Public Abstract

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Title:Molecular Dynamics Simulations of Pressure Shocks in Liquid Phase Nitromethane

We have investigated the phenomenon of high pressure shock waves traveling through liquid phase nitromethane (NM). Nitromethane is a commonly encountered high energy fuel additive, it is a stable explosive material, and it is also commonly used in the synthesis of many other explosive and nonexplosive organic materials. The speeds of these pressure shock waves depend on the strength of the shock and the initial temperature of the liquid. The liquid NM is initially equilibrated under zero atmospheric pressure. We use Classical Molecular Dynamics Computational methods to carry out computer simulations from which we obtain and extract the data that is compared to various experimental results. Among these results is the sound speed through liquid NM as a function of its temperature at constant ambient pressure. The sound speeds from our simulation model are between 15-30 percent too high. We also have general results of shock speeds, densities and pressures all as functions of the particle speeds which give the shock strength. These results are commonly referred to as Hugoniot data and ours spans the entire temperature range of liquid NM initially under ambient pressure. Our simulations are on the scale of less than ten picoseconds and up to about 160 angstroms. At this scale the applicability of the commonly used continuum based shock equations known as the Rankine-Hugoniot equations is called into question. We have found that while these equations are applicable to the shocked densities and pressures on this picoscale, they are not applicable to the shocked energies obtained behind fronts. In other words, the density and pressure behind shock fronts appears to obtain expected equilibrium values on this scale but the energy does not. This is relevant in helping to determine precise mechanisms of energy transfer in liquid NM that can or will lead up to its reaction or detonation.