ABSTRACT

IMPLEMENTATION OF AUTOMATICALLY SIMPLIFIED CHEMICAL KINETICS THROUGH INTRINSIC LOW-DIMENSIONAL MANIFOLDS FOR GASEOUS HMX

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An automated method to generate, validate, and implement an Intrinsic Low-Dimensional Manifold (ILDM) has been developed. This method has been applied to a detailed gaseous HMX (Octahydro-1,3,5,7-Tetranitro-1,3,5,7-Tetrazocine) mechanism that contains 44 species and 232 reactions. A three-dimensional manifold tracked detailed chemistry based on enthalpy, pressure, and mass fraction of N_2. A four-dimensional manifold adds the mass fraction of NO. A one-dimensional (in space) BYU combustion program has been used to compare the three- and four-dimensional manifolds with a full kinetic mechanism. Simulations show that the three-dimensional manifold is an adequate representation of the full kinetic mechanism away from the reacting surface (> 60 μm at 20 atm). The four-dimensional manifold is an adequate representation of the

full kinetic mechanism closer to the reacting surface (>19 μm at 20 atm). An advantage of the ILDM method is that computational time is reduced by an order of magnitude. However, this advantage can be offset by the development time required to create and implement the ILDM method. Another portion of this project is two-dimensional (in space) simulations that model high explosives in a container. Even though this portion of the project does not implement an ILDM, it gives insight to meaningful simulations that can be performed with an ILDM. The simulations explore heat feedback of equilibrium gases in a heated container filled with solid HMX. Heat feedback is calculated to investigate flame propagation and burning characteristics of the solid HMX. Further work is necessary to implement the ILDM approach in similar container simulations. The methodology used to implement the four-dimensional ILDM into the one-dimensional (in space) combustion code is available to be used in other applications. One application of interest is the University of Utah's three-dimensional (in space) CFD code, ARCHES.