Abstract Submitted for the SHOCK05 Meeting of The American Physical Society

Molecular dynamics analysis of a liquid explosive reaction zone LAURENT SOULARD, BLANDINE CROUZET, CEA-DAM Ile de France, bp 12, 91680 Bruyeres-le-Chatel — We present in this work a detailed analysis by molecular dynamics of the reaction zone of a stationary planar detonation. In particular, we look at the influence of chemical characteristics such as the reactions reversibility and endothermicity. So, equilibrium and frozen Hugoniot of the reactive system are calculated by a specific molecular dynamics method. These results can be used to a predict the detonation characteristics such as the thermodynamic properties of ZND spike and the CJ point. We observe in particular the influence of the preliminary endothermic phase on the detonation velocity and its stability. The comparisons between these predictions and non equilibrium molecular dynamics results confirm the results of this first theoretical part. In a second step, the main hypotheses of a ZND model are extracted from the MD simulations (mainly the formalism of the reactive EOS in the reaction zone). The parameters of the corresponding model are then fitted on MD results. The final step is the implementation of the model in an hydrodynamic code. Direct comparisons between molecular dynamics simulations and hydrodynamics calculations for various 1D and 2D (in the hydrodynamics sens) configurations are presented.

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Date submitted: 07 Apr 2005

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