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Phase separation in H2O:N2 mixtures and implications for detonation. LAURENCE FRIED, AMITESH MAITI, Lawrence Livermore National Lab, RICHARD GEE, SORIN BASTEA — A class II atomistic force field with Lennard-Jones 6-9 nonbond interactions is used to investigate equations of state (EOS) for important high explosive detonation products N2 and H2O in the temperature range 700-2500 K and pressure range 0.1-10 GPa. A standard 6th order parameter-mixing scheme is then employed to study a 2:1 (molar) H2O:N2 mixture, to investigate in particular the possibility of phase-separation under detonation conditions. The simulations demonstrate several important results, including: (i) the accuracy of computed EOS for both N2 and H2O over the entire range of temperature and pressure considered; (ii) accurate mixing-demixing phase boundary as compared to experimental data; and (iii) the departure of mixing free energy from that predicted by ideal mixing law. The importance of supercritical phase separation during detonation will be discussed. The work was performed under the auspices of the U.S. Department of Energy by the University of California Lawrence Livermore National Laboratory under Contract W-7405-Eng-48.

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