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Phase equilibria computations of multicomponent mixtures at specified internal energy and volume[1] PHILIP C. MYINT, ALBERT L. NICHOLS III, H. KEO SPRINGER, Lawrence Livermore National Laboratory — Hydrodynamic simulation codes for high-energy density science applications often use internal energy and volume as their working variables. As a result, the codes must determine the thermodynamic state that corresponds to the specified energy and volume by finding the global maximum in entropy. This task is referred to as the isoenergetic-isochoric flash. Solving it for multicomponent mixtures is difficult because one must find not only the temperature and pressure consistent with the energy and volume, but also the number of phases present and the composition of the phases. The few studies on isoenergetic-isochoric flash that currently exist all require the evaluation of many derivatives that can be tedious to implement. We present an alternative approach that is based on a derivative-free method: particle swarm optimization. The global entropy maximum is found by running several instances of particle swarm optimization over different sets of randomly selected points in the search space. For verification, we compare the predicted temperature and pressure to results from the related, but simpler problem of isothermal-isobaric flash. All of our examples involve the equation of state we have recently developed for multiphase mixtures of the energetic materials HMX, RDX, and TNT.

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