM enhance reproducibility and enable seamless integration with external analytical platforms. In summary, the study demonstrates the technical soundness of DWSIM in modeling and optimizing LNG BOG re-liquefaction cycles, highlighting its potential as a low-cost and reliable alternative for advanced cryogenic process development.
Keywords: Boil-Off Gas, LNG, Cryogenics, DWSIM, Re-liquefaction, Multi-Layer Perceptron, surrogate model

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