Abstract

The present dissertation addresses the development of EUDETCODE (EUropean DETonation CODE), a unified thermochemical code for the modeling and simulation of detonation and combustion processes in energetic materials. The research has been conducted within the framework of the European Defence Agency project EUDETCODE, involving several European industrial and academic partners, to consolidate expertise in the field and provide the defence community with a robust, modular, and extensible computational tool.

From a physical perspective, the theoretical foundations of detonation and combustion are recalled, and the governing equations of state (EoS) are critically assessed, ranging from the ideal gas approximation to advanced intermolecular potential-based and multiphase models. Both fluid and condensed phases of the chemical reaction products are treated, with special attention devoted to carbon allotropes and metallic additives, which are often critical for the accuracy of predictions.

From a numerical standpoint, the thesis introduces efficient and problem-tailored algorithms for chemical equilibrium and parameter fitting. A nonlinear constrained minimization strategy is designed for equilibrium composition calculations; a least squares method is implemented for the determination of Jones–Wilkins–Lee parameters, ensuring consistency between equilibrium thermodynamics and hydrodynamic simulations. The software architecture is conceived to be modular, object-oriented, and equipped with a graphical interface facilitating extensibility and usability.

Benchmarking has been performed against state-of-the-art thermochemical codes (CHEETAH, EXPLO5, THOR, among others) and validated against experimental data, including detonation velocity measurements and cylinder tests with aluminized formulations. Results confirm the capability of EUDETCODE to reproduce experimental trends with high accuracy, while overcoming convergence issues and limitations of existing codes.

The scientific contributions of this work lie in the integration of advanced thermo-

dynamic models into a unified, validated numerical framework, the development of robust algorithms for equilibrium and fitting procedures, and the demonstration of EUDETCODE as a high-performance, extensible platform for energetic materials research. Beyond its immediate applications, the code establishes a foundation for future extensions, including the treatment of non-ideal detonation models and the coupling with hydrocodes.