Entropy Production in a Shock Wave

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We consider a shock wave propagating in the x-direction a one-component 3D gas. The shock wave (Mach number ≈ 8) induces a sharp density gradient, which we treat as a surface. The entropy production is determined using non-equilibrium thermodynamics for surfaces [1]. We define the equimolar surface according to Gibbs [2] and obtain surface excess properties. Using the Gibbs equation for surfaces we find that the surface excess entropy production (in excess of the adjacent bulk phases) can be written in the form σs = $\sum[JiXi]$- where Ji are fluxes and Xi are driving forces. The bracket with the subscript "-" means that each product is taken as a difference across the wave. Constitutive equations for heat- and mass fluxes across the wave front follow from the excess entropy production.

The theory is combined with non-equilibrium molecular dynamics simulations of a blast wave in a moderately dense Lennard-Jones/spline gas, which gives numerical values to the analysis. We show that most of the kinetic energy in the wave is converted reversibly to enthalpy and a smaller amount is dissipated. The surface excess entropy production is found to agree with the local entropy production integrated over the shock wave and with the entropy balance equation. The use of non-equilibrium thermodynamics for surfaces offers a new way to determine the entropy production in shock waves and an alternative to earlier work [3].

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References

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[3] See e.g. B. L. Holian, M. Mareschal, and R. Ravelo, J. Chem. Phys. 133, 114502, 2010.