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Vortex Formation in a Proposed Detonation Internal Combustion Engine

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A possible configuration for taking advantage of detonation combustion in an internal combustion engine is described, which uses a separate detonation combustion chamber that discharges tangentially into a vortex chamber formed by the piston and cylinder at top dead center. The vortex chamber is designed to efficiently store a portion of the kinetic energy produced by the detonation wave in the form of a vortex, which would subsequently be converted into static pressure. By placing this chamber above the piston surface, the detonation and primary shock waves are directed parallel to the piston surface, thus avoiding potentially destructive loads to the piston. The rapid burning followed by mixing with air in the vortex chamber may reduce the formation of NOx and unburned hydrocarbons as compared to conventional combustion. Such a configuration may efficiently take advantage of clean-burning slow-deflagrating fuels such as natural gas to yield constant volume-type efficiencies. Shock wave propagation through the vortex chamber was simulated to qualitatively observe the vortex storage and rapid mixing characteristics.

I. Introduction

A. Natural Gas Internal Combustion Engines

SINCE the U.S. Clean Air Act was introduced, there has been strong interest in cleaner burning and more thermally efficient operating internal combustion (IC) engines.[1] Alternative fuels show promise in reaching such goals. One such fuel, natural gas, is an abundant, inexpensive, and desirable fuel for IC engines, it is clean burning with high octane and cetane numbers and is thus capable of tolerating high piston compression ratios without knock. Ignition is easy due to the wide ignition limits of natural gas/air mixtures. New generation natural gas engines have turned to stratified charge chambers that enrich the mixture around the igniter and enhanced turbulence (high "squish") to increase flame propagation speeds for an overall lean mixture.[2–4] However, current efforts to substitute such alternate fuels for conventional liquid fuels in internal combustion engines face many obstacles. They include problems with storage, distribution, ignition, slow burning, low fuel efficiency, and emissions. The latter three problems may be reduced by means of the proposed modifications to the IC engine.

The amount of work that can be produced by combustion products inside an internal combustion engine is proportional to the combustion products pressure relative to the surroundings. Consequently, a higher pressure at the end of the combustion process results in more power produced during the piston expansion (power stroke). The obtainable combustion product pressure is not only a function of supercharging and piston compression, but also of the combustion process. The ratio of the peak cylinder pressure achieved with and without ignition is defined herein as the combustion pressure ratio (CPR). The ideal Otto cycle has instantaneous constant volume heat addition with a CPR about equal to the temperature ratio due to combustion. Such a cycle is more efficient than the ideal constant pressure combustion Diesel cycle at the same mechanical compression ratio. For slow burning fuels where the heat is still released during the piston expansion instead of instantaneously at top dead center (TDC), the result is a lower CPR. For example, the low deflagration flame speeds noted in spark-ignited natural gas engines can result in up to 45 deg of crank angle for complete combustion, which can contribute to lower thermal efficiencies.

While higher compression ratios increase efficiency, the piston compression in the spark-ignited Otto cycle is limited in order to avoid "knock" and the high temperatures that may lead to additional NOx emissions. Knock is caused by autoignition (and in some cases, end-gas detonation), which results in rapid local pressure rises and impulses to the piston surface, which are unfavorable to the shaft bearings and also lead to undesirable high heat transfer rates to the piston head.[1] Knock prevention is considered a controllable nuisance because it requires the use of expensive high octane fuels in engines with high compression ratios. To maximize cycle efficiency for an internal combustion piston engine, one would like to combine high piston compression and rapid combustion if no pressure limiting is necessary.

B. Detonation Combustion Aspects

The fastest combustion heat release rate occurs when a mixture is ignited by shock-wave-induced heating, called detonation. Controlled detonation can be achieved in a laboratory device such as a shock tube, for which the resulting pressure, temperature, and velocity increase have been carefully studied and published by many researchers (e.g., Ref. 5).

Previous attempts to harness detonation combustion for nondestructive purposes have included rotating detonation wave rocket engine designs.[6,7] However, the spinning (rotationally propagating) detonation necessary for this application was found to be unstable and could not be continuously maintained.[6] Recently, detonation behavior has been investigated for aerospace propulsion systems for other configurations.[8–11] Helman et al.[8] conducted pulsed detonation rocket engine experiments to demonstrate its feasibility, which has since been studied computationally.[10] Another application by Wortman considered detonation ducts to augment gas turbine efficiencies.[11] However, the above studies indicate several difficulties that must be overcome in order to allow practical application of a detonation engine.

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One-dimensional detonation allows the minimum entropy rise for the combustion process as compared to constant volume or constant pressure combustion.[12,13] However, if the kinetic energy of detonation is dissipated by turbulent reflecting waves inside a constant volume combustor yielding shock and viscous losses, then the detonation entropy rise increases to that of a subsonic combustion constant volume entropy rise. To avoid this loss, the kinetic energy would have to be isentropically stored and converted to pressure for power extraction, which is in general impractical for an IC engine, given the speed of the detonation wave as compared to typical piston translational velocities. However, even an entropy rise approaching that of constant volume combustion would be desirable from an efficiency standpoint as compared to those associated with the slower heat input of deflagration, which result in pressure-limited or constant pressure combustion efficiencies.

Another potential advantage of detonation combustion is reduced NOx production. This is possible because the NOx formation reactions are very slow[3,14] compared to the time scales associated with the primary detonation reactions.[6] If the temperature can be significantly reduced through leaning immediately following the detonation combustion, then NOx formation may be substantially reduced. At the same time unburned hydrocarbons (HC) can be afterburned in the leaned mixture, if it contains sufficient excess oxygen and a high enough overall temperature. This afterburning is particularly helpful for natural gas since a high fraction of its HC emission typically results from unburned fuel (~95%), although its total HC emissions is quite low compared to other fuels.[15] In addition, the high local temperatures of the detonation process may yield less unburned fuel than low-speed deflagration combustion.

However, a significant problem of detonation combustion is withstanding the propagation of its strong shock wave within the engine containment. For an internal combustion engine, such a high kinetic energy wave directly impacting the piston surface would certainly cause exaggerated knock-like problems. Therefore, to take full advantage of the rapid combustion benefits of detonation in an IC engine, the associated shock wave kinetic energy must not impinge directly on the piston surface and the combustion products need to be quenched rapidly by leaning. An engine design that may be capable of realizing such objectives is described in the following, and has been named the detonation internal combustion engine (DICE).[13,16]

II. Detonation Internal Combustion Engine (DICE)

A. Configuration

The concept for a detonation internal combustion engine is designed to increase thermal efficiency through increased flame speed, and reduce pollutant emissions through fast leaning. While the concept is not fuel specific, natural gas is especially appealing due to its gaseous form, which is more readily detonable and does not yield as much particulate emissions. Liquid fuels would have to be atomized or subsequently evaporated to droplet sizes of less than 10 μm to achieve detonation, due to the time scale associated with droplet evaporation.

The DICE configuration is shown in Fig. 1 and described as follows. A conventional piston cylinder configuration is modified to incorporate a separate combustion chamber, referred to as the detonation chamber, which is isolated with a valve from the compression chamber during fuel injection. During the compression stroke, fuel is injected in the detonation chamber providing a turbulent near-stoichiometric fuel-air mixture, while maintaining fuel-free compressed air in the piston/vortex chamber. Note, this is different from the two-stage combustion in stratified natural gas internal combustion engines,[17] which includes a small pilot chamber of stoichio-

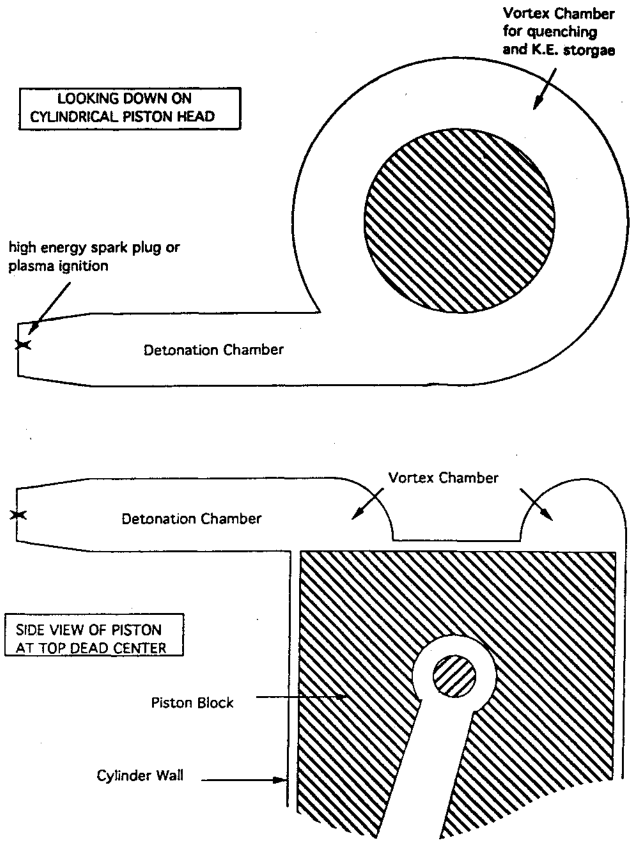

Fig. 1 Schematic of proposed DICE configuration.

metric fuel mixture to initiate combustion and a lean mixture in the main chamber where the majority of the combustion takes place.

The DICE cycle requires the generation of a properly timed, unidirectional detonation wave in the detonation chamber. This controlled detonation must occur over a short distance and is initiated at the beginning of the detonation chamber once the piston has reached top dead center. The initiation may be in the form of a high energy spark plug (e.g., 1 J) or a plasma ignition device to accelerate detonation initiation. The rapid release of heat leads to a series of pressure waves that coalesce to form a shock wave designed to be of sufficient strength to detonate the fuel-air mixture in the detonation chamber by shock wave heating. The distances required for such formation would have to be short to allow practical application of this concept. However, Helmen et al.[8] were able to repeatedly produce detonations in less than 5 cm for several ethylene-oxygen mixtures with speeds ranging from 750 to 950 m/s, which is lower than the Chapman-Jouget wave speed indicating the detonation was still developing. These detonations were created in a tube approximately 1 cm in diam, with an automotive spark plug firing mechanism at 1 atm that generated peak pressures as high as 30 atm. Similarly, Nichols et al.[6] rapidly ignited methane-oxygen mixtures in 80–90 μs using conventional spark plug ignition of about 30 mJ. Recent computations by Kaplan and Oran[18] of a Mach 2 reflecting wave in stoichiometric propane-air mixture were also able to initiate detonation in distances of less than 7 cm. To enhance the detonation formation, high tube wall temperatures could be maintained. In addition, by providing strong mixing and high turbulence levels in the detonation tube before ignition, the deflagration-to-detonation transition times and distances can be reduced.[6]

Detonation propagation is controlled by activation energy and fuel equivalency of the mixture as well as the precombustion geometric and state conditions.[19,20] Typical cell sizes for methane gas are very large at 1 atm or lower pressures (~0.4 m) resulting in longer deflagration-to-detonation (DDT) transition times and distances than seen at elevated pressures and temperatures.[21,22] Thus, the conditions produced by the mechanical piston compression allow for detonation to occur more readily, which is one reason for knock-limited compression ratios of natural gas engines. It is important to note that high purity methane is extremely resistant to detonation even under such high pressure and temperature conditions, but the addition of other hydrocarbons such as ethane (typically the second most prominent constituent in natural gas after methane[23]) greatly increases the susceptibility to detonation.[24,25]

While the minimum entropy rise is achieved with a fully developed Chapman-Jouget wave,[12] it is only critical to produce at least a rapid combustion wave that maintains its stability for the length of the detonation chamber. This is because the failure to convert any of the associated kinetic energy should still result in at least a constant volume-type efficiency, which is better than the case where slow deflagration burning leads to significant heat release during piston expansion. Thus, the proposed engine may allow exploitation of both the high piston compression ratios possible with high octane methane mixtures as well as the high CPR's characteristic of an ideal Otto cycle.

The high speed of the detonation combustion products is so far in excess of the piston speed that its momentum cannot be harnessed directly to produce piston power, i.e., the excess kinetic energy is difficult to utilize. This is one of the reasons why detonation combustion is difficult to apply in mechanical power production. To solve this problem and minimize the problems associated with knock, the kinetic energy of the combustion products is directed parallel to the piston surface to avoid direct impingement of the residual shock waves on the piston surface. This yields a more gradual buildup of pressure on the piston surface as the shock propagates around the doughnut-shaped vortex chamber, as compared to a normal shock impingement. The piston surface is intended to be exposed only to the combustion products and not the high local temperatures associated with the detonation front. However, residual transverse waves from the expired detonation and the vortex chamber curvature will likely produce increased thermal loads that require much more stringent requirements on surface materials, e.g., the use of plasma spray coating.

As the high-pressure combustion products are injected tangentially into the vortex chamber, they mix with and compress the dilution air in the chamber. Therefore, the high kinetic energy, which is only available for a fraction of a millisecond, can be temporarily stored in the form of a vortex positioned above the piston. An experiment would be needed to determine the extent of specific kinetic energy available of the mixture of combustion gases and dilution air, but it may be crudely estimated by taking the fuel-air interface expansion distance (through detonation) over the time for it to occur (approximately the DDT time) and multiplied by the mass fraction constituted by the combustion gases. During the piston power stroke, which takes several milliseconds, the vortex kinetic energy is partially recovered as static pressure as it is slowed by wall shear stress forces and flow turbulence. If one "freezes" the piston motion to examine the effect of the vortex decay, the nonisentropic conversion can be considered as a constant volume process whereby conservation of energy of the static temperature approaches its isentropic stagnation value, e.g., for a vortex Mach number of M_v, the static temperature would rise by a factor of $[1 + \frac{1}{2}(\gamma - 1)M_v^2]$. However, the static pressure would only rise by the same factor since density is constant. Taking into account the piston movement, the vortex conversion reduces the rate of pressure drop during expansion as compared to expansion without vortex decay; thereby allowing for a relative increase of the average pressure force on the piston and the associated power produced. However, all of the kinetic energy would have to be recovered instantaneously to approach the theoretical Otto efficiency associated constant volume combustion. In addition, the high convection velocities of the gases would lead to higher heat transfer losses as compared to a conventional low-speed deflagration combustion.

To quantify some of these effects, a nonadiabatic zero-dimensional cycle analysis with stroke integration has been conducted with finite flame speed, a variable specific heat ratio, and a turbulent convective heat transfer model for potential DICE conditions.[26] The adiabatic results for an 8:1 compression ratio showed that significant increases in thermal efficiency were possible for instantaneous combustion associated with detonation, as opposed to conventional flame speeds associated with deflagration (63 vs 36%). However, heat transfer losses were much greater for the detonation case, such that even with 2:1 leaning the improved efficiency of instant combustion for the nonadiabatic cases was not as striking (42 vs 33%). The physical complexity of the detonation and mixing process as compared to the simplifying assumptions renders such trends to be primarily qualitative.

By diluting the combustion products with the compressed air inside the vortex chamber, the rapid quenching may minimize the formation of both NOx and unburned hydrocarbons. This quenching is important to reduce NOx levels since they are controlled by reaction times and reaction temperature. Time scales for NOx to reach equilibrium are of the order of 1–2 ms,[14] much larger than 0.1–0.2 ms expected for detonation[6] and mixing (see below) to occur. Meyer et al.[2] as well as Rizk and Mongia[3] showed that significant quantities of NOx are produced only at temperatures in excess of 1800 K. Therefore, the compressed air temperature must be sufficiently low to bring the subsequent mixture with the burned gasses below this value. For example, if the precombustion fuel-free vortex mass is twice that of the precombustion fuel-air detonation chamber mass, then mechanical compression ratios of 15:1 or less with assumed complete postcombustion mixing are estimated to result in overall mixed temperatures below the critical 1800 K. Such a 2:1 mass ratio also reduces the overall mixture ratios well below the stoichiometric levels.

While the potential impact of such engines may be significant in that nonrenewable fuel consumption and pollution abatement are of national concern, several potential problems of the DICE configuration should be mentioned. These include the degree to which one may achieve proper stratification and fuel injection for the various chambers; the additional heat transfer and material design aspects that will be necessary to withstand the higher thermal transient loads, especially on the detonation chamber housing; and the development of a system to yield short distance deflagration to detonation transition. This last problem of rapid detonation formation may result in the DICE configuration being practical only for very large piston engines.

B. Computations of a Shock Wave Entering the Vortex Chamber

To study some of the unsteady wave characteristics of the proposed DICE flowfield, a noncombusting portion of the cycle was simulated to model the high-speed vortex and mixing dynamics. This nonreacting simulated portion begins as the detonation wave has terminated due to fuel absence and the residual shock wave enters the vortex chamber, and the simulation ends once a reflected shock wave reaches the upstream boundary of the computational domain. To approximate this flow, an initially one-dimensional shock wave entering a vortex chamber containing nonreacting inviscid fluid was simulated to characterize the unsteady gasdynamics. However, an actual terminated detonation wave would be much more complex due to residual transverse shocks and trailing expansion waves. Since the acoustic speeds are significantly higher than the piston translation speed, the piston was simply considered to be frozen at top dead center (maximum compression), thus, all boundaries were considered static and two dimensional for the calculations. The computations were completed using the finite element method with flux corrected transport (FEM-FCT), which incorporates a monotonic shock-capturing scheme combined with an unstructured transient adaptive refinement scheme for the mesh, formulated by Lohner et al.[27]

The following is a brief summary of the numerical method and the conservation form implementation of the Euler equations used in this study:

$$\frac{\partial U}{\partial t} + \frac{\partial F_j}{\partial x_j} = 0 \tag{1}$$

where the summation convention is used for the four conservation equations of mass, momentum, and energy:

$$U = \begin{bmatrix} \rho \\ \rho u_i \\ \rho e \end{bmatrix}, \qquad F_j = \begin{bmatrix} \rho u_j \\ \rho u_i u_j + p\delta_{ij} \\ u_j(\rho e + p) \end{bmatrix} \tag{2}$$

with the state equation is

$$p = (\gamma - 1)\rho(e - \tfrac{1}{2}u_j u_j) \tag{3}$$

where ρ, p, e, and γ, are density, pressure, specific total energy, temperature, and the ratio of specific heats (=1.4), respectively, and u_i is the component of the fluid velocity in the direction x_i of a Cartesian coordinate system.

The higher-order solution chosen for FEM-FCT is obtained via a two-step form of the second-order Taylor-Galerkin scheme. Solution of the consistent mass matrix form is achieved by iterating with the lumped mass matrix. A low-order monotonic scheme is also produced by adding "mass-diffusion" to the high- (second-) order scheme. The low-order solution and the high-order solution can then be combined to yield monotonic conditions for the conserved quantities near discontinuities and a second-order solution in the rest of the domain, through the FEM-FCT formulation. Adaptive H-refinement was employed to optimize the distribution of grid points by refining areas with high gradients of density and coarsening areas of low gradients of density. This adaptivity allows efficient use of memory and computational time. A local "error indicator" based on density gradients was used to determine if a given element needed to be refined, coarsened, or left alone based on the H_2-seminorm. This scheme has been shown to provide excellent flowfield predictions for nozzle flows[28] and shock-wave-generated vorticity.[29]

For simplicity, the computations assume a Mach 2.95 planar shock in the detonation chamber (4 cm wide), which is just about to enter the vortex chamber (o.d. of 16 cm, and i.d. of 8 cm). Such a shock yields a static pressure ratio of 10.0 and a fixed inflow of Mach 1.35. Time integration is referenced to an initial vortex chamber temperature of 690 K, which corresponds to an 8:1 mechanical compression ratio at top dead center.

Figures 2a–2f depict density distributions for sequential time steps. Figure 2a shows density values at 1500 time steps (~100 μs) from the initial conditions described above. As the shock enters the chamber, it is planar across the lower section of the chamber, however, near the convex corner formed at the intersection of the detonation and vortex chambers, an expansion wave forms as the flow turns and heads upward with a weak secondary shock. In addition, some reflection from the i.d. of the vortex chamber may be seen. In Fig. 2b (2000 time steps), the planar shock impinges on the o.d. and reflects in a manner similar to a curved compression corner as the primary shock moves counterclockwise. The secondary curved shock continues in a clockwise motion, while the reflection off of the i.d. reaches the bottom of the computational domain. In Fig. 2c (3000 time steps) the primary shock and the weak shock interact near the one o'clock position of the vortex chamber and a nearly stationary reflected shock wave causes a Mach stem to appear at the 6 o'clock position. There are strong radial gradients behind the primary shock, partly due to the constant local compression that results in a lower velocity along the o.d. The primary shock dominates the shock-shock interaction (Fig. 2d, 4000 time steps), and eventually interacts with the reflected shock below (Fig. 2e, 5000 time steps), and sends a normal shock moving upstream into the detonation chamber with subsonic flow behind it (Fig. 2f, 6000

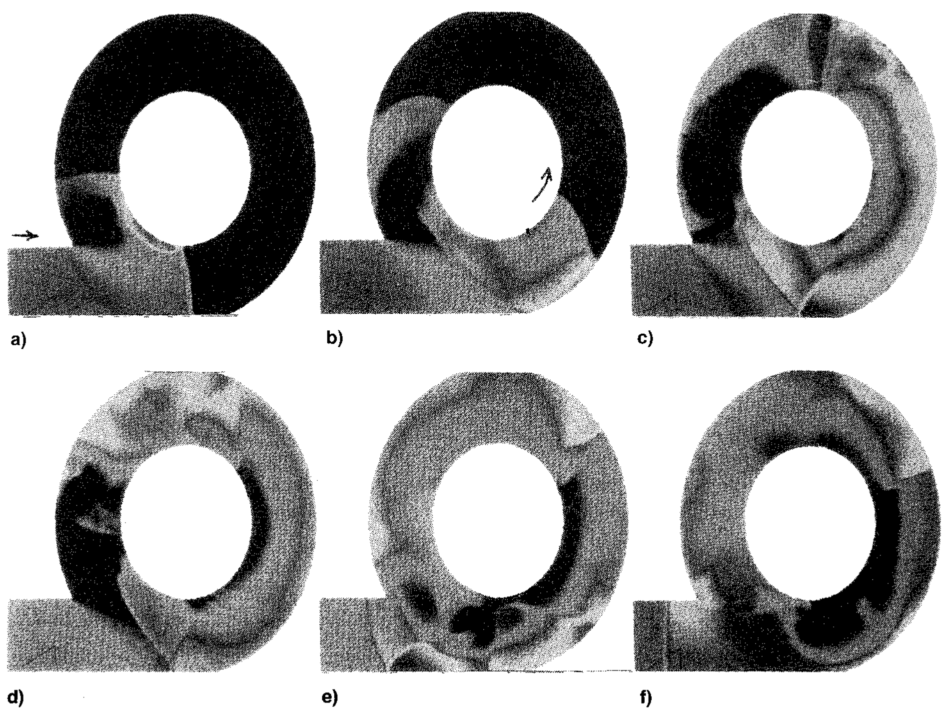

Fig. 2 Density shaded distribution of right-running Mach 2.95 shock entering quiescent vortex chamber: a) 1500, b) 2000, c) 3000, d) 4000, e) 5000, and f) 6000 time steps.

time steps). The computation was concluded as the shock was about to reach the inflow boundary with a total simulation time of ~0.51 ms for the 7000 time steps. In general, the density results show the preferential direction of compression, which stores the kinetic energy; the transverse wave dynamics, which should enhance mixing rates as compared to a conventional cylinder flowfield; and the finite time associated with a pressure increase across the piston head surface, which was equivalent to about 5 deg of revolution for a 1600-rpm engine, and significantly less than that for NOx formation.[3]

Velocity vectors and Mach number distributions at 4000 time steps are shown in Figs. 3 and 4, and velocity vectors and Mach number distributions for 7000 time steps are shown by Figs. 5 and 6. At 4000 time steps, the right side of the chamber remains supersonic, whereas complex shock-vortex dynamics with large scale eddies are found on the left side. Refinement may be observed in the concentration of velocity vectors along portions of the flow with high gradients. At 7000 time steps, a normal shock is just about to reach the inflow boundary, while supersonic flow is maintained in portions of the chamber and a somewhat uniform vortex flowfield has resulted with an average Mach number of about 0.6. Thus, through the processes of multiple shock and expansion waves, a portion of the linear kinetic energy of the shock-induced flow is transformed and stored into the rotational kinetic energy of a vortex. It can also be expected that this process will allow rapid mixing of the combustion products issuing into the cooler fresh air of the vortex chamber. Such mixing is important to moderate the overall temperatures below that of significant NOx production. In a similar flow, rapid quenching and strong mixing were experimentally observed in a shock channel generated confined vortex by Chan et al.[30] with circulation velocities as high as 450 m/s, which lends support to the above conclusions. Finally, computations for a shock entering a vortex chamber without a solid core indicated significantly less mixing and less vortex energy storage as compared to the present preferred "doughnut" configuration.[16]

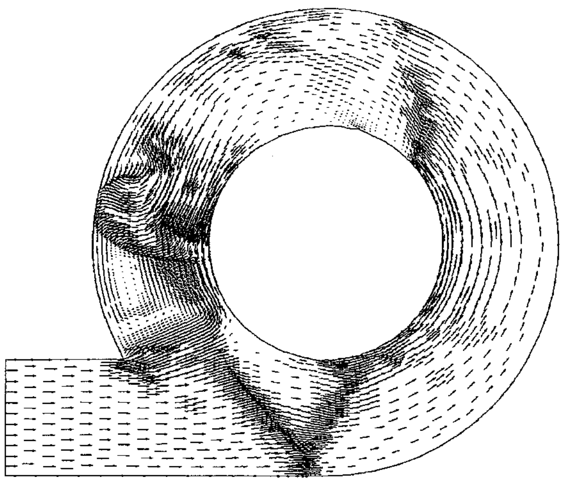

Fig. 3 Velocity vectors of Mach 2.95 shock entering vortex chamber at 4000 time steps (size varies according to Mach number). Strong mixing is noted due to multiple curved shock propagation and interaction.

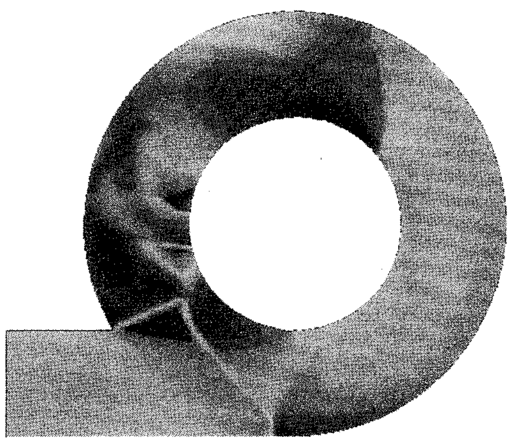

Fig. 4 Mach number distribution (minimum = 0.1 and maximum = 1.8) of Mach 2.95 shock entering vortex chamber at 4000 time steps.

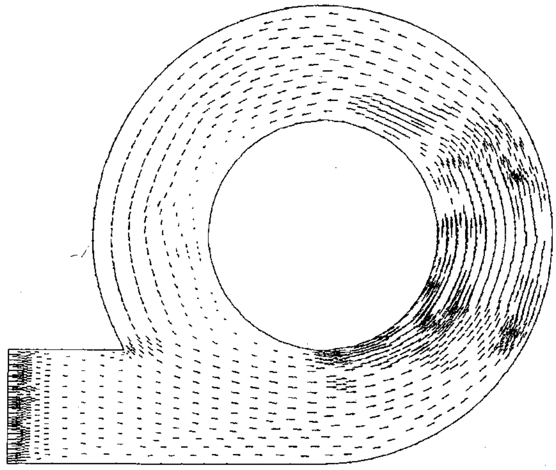

Fig. 5 Velocity vectors of Mach 2.95 shock entering vortex chamber at 7000 time steps (size varies according to Mach number). High-speed vortex ($M_v \sim 0.6$) has been established.

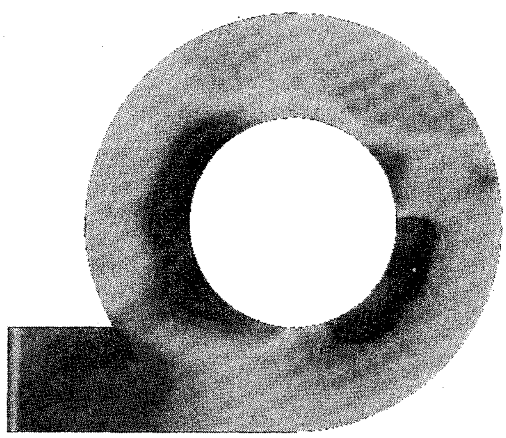

Fig. 6 Mach number distribution (minimum = 0.1 and maximum = 1.4) of Mach 2.95 shock entering vortex chamber at 7000 time steps. Note, reflected shock waves have coalesced into a planar shock, which is moving upstream and is just about to reach the inflow boundary.

III. Conclusions

Controlled detonation combustion may be used in future internal combustion engines to achieve efficiencies similar to that of constant volume burning and minimize pollution emission formation. Such an engine is herein proposed that uses a separate detonation combustion chamber that discharges tangentially into a vortex chamber formed by the piston and cylinder at top dead center; this prevents direct impingement of shocks on the piston surface. The rapid near stoichiometric combustion is followed by rapid dilution through mixing with air in the vortex chamber to reduce the formation of NOx and unburned hydrocarbons and to achieve an overall lean mixture. The vortex chamber is designed to store a portion of the detonation wave's kinetic energy in the form of a vortex, which reduces the rate of pressure drop during piston expansion. While efficient conversion of some of this kinetic energy can yield a thermal efficiency somewhat better than that of constant volume subsonic combustion, the most significant benefit realized is relative to the case of slow deflagration burning, which typically exhibits nearly constant pressure combustion. The propagation of a detonation-formed shock wave into the fuel-free vortex chamber was simulated with a shock-capturing finite element Euler flow code and the results supported the feasibility of vortex storage and rapid leaning. Thus, the proposed internal combustion engine modification can take advantage of the low emission benefits of natural gas as a fuel, while providing rapid combustion through detonation and rapid dilution due to the high-speed vortex flowfield. Potential problems and issues of the detonation engine technology have also been addressed in this study. In addition, much work is needed to seriously assess the viability of this proposed technology in view of the potential problems.

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