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Supersonic nozzle flow and condensation analysis by the non-equilibrium molecular dynamics YUYA MATSUMURA, SHINTARO IMAYAMA, DAIJI ICHISHIMA, Sumitomo Heavy Industries — In this research, we study supersonic inviscid flow through a Laval nozzle by means of the non-equilibrium molecular dynamics, and demonstrate the capability of the method for analysis of the nozzle flow and condensation. The flow is driven by the pressure difference imposed by heat baths attached to both ends of the nozzle. Only the repulsive force is applied between molecules and the nozzle wall to minimize the viscous effect. With Argon gas (Lennard-Jones potential), the flow properties follow the isentropic expansion except on the nozzle end. Water vapor flow is also investigated with the modified Lennard-Jones potential to observe the condensation of the water through the isentropic expansion. The result shows the nucleation and growth of molecule clusters in the region after the nozzle throat.

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