NUMERICAL SIMULATION OF COMBUSTION PHENOMENA pdf

1: Numerical Simulation of Pulse Detonation Engine Phenomena | Ann Karagozian - www.enganchecuban

Numerical Simulation of Combustion Phenomena Proceedings of the Symposium Held at INRIA Sophia-Antipolis, France, May , Editors: Glowinski, Roland, Larrouturou, Bernard, Temam, Roger (Eds.).

He 1 and A. Karagozian 2 Received June 17, ; accepted in revised form October 25, This computational study examines transient, reactive compressible flow phenomena associated with the pulse detonation wave engine. The PDWE is an intermittent combustion engine that relies on unsteady detonation wave propagation for combus- tion and compression elements of the propulsive cycle. The present computations focus on high order numerical simulations of the generic PDWE configuration with simplified reaction kinetics, so that rapid, straightforward estimates of engine per- formance may be made. Both one- and two-dimensional simulations of the high speed reactive flow phenomena are performed and compared to determine the appli- cability of 1D simulations for performance characterization. Examination of the effects of the combustion reaction mechanism and the use of a pressure relaxation length for 1D simulations is made. Characteristic engine performance parameters, in addition to engine noise estimates within and external to the detonation tube, are presented. Detonations; gasdynamics; reactive Euler equations; shock capturing schemes. While specific configurations vary, in general the PDWE consists of propagating detonation waves generated periodically within an engine tube, with associated reflected expansion and compression waves which can act in periodic fashion to produce high forward thrust [1â€”3]. The generic reactive and non-reac- tive wave phenomena occurring in the PDWE cycle are described in Fig. The propagating detonation leaves a mixture of combustion products behind the wave. The detonation reaches the end of the tube, propagates outward as a shock into the surrounding air, and an expan- sion wave simultaneously reflects back into the tube Figs. The expan- sion wave produces lower pressure gas in its downstream region, further expelling the combustion products situated behind the wave. When the expansion reaches the thrust wall or plate at the forward end of the thrust tube, it is reflected as an expansion wave Fig. When the expansion wave reaches the exit Fig. The reflection of the wave at the thrust wall delivers thrust to the vehicle and is reflected as a shock, allowing the combustible mixture of reactants to ignite, with transition to a propagating detona- tion wave Figs. Numerical Simulation of Pulse Detonation Engine Phenomena During propagation of the detonation, combustion of reactants takes place so rapidly that the process effectively takes place at a constant volume, which is theo- retically more efficient than a constant pressure combustion process as essentially occurs in conventional airbreathing or rocket engines. The absence of rotating machinery suggests that the PDWE concept holds real promise for high thrust density, low fuel consumption propulsion applications, either in an airbreathing or rocket engine mode. A number of alternative configurations for the PDWE have been proposed and tested [4], and numerical simulations of PDWE phenomena are being actively pursued. Since then, extensive testing has been and continues to be pursued by a variety of groups [3, 4]. An excellent historical overview of the development of the PDWE as a constant volume combustion engine concept is provided in Eidelman et al. Overviews of past and ongoing numerical simulations of PDWEs are described in recent articles by Kailasanath [2, 6â€”8]. The relaxation length is used in order to mimic mul- tidimensional wave effects in the pressure near the tube exit when using a 1D simu- lation, in particular when the local exit flow is subsonic over a portion of the cycle. Kailasanath and Patnaik find that the relaxation length can have a significant effect on engine performance, with increases in relaxation length leading to increases in engine impulse. The impulse I is typically defined as. I â€” A F Dptw t dt 1 0 where A is the area of the thrust wall and Dptw t is the time-dependent pressure differential compared with initial tube conditions at the thrust wall. An alternative performance parameter, the fuel-based specific impulse, Isp, f , is defined as Isp Isp, f â€” 3 Yf where Yf is the fuel mass fraction present within the initial premixed reactants in the tube. The effect of partially filling the detonation tube with reactants, in the vicinity of the thrust wall, and having the remainder of the tube filled with air, is explored by Cambier and Tegner [10] and by Li et al. Reducing the region of the tube occupied by reactants results in a higher Isp, f for a given engine cycle, clearly, due to the reduction in the effective Yf. This occurs He and Karagozian despite the fact that when the detonation propagates through the interface between reactants and

air, reflected expansion waves return to the thrust wall and reduce the pressure at the wall at an earlier time than the reduction that occurs when the expansion waves reflected from the tube exit encounter the wall. An analytical model for the impulse of the single cycle PDWE has been devel- oped by Wintenberger et al. Employing a similarity solution for the tem- porally constant pressure region within the tube as occurs during the portion of the cycle shown in Figs. Correspondence of the model results to performance parameters quantified in experiments and in numerical simulations is quite good. The present study focuses on both one- and two-dimensional simulations of the pulse detonation engine using high order numerical schemes, developed over the years by Stanley Osher and collaborators. Governing Equations The governing equations which describe the flow and reaction evolution in the PDWE with a single step, irreversible chemical reaction consist of the conservation of mass, momentum, energy, and species. The following representation was used, for example, in simulations of the two-dimensional planar PDWE configurations under investigation: Y is the reactant mass fraction, which varies from 0 to 1, while K is the reaction-rate multiplier for the reaction, which also sets the spatial and temporal scales in the problem. One-step chemical reactions were considered in the present study, mostly for the methane-oxygen reaction, but also for the hydrogen-oxygen reaction. These were sufficient to enable reasonable estimates for performance parameters to be derived from the computations. The reaction terms K and Ti were determined for the methane-oxygen reaction from data provided in [15]. We found that the PDWE cycle results were not sensitive to our selections of K and Ti , within reasonable limits, for this reaction, and hence these values were chosen to be the same as those for the methane-oxygen reaction. The values of these reaction quantities for the two reactions considered are shown in Table I. Two methods for initiation of the detonation reaction were explored. The second method initiated the computation via an incoming shock moving through the reactants toward the thrust wall, which reflected from the wall and ignited the detonation. These initia- tion mechanisms produced virtually the same overall performance parameters, since the incoming shock strength in the second method could be chosen so that the pressure at the thrust wall rapidly rose to the same extent using either ignition method. At much lower spark region initial temperatures and pressures, of course, there would be a much more gradual transition from the deflagration sub- sonic combustion to the detonation process [16]. Both one- and two-dimensional numerical simulations were performed in this study. In addition to the 2D planar problem described in Eq. In the case of the 1D simulations, the use and effect of employing a pressure relaxation length exterior to the end of the detonation tube, after Kailasanath and Patnaik [9], was also explored. When the relaxation length l was set to be greater than zero, the external pressure was allowed to spatially decay in a linear fashion over the length l to atmospheric pressure, rather than having the exit plane pressure exposed immediately to atmospheric pressure. The relaxation length assumption is suggested by Kailasanath and Patnaik [9] to enable the flow interior to the PDWE tube i. In the present 1D simulations, however, the computational domain consisted primarily of the detonation tube containing grid points , since the effect of a pressure relaxation length on the wave reflected back into the detonation tube could be represented using only a few grid points beyond the tube end in order to capture the spatial slope in pressure. In the 2D simulations, on the other hand, the air external to the detonation tube was assumed to be uniformly at atmospheric pres- sure, and the computational domain extended well downstream of the end of the tube, in general at least one and one half tube lengths downstream. The 2D domain extended at least two tube diameters away from the detonation tube in the dimen- sion perpendicular to the axial dimension. Hence for the 2D simulations, no relaxation length approximation was necessary, and outflow boundary conditions were employed at the edges of the computational domain. Comparisons were thus possible between the 2D simulations, which captured flow characteristics external and internal to the PDWE, and 1D simulations with and without a pressure relaxation length, in which only the interior of the PDWE and a few exterior grid cells were resolved. ENO methods constitute a class of high accuracy, shock capturing numerical schemes for hyperbolic systems of conservation laws, based on upwind biased differencing in local characteristic fields. It has high accuracy third order or higher in smooth regions of the flow, and cap- tures the motion of unresolved steep gradients in general without introducing spurious oscillations. Hence ENO is particularly well suited for resolution of Numerical Simulation of Pulse Detonation Engine Phenomena flowfields in which there are shocks or flame fronts. ENO uses an adaptive poly- nomial

interpolation constructed on the basis of decisions to avoid steep gradients in the data; these decisions involve selection of the smoothest computational stencil in the vicinity of the gradient to approximate fluxes. The polynomial is also biased to extrapolate data from the direction of information propagation i. WENO schemes, developed by Jiang and Shu [17], are based on ENO and incorporate all possible stencils in approximating fluxes, so that higher order accuracy may be achieved with a smaller number of points in a given stencil [22]. For example, with 3 points per stencil, an ENO scheme becomes third order in accuracy, but a WENO scheme becomes fifth order accurate in smooth regions and remains third order accurate in the vicinity of discontinuities. To avoid entropy-violating expansion shocks near sonic points, where charac- teristic velocities change sign, high order dissipation was added in the present study via the Local Lax Friedrichs LLF scheme [23], which adds extra numerical vis- cosity throughout the computational domain at each time step. This feature ensures that for a sufficiently small time step according to the Courantâ€"Friedrichsâ€"Levy or CFL condition , the time discretization will not introduce spatial oscillations to the result. Since the current simulation only involved a single step reaction, use of the TVD Rungeâ€"Kutta method was pre- ferred. The CFL condition in this case incorporated the source term to insure sta- bility, since reaction rates often impose the greatest constraints on time integration. It is found that the degree of spatial resolution of the reaction zone can have a profound effect on the peak pressure amplitude and period of oscillation of the overdriven pulsating detonation wave. A minimum required resolution of 20 grid points per detonation reaction zone half-length is suggested in [24] for the canonical pulsating detonation problem with an overdrive of 1. Grid resolution tests in the present PDWE study, however, suggested that even 5 grid points per reaction zone half-length were sufficient for the cases under consideration. The present WENO scheme was also tested on a non-reactive problem with an analytic solution, that of the one-dimensional propagation of a normal shock wave out of a straight tube into air at atmospheric conditions. This problem yields reflection of an expansion fan back into the tube, mimicing the processes taking place when a detonation leaves the PDWE tube see Figs. Validation of the 3rd order WENO scheme on a one-dimensional, non-reactive problem with an analytic solution. Shown are spatial distributions of pressure in the vicinity of the open tube end within the tube at various times: Comparisons are made among simulation results for various spatial grid sizes symbols and the analytic or exact solution lines. Propagation of the shock wave to the right a , b , out of the tube, results in reflection of an expansion wave back into the tube c , d. Here the flow throughout the domain shown remains subsonic in the labo- ratory reference frame for all times shown. Figure 2 shows the computed pressure distribution in this non-reactive test problem at four different times. There was virtually no difference between the 3rd order WENO-computed solution and the analytic solution when the spatial grid spacing was less than about 2 cm in this test case. While ENO schemes can become expensive due to the required decisions on the stencils, WENO schemes were found to be less costly, and moreover, the ability to use relatively coarse grids, as seen in [24], helps to reduce Numerical Simulation of Pulse Detonation Engine Phenomena the overall computational time. Both the shock propagating out of the tube right side of Figs. The flow throughout the tube remained subsonic or, prior to passage of the shock, quiescent during the computation. This comparison lends confidence that the present scheme and boundary conditions, even in 1D, were capable of cap- turing important compressible wave dynamics at the end of the detonation tube. Noise Estimates As described above and in Wintenberger et al. In addition to the impulse I, spe- cific impulse Isp , and fuel specific impulse, Isp, f , the sound pressure level SPL at various locations within and external to the detonation tube were computed in this study. These noise levels were roughly estimated by examining the Fourier trans- form of the time-dependent pressure measured at various locations within the computational domain. A peak in the spectrum often appeared at roughly Hz, which corresponded to the inverse of the period of the PDWE cycle for a tube length of one meter and a CH 4 â€"O2 reaction. Smaller peaks at higher harmonics were usually observed. Hence the present computations allow rough estimates of the distribution of sound pressure level, or noise, emanating from pulse detonation engine to be made. A straight, planar PDWE tube one meter in length and 0. The tube was assumed here to be completely filled with a stoichiometric mixture of methane and oxygen at atmo- spheric pressure. A CFL number of 0. The propa- gation of the detonation to the right, within the tube, is readily apparent; its exit from the tube end resulted in the propagation of a vortical structure, coincident with the leading shock, into the

surrounding air. Simultaneous to the exit of the shock and initiation of the vortex, a reflected expansion fan entered the detonation He and Karagozian Fig. Temporal evolution of the 2D planar pressure field within and external to the PDWE over one cycle, with data shown at times corresponding to a 0. A CH 4 â€”O2 reaction was simulated here. The color map for the pressure distribution is shown, with units of Pascals. Temporal evolution of the centerline pressure within and external to the PDWE over one cycle, extracted from a 2D planar simulation of the flowfield, as in Fig. Detonation tube Patm Fig.

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2: "Numerical Simulation of Combustion in the Ironmaking Blast Furnace Rac" by Tyamo Okosun

*Numerical Simulation of Combustion Phenomena: Proceedings of the Symposium Held at INRIA Sophia-Antipolis, France, May , (Lecture Notes in Physics) (English and French Edition) [Roland Glowinski, Bernard Larrouturou, Roger Temam] on www.enganchecubano.com *FREE* shipping on qualifying offers.*

To quickly perform the highly resolved simulations with limited processing resources of large-scale hydrogen combustion, a method based on thermal theory was developed to obtain kinetic parameters of global reaction mechanism of hydrogenâ€”air combustion in a wide range. Good agreement between the model prediction and the experimental data was achieved, and the comparison between simulation results by the detailed mechanism and the global reaction mechanism show that the present calculated global mechanism has excellent predictable capabilities for a wide range of hydrogenâ€”air mixtures. Introduction Nuclear power as a clean and sustainable energy has ignited the interests of the researchers worldwide Momirlan and Veziroglu, However, significant safety issues associated with hydrogen occur in pressurized water reactors and boiling water reactors of nuclear power plants Yanez et al. The interaction of the melted core with the cooling water can generate large quantities of hydrogen during a severe accident, which can results in a flammable mixture being formed. The hydrogen can be ignited leading to explosion which will threaten the integrity of containment I. Due to shorter time period and lower cost, numerical simulation appears to be an appropriate tool to assess the hydrogen risk, which emphasizes the importance of chemical reactions to combustion Kuo, Therefore, the rational reaction mechanisms and kinetic parameters are significant to accurately reflect combustion process in the numerical simulation. Nowadays, the detailed or global mechanisms can be used to simulate combustion process and provide insight into combustion phenonmena. Obviously, a detailed mechanism involving a large number of species and reactions requires high computational costs and performs highly resolved simulation slowly, which in turn a global mechanism is required to predict the combustion characteristics in great accuracy with limited processing resources Kim et al. Global chemistry models are often implemented in large-scale simulations of combustion in nuclear power plants Manninen et al. Presently, several researches Sung et al. However, those methods require strong mechanism-dependent knowledge and are generally time-consuming due to the iterative procedure and validation process for eliminating species Lu and Law, Therefore, it is necessary to establish a reasonable and simplified method to obtain single-step chemistry model. The researches of mechanisms using laminar flame propagation velocity have been globally conducted. Egolfopoulos and Law , based on the relationship between laminar propagation velocity and pressure, studied the laminar propagation velocity varying with pressure due to chain termination when the pressure exceeded a certain range. However, the model was based on detonation velocity and thus the established mechanism ignored the effect of laminar flame. With the aim to simulate large-scale hydrogen combustion and explosion, Wang et al. On the basis of thermal theory, Khaikin and Merzhanov proposed the relation between combustion velocities and reaction order, activation energy of gasâ€”solid reaction under the condition of steady combustion, which was applied widely in heterogeneous combustion Merzhanov et al. The activation energy can be obtained by fitting experimental velocities at adiabatic flame temperature. However, these expressions are not suitable for homogeneous gas phase reactions. In this paper, a method based on thermal theory was developed to obtain reaction rate parameters for global model. Global Mechanism The following assumptions are made for the detailed model establishment in this study: The thermal theory Chatelier, ; Evans, deals with phenomena about heat release and propagation without taking the diffusion factors into account. In addition, the thermal theory lays barely on the physical process and couples the principles of heat transfer, chemical kinetics, and thermodynamics without referring to a great deal of mathematics. Therefore, in this paper, a method is developed for one-step hydrogen combustion mechanism and the activation energy and pre-exponential factor are derived based on the thermal theory. The ignition process of mixture can be divided into two regions: In preheating region, the gas is heated from the initial temperature T0 through heat conductivity and ignited on the boundary; in chemical reaction region the chemical latent enthalpy of gas transfers to sensible enthalpy of products. The heat flux transferred by

conduction between T0 and Ti is Q.

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