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Modelling temperatures of reacting nitromethane ROBERTA MULFORD, DAMIAN SWIFT, Los Alamos National Laboratory — Detonations are chemical reactions and as such may appropriately be modelled using a temperature-dependent rate model. We test the predictions of such a model against temperatures reported for shock-loaded and reacting nitromethane liquid. Liquid nitromethane has the advantage of being largely free of pores, and thus reacting homogeneously to produce a single uniform temperature, rather than exhibiting "hot-spots." The liquid is also transparent, allowing observation of emission from the shocked and reacting state rather than the surface. A thermodynamically complete EOS is necessary in order to apply a temperature- dependent rate model within a hydrocode. A quasiharmonic EOS is used to determine an adequately reliable temperature for a given state in pressure and energy. The temperature is determined by assuming that available energy is distributed over vibrational modes for the reactant molecule. The model has previously been shown to reproduce measured particle velocity profiles that compare well with published reactive behavior.

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