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Energetics of a Heat Engine: A Molecular Dynamics Simulation Study
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KUMNEGER TADELE, Department of Physics, Dire-Dawa University, YERGOU TATEK, Department of Physics, Addis Ababa University, STATISTICAL AND COMPUTATIONAL PHYSICS TEAM — We perform a classical molecular dynamics simulation study of a heat engine operating between two heat reservoirs and performing a Carnot-like cycle in a finite time over a wide range of process rates. The working substance of the heat engine is made of highly concentrated interacting Lennard-Jones particles with the aim to simulate a real gas. The piston speed and temperature ratio of the cold and hot heat reservoirs are used as control parameters whereas efficiency and power output per cycle are the physical quantities of interest. The variation of these quantities as a function of the independent parameters is studied with the objective to investigate the validity of relevant theoretical predictions. For instance, for small process rates, the linear dependence of the heat engine efficiency with temperature ratio, in agreement with theory, has been demonstrated. Finally, a unified optimization criterion is applied to determine optimum operation conditions of the engine that make the best trade-off between efficiency and power output.

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