A NUMERICAL STUDY OF PLANAR DETONATIONS

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Abstract t— **A numerical study on the buildup and propagation of planar detonation waves in H_2 + *Air* combustible mixtures, based on the use of unsteady Euler equations coupled with source terms to account for rates controlled chemical activity, is presented. The computer solver works with 13 chemical species and 33 different one step reactions of a H_2-O_2 - N_2 combustion mechanism. The detonation process is initiated via the energy provided by an igniter which acts as a driver of a shock tube driving through a combustible mixture a blast (or strong shock), accompanied by exothermic chemical changes. It is shown that for each equivalence ratio of the combustible mixture, the detonation can only be triggered if the igniter energy deposition equals or exceeds a computed minimum value. When the igniter energy deposition is less than this minimum, the combustion zone start to decouple from the blast front and if that energy is diminished even more, the combustion could not take place. A particular way of generating sustained overdriven detonations, is also considered.**

Keywords— **unsteady flow, chemically reacting flows, ignition, Chapman-Jouguet detonations, overdriven detonations.**

I. INTRODUCTION

It is well known that any explosive mixture, can in general, go through two extremes modes of combustion. One extreme is the slow laminar deflagration mode; here the flame propagates at typical velocities of the order 1 ms^{-1} relative to the unburned gases and the overpressure is small. The other extreme is the detonation mode, in which the detonation wave propagates at velocities of the order of 2000 ms^{-1} and with an overpressure rise across the wave of almost 20 times the initial value. The propagation of laminar deflagrations is governed by the molecular diffusion of heat and mass from the reaction zone to the unburned mixture. On the other hand, the propagation of detonations depends on the adiabatic shock compression of the unburned mixture to increase its temperature to bring autoignition. The strong exponential temperature dependence of chemical reactions rates, makes possible the rapid combustion in the detonation mode. In between the two extremes of laminar deflagration and detonation, there is an almost continuous spectrum of burning rates, however in this work, only detonations in homogeneous gaseous mixtures of H_2 and *Air* are considered.

The classical Chapman-Jouguet theory, seeks the unique solution of the one-dimensional conservation equations across the detonation front in which the flow behind the wave is sonic. It involves only an equilibrium thermodynamic calculation for the detonation states (i.e. the detonation velocity, pressure, temperature, and density ratios across the wave, and the equilibrium composition of the products gases). These detonation states calculated using the classical approach agree well with experimental observations. However, parameters like the initiation energy, detonability limits, the thickness of the reaction zone and the critical tube diameter, are requiring a knowledge of the structure of the wave itself, and hence the chemical reaction rates. Following Lee (1984), these parameters are referred as the *dynamic*s *detonation parameters* to distinguish from the equilibrium *static detonation state*s obtained from the Chapman-Jouguet theory.

A century after the formulation of the successful Chapman-Jouguet theory, the estimation of dynamics detonation parameters continues being mostly, based on experimental data, see Kaneshige and Shepherd (1997). In the 1960s, experiments revealed that gas-phase confined detonations are most often characterized by unsteady, three-dimensional cellular structures, which can only in an averaged sense be predicted by one-dimensional steady theories. Since then, numerical modeling has steadily advanced to predicting the flow field behind shock induced reactions (Sharpe and Quirk, 2008), nevertheless and to the degree of our knowledge, no theory has yet described how the cellular structure is formed and sustained behind unconfined waves.

To totally preserve the concept of one dimensional planar detonation, the ignition source should also be planar. Similarly, if the flow has spherical symmetry and it is wanted to preserve, then the ignition source should also have spherical symmetry. However, if inside a duct filled with combustible mixture, the detonation is started by an ignition source which provides a 3D blast, the production of a highly three-dimensional structure of interacting and reflecting longitudinal and transverse waves should be expected. The longitudinal ones, could associate with the propagating detonation, while the transverse ones propagating normal to the direction of the detonation motion, distort the wave front. This structure will last until full equilibrium between the transverse shocks is reached and the flow becomes essentially one-dimensional. This transition from a 3D start to a final 1D detonation state cannot yet, be approached with our solver.