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Comparative analysis of the data on shocked benzene properties obtained in MD simulations with different interatomic potentials VLADIMIR DREMOV, GENNADY IONOV, FILIPP SAPOZHNIKOV, ILYA DERBENEV, Russian Federal Nuclear Centre - Institute of Technical Physics, 456770 Snezhinsk, Russia, JEAN-BERNARD MAILLET, NIKOLAS PINOT, LAURENT SOULARD, CEA, Centre DAM-Ile-de-France, Bruyeres-le-Chatel 91297, France — We present in the paper the results of reactive MD simulations of shock loading of liquid benzene. The Hugoniot of benzene was calculated with the hugoniostat technique in the pressure range 0-100 GPa. The AIREBO potential was used as the model of interatomic interactions. The number of benzene molecules in the simulation was about 1000. Timescale of the MD simulation for each Hugoniot point is several nano-seconds. Obtained results were compared with the experimental ones and with simulation results obtained early with ReaxFF and LCBOPII potentials. The key questions under investigation are the kinetics of polymerization at moderate pressures (10-20 GPa) and the kinetics of the formation of condensed carbon clusters at high pressures (>40 GPa). The AIREBO was tested from the point of view of minimal model adequately reproducing the properties of shock compressed hydrocarbons.

Vladimir Dremov
Russian Federal Nuclear Centre - Institute of Technical Physics

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