Numerical Simulation of Detonation with Detailed H2/O2 Reaction Mechanisms

P.Pradeep Kumar[*], Jeong-Yeol Choi[*†]

ABSTRACT

Detonation propagation studies is recently getting more attention in these days for its feasibility in aerospace application. Another motivation for this study is the safety concern in industries, since the detonation can cause failure to the mechanical components particularly when the flame accelerates within a pipe or tubes. In this study we numerically simulated a Moderately unstable detonation case with various grid systems and fluid dynamic length scales and have compared in the contents. Moderately Unstable detonation case was selected for this study and detailed Hydrogen-Air Reaction Mechanisms proposed by Jachimowski was used in this study with N2 as inert species.

Key Words : Detonation Simulation, Detailed Hydrogen reaction Mechanism, ZND structure, CFD

Studies on Hydrogen detonation has always been an important considering the safety factor and has been increased in the recent years considering its propulsive application in aviation propulsion. Various studies and experimental researches claim that the propulsive cycle involving detonation increases the propulsive efficiency considerably. And hence research on engines involving detonation propulsion such as PDE′s, RDE′s and CRWE′s have been increased in the last decade. Hydrogen has wide range of flammability limits and ignites more rapidly than the other fuels. Thus Hydrogen can easily detonate in closed tubes and the detonative force causes mechanical failure particularly when detonation gets accelerated within a closed pipe or duct.

Various numerical studies have been conducted in the past on detonation and related studies. Choi.et.al[1] investigated the numerical issues in simulating the Detonation and gave an insight into the computational problems one may incur during the simulation as well as given a direction to predict for grid cell size requirement for detonation prediction. Similarly various researchers have attempted

to simulate the detonation, but most of them relied on the one-step kinetics model. But for an accurate prediction, detailed kinetics model always serves better than the one-step models which comes with computational costs.

In this paper, we have studied the Detonation propagation in a tube with the single step induction parameter model as well as with the detailed kinetic mechanisms. An Experimental case was selected for this simulation with mixture 2H2 + O2+ 3.5N2 at detonation velocity of 1.958 Km/s. Single step model requires seven parameters such as specific heat ratios(γ_1 & γ_2) and gas constants of the reactants and products(R_1 & R_2), the heat release q, the pre-exponential factor K, and the activation temperature T_a. The ZND structure calculation for the detonation wave for one step model was defined in [1] whereas for the detailed kinetics were calculated from the Caltech code. The strong shock, inclined for initial perturbation, initially compresses the propellant and the high temperature and high pressure is sufficient enough to ignite the compressed propellant. the reaction zone thickness depends on the inflow condition and gets thermally chocked at which the propellants are completely burned. the temperature pressure density ratios along with mach number are depicted in Fig. 1 and the

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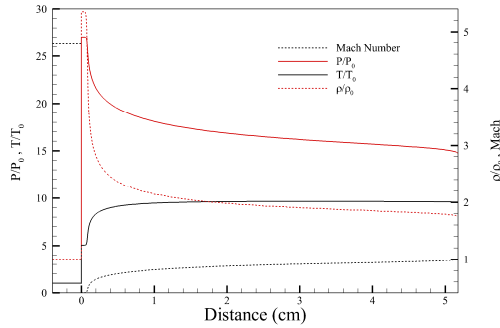mole fraction along the reaction zone were depicted in Fig. 2.

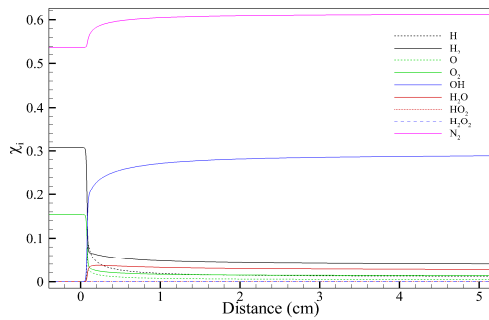Fig. 1 Flowfield variables along the ZND structures calculated for 2H2+O2+3.5N2.

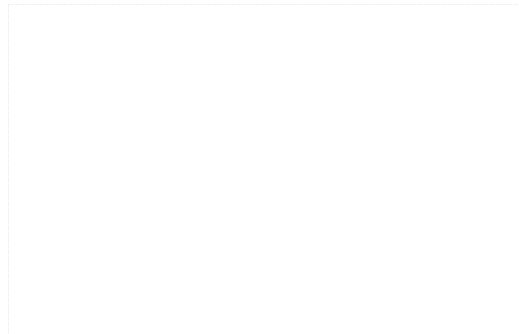Fig. 2 Species Mole Fraction along the ZND structures calculated for 2H2+O2+3.5N2.

Fig. 3 Flowfield variables along the ZND structures calculated for 2H2+O2+3.5N2.

ZND structure is used as the initial condition with an inclined shock to create the initial perturbation. The numerical method for this problem includes the governing equations solved using a cell-vertex finite-volume method. The convective fluxes are calculated by AUSMDV scheme with the primitive variables interpolated by a third order WENO scheme. the discretized equations were integrated in time using a fourth-order accurate Runge-Kutta scheme. More details of the implementation were reported in [4-5].
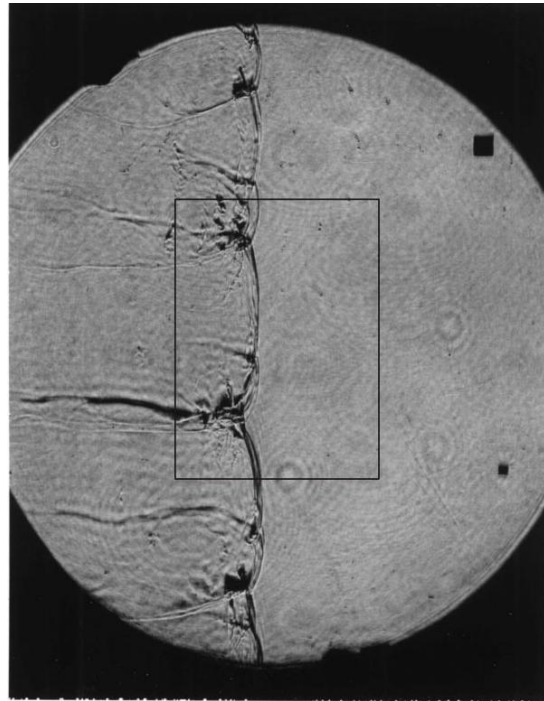
Fig. 4 Experimentally observed Detonation front. (Pic Courtesy: J. Austin [6])

For this study, a more reliable Jachimowski reaction mechanisms was selected, which was widely used over the past decade for various combustion models. A more detailed issues related to detonation simulation were discussed in [1]. For this study, A moderately Detonation case with the inflow conditions at 297K, 20Kpa with a detonation velocity of 1958 m/s for the above mentioned mixture was selected. A uniform tube of dimension 3.0x1.0 with an extended length in the extension ratio of 1.02 further is selected. for this study. A pre-exponential factor of k=4000 was used for this study, while the other properties for the induction model calculations were defined from the experimental conditions [6]. The VN Pressure behind the propagating shock wave dictates the stability of the detonation propagation. and were plotted in Fig. 4&5 for detailed reaction mechanisms and for 1-step model.
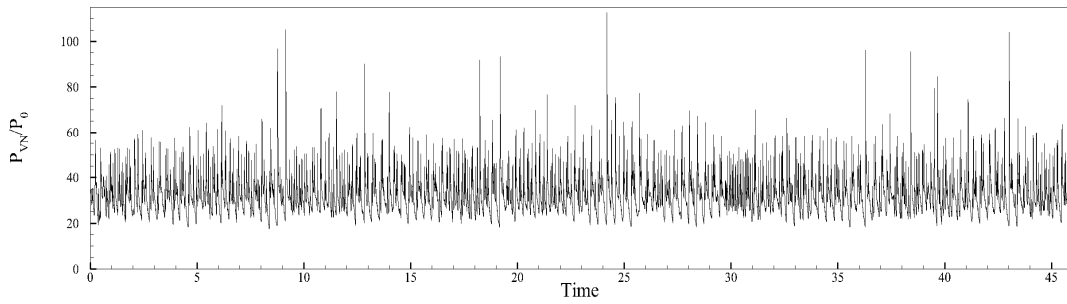
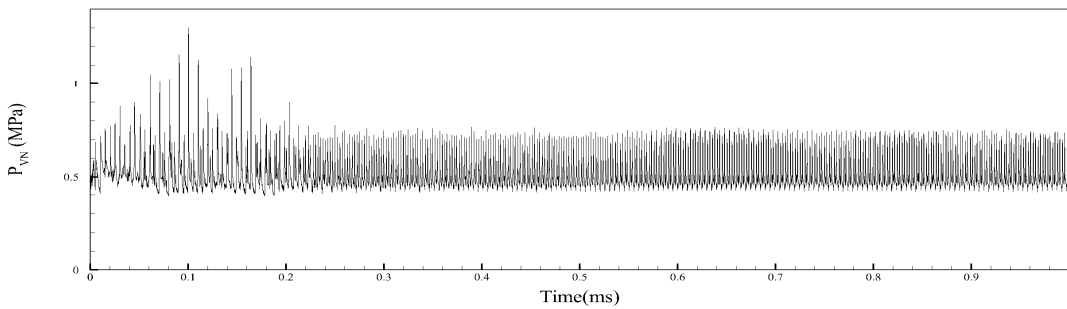Fig. 2 Pressure History with 1-Step induction Model

Fig. 3 Pressure History with Detailed Reaction Mechanisms

The contours of the pressure, temperature and product fraction are depicted in Fig. 4-7 for 1-step kinetics model.
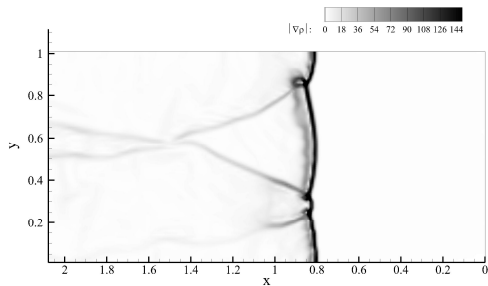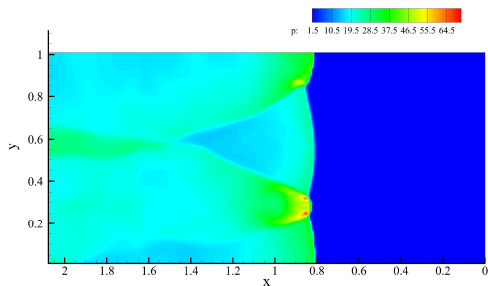

Fig. 4 Density Variation Contour with 1-Step
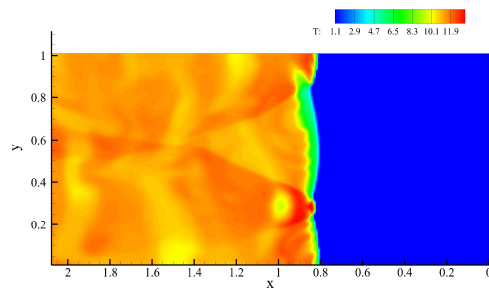

ModelFig. 5 Pressure contour with 1-Step Model
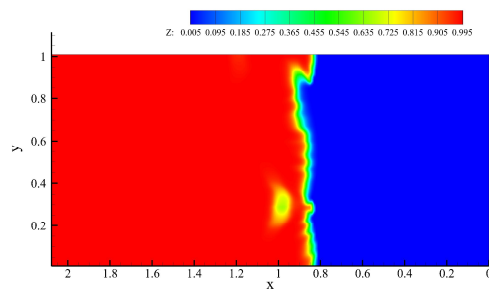

Fig. 6 Temperature History with 1-Step Model

Fig. 7 Reaction Progress Variable with 1-Step Model

The contours of pressure, Temperature, density variation and mole fraction were depicted in Fig.8-17 and the smokefoil record

obtained from these simulations were plotted in Fig. 18-19.
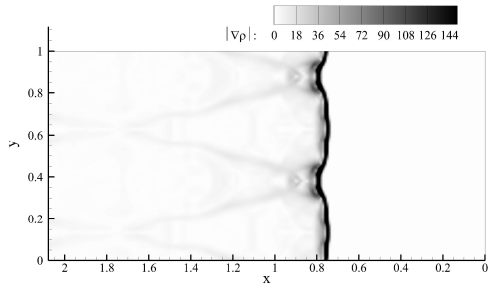
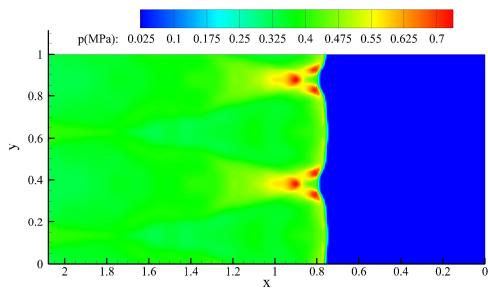Fig. 8 Density Variation Contour with Detailed Reaction Mechanisms

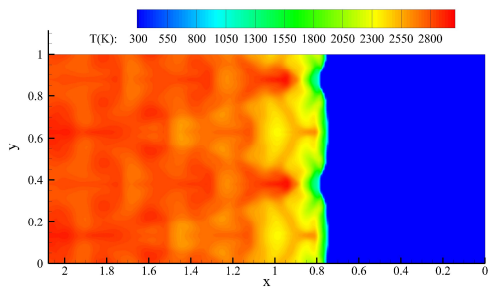Fig. 9 Pressure Contour with Detailed Reaction Mechanisms

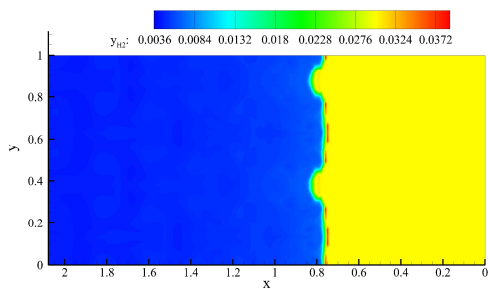Fig. 10 Temperature Contour with Detailed Reaction Mechanisms

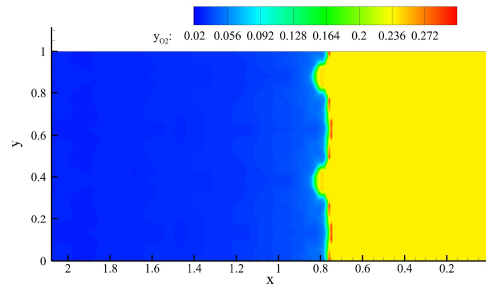Fig. 11 Mass fraction distribution of H_2 species with Detailed Reaction Mechanisms

Fig. 12 Mass fraction distribution of O_2 species with Detailed Reaction Mechanisms

Fig. 13 Mass fraction distribution of H_2O species with Detailed Reaction Mechanisms

Fig. 14 Mass fraction distribution of OH species with Detailed Reaction Mechanisms

Fig. 15 Mass fraction distribution of H species with Detailed Reaction Mechanisms

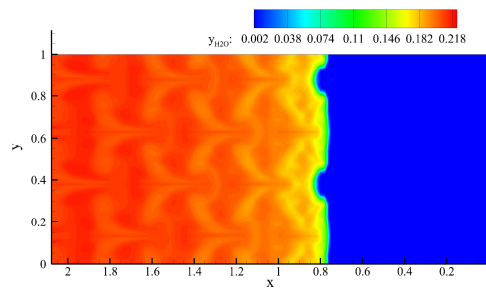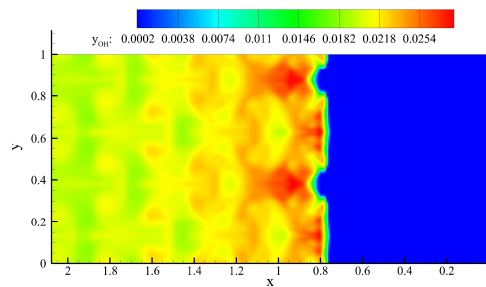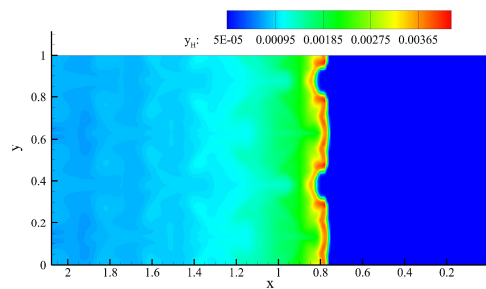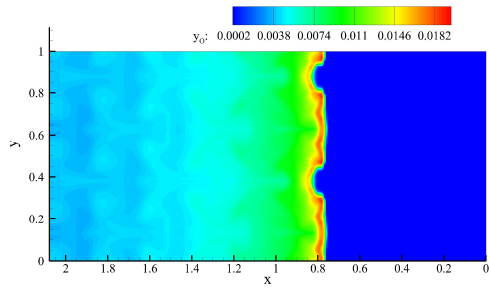Fig. 16 Mass fraction distribution of O species with Detailed Reaction Mechanisms
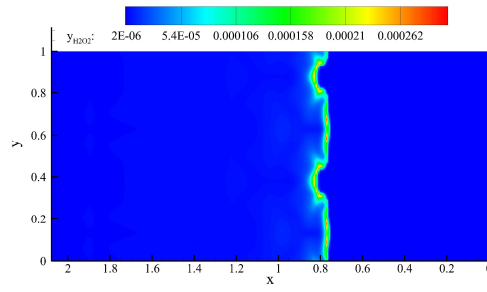

Fig. 17 Mass fraction distribution of H_2O_2 species with Detailed Reaction Mechanisms
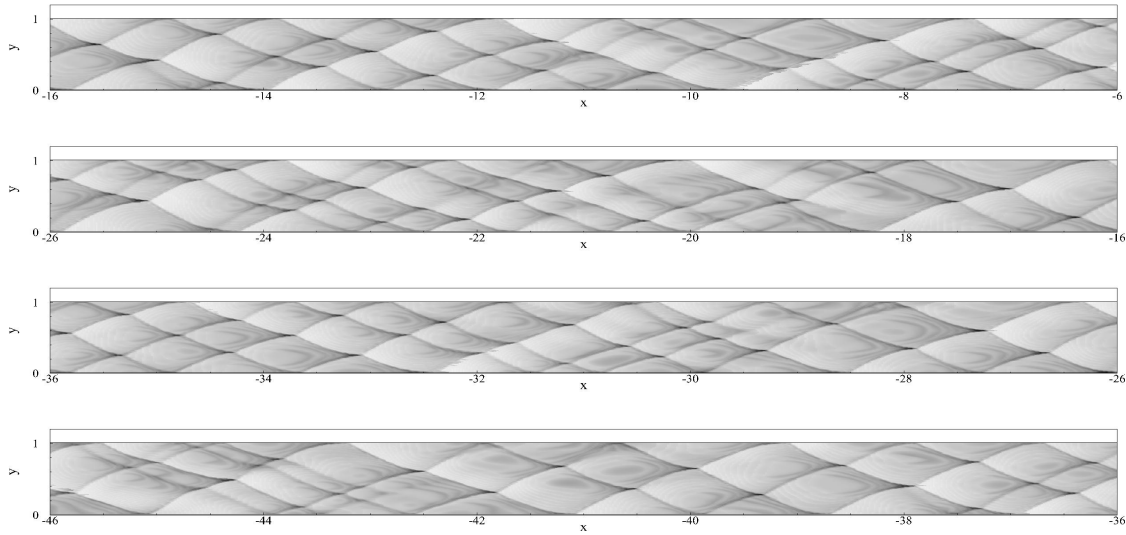

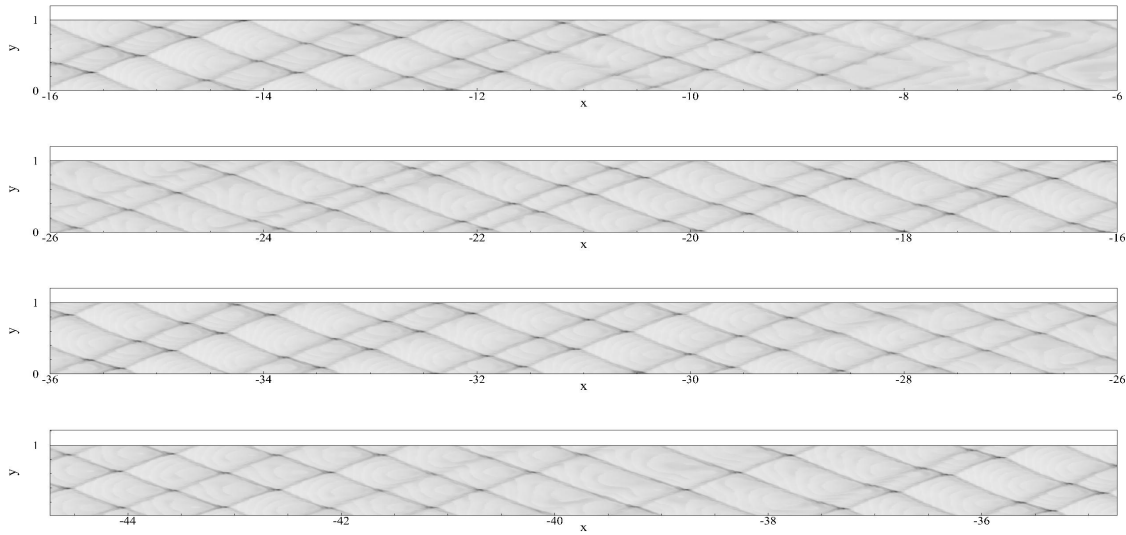Fig. 2 Smoke-Foil Record with 1-Step Reaction model

Fig. 3 Smoke-Foil Record with Detailed Reaction Mechanism.

Detonation propagation was simulated with detailed chemical kinetics and 1-step induction model. One particular case of moderately unstable detonation was selected and compared with that of the 1-step model as depicted. Even though 1-step induction model efficiently analyzes the key features in a detonation, detailed chemical kinetics is preferred for a complete understanding of the combustion taking place behind the detonation wave.

Reference

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