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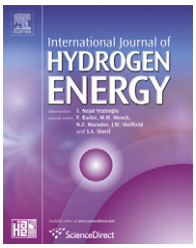

LES model of large scale hydrogen–air planar detonations: Verification by the ZND theory

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ABSTRACT

The large eddy simulation (LES) model of hydrogen–air detonation at very large scales, which doesn't require Arrhenius chemistry, is presented. The progress variable equation is applied for the first time to simulate propagation of a reaction front following and coupled with a leading shock. The gradient method, based on a product of pre-shock mixture density and detonation velocity, is employed as a source term in the progress variable equation. Chemical kinetics enters the combustion model only through its influence on the detonation velocity and modelling of detailed chemistry is omitted. The LES model is verified against theoretical solution by the Zel'dovich–von Neumann–Doring (ZND) theory for a case of planar 29.05% hydrogen–air detonation in elongated $3 \times 3 \times 100$ m calculation domain. Thermodynamically calculated values of the specific heats ratio for burned mixture $\gamma = 1.22$ and the standard heat of combustion $\Delta H_c = 3.2$ MJ/kg are applied without any adjustment often applied in other models. Numerical simulation reproduced theoretical values of von Neumann spike, Chapman–Jouguet pressure, Taylor wave and detonation propagation velocity. There are no adjustable parameters in the model. Practically no grid sensitivity for the planar detonation wave is demonstrated by the LES model. Detonation velocity and pressures are shown to be nearly independent of the computational cell size in a wide range of cell sizes 0.1–1.0 m. Impulse depends to some extent on a cell size. Three-dimensional version of the LES model is under development to simulate pressure effects and identify design solutions, including mitigating techniques, for hydrogen safety engineering. There is no intention to use this oriented on large scale applications engineering LES model to reproduce fine structure of the detonation wave.

1. Introduction

Hydrogen is increasingly used as an energy carrier in transport, stationary and other applications. Detonation is a worst case scenario for accidents with unscheduled hydrogen release. Higher propensity of hydrogen–air mixtures to deflagration-to-detonation transition (DDT) compared to hydrocarbon–air mixtures, along with lower ignition energy and wider detonability limits, requires special technical and organizational measures to guarantee the same level of safety for emerging hydrogen-fuelled technologies as for today's fossil-fuelled economy. Contemporary engineering tools are needed to simulate pressure effects of hydrogen explosions in the open atmosphere and complex geometries at practical scales. Prediction of detonation parameters, i.e. pressure and impulse, as well as blast parameters beyond the detonation

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Nomenclature

c	progress variable (normalised product mass fraction)
D	detonation velocity, m s^{-1}
ΔH_c	heat of combustion, J kg^{-1}
S_c	source term in conservation equation for progress variable, kg m^{-3} s^{-1}
S_e	source term in energy conservation equation, J m^{-3} s^{-1} $S_e = S_c \cdot \Delta H_c$
t	time, s

Greek letters

μ	dynamic viscosity, Pa s
ρ	density, kg m^{-3}

Subscripts and superscripts

c	source term in progress variable equation
e	source term in energy conservation equation
eff	effective value
u	unburned mixture

Bars

–	LES filtered quantity
~	LES mass-weighted filtered quantity

zone is important for hydrogen safety engineering, particularly for risk assessment through realistic safety distance assessment for hydrogen infrastructure [1,2] and development of mitigation technologies.

The Zel'dovich–von Neumann–Doring (ZND) theory, developed by Zel'dovich [3], von Neumann [4] and Doring [5] following the analysis of one-dimensional shock with energy feeding performed earlier independently by Chapman [6] and Jouguet [7], implies that detonation is a complex of precursor shock and combustion wave. Detonation propagates with a speed of von Neumann shock. This shock compresses the fresh mixture and enables it to react. The end of reaction zone is defined by the Chapman–Jouguet (CJ) condition (sonic plane) [6,7]. Detonation front thickness is a distance from the precursor shock to the end of reaction zone where the CJ condition is reached. Thickness of the detonation front increases with decreasing Mach number [8]. The flow in the reaction zone is subsonic relative to the shock and is acoustically isolated from the flow structure downstream of the sonic plane, and the local Mach number is $M < 1$ and increases with the distance from the leading shock due to the heat release by the chemical reaction [8]. Each wave of the ZND type has a minimum sustainable detonation speed known as the CJ speed in which a sonic plane (relative to the detonation shock speed) arises at the CJ point. Combustion energy released in reaction front feeds the leading shock by sonic waves. The speed of detonation wave and the thermodynamic state at the CJ point are determined by the initial upstream shock state and by the equation of state for the reaction products alone. Rapid combustion occurs in the detonation as a result of the exponential dependence of the chemical reaction rate on temperature which in consequence supports the shock [8,9,10]. The particular form of the reaction rate law and the equation of state for partially reacted material affect only the interior structure of the reaction zone [11,12].

The detonation simulated in this study, i.e. near stoichiometric 29.05% hydrogen–air mixture at initial conditions of 0.099 MPa and 304 K, travels at 1954 m/s with a propagation Mach number $M = 4.8$ and the detonation front thickness 5.21 mm according to the ZND theory [13].

Downstream of the sonic plane is a region where an expansion wave, i.e. Taylor wave, connects the state at the CJ plane to the rear boundary. The Taylor wave does not have to be attached to the final point (CJ point) [11,12]. The expansion fan is not strictly a part of either the CJ or ZND models. The products beyond the CJ plane continue to accelerate as they expand and their temperature and pressure continue to drop. Taylor [14] was the first to examine the distribution of velocity in this region. Gas velocity at the CJ plane is about 1/3 of D [15]. The pressure gradient in the expansion wave for particular pressure depends only on the distance of the front from the detonation origin. At the end of the Taylor wave for planar detonation the pressure is about 0.375 of P_{CJ} [15].

Euler equations with Arrhenius chemistry are commonly used for numerical simulation of detonations. The application of Navier–Stokes (NS) equations is more promising approach [16] enabling DDT modelling and simulation. However, as mentioned in Ref. [17] the unsteadiness in multi-dimensional detonation makes it extremely difficult to use NS equations, because of a number of unsteady shear layers existing not only on the tube walls but also downstream of the curved and intersecting shock waves. Over 100 points are required in the half-reaction length of steady planar detonation to obtain a truly converged solution when Arrhenius chemistry is applied [18]. Resolutions of less than about 20 points per half-reaction length give very poor or else entirely spurious solutions. Short and Quirk [19] have shown that for pulsating detonations with realistic chain-branching reactions, a few hundred points per half-reaction length may be required to obtain even the qualitatively correct solutions. The resolution required to obtain converged solutions in multi-dimensional cellular detonation simulations is likely to be higher than that for the simpler pulsating detonations. Generation of high-accuracy solution-adaptive grids resolving all such highly-unsteady shear layers is impossible within the present computational capabilities as a required mesh of 1 micron necessitates 2×10^{10} grid points for a 2D domain of only 10×20 cm which is far too small for accident scales of ten and hundred of meters. Increase of cell size makes even one step irreversible Arrhenius chemistry incapable of reproduction of experimental explosion characteristics without ''recalibration'' for each particular grid.

Thus, Arrhenius chemistry approach can hardly be suggested as a grid independent tool for hydrogen safety engineering to tackle large scale problems. Alternative methods of detonation modelling should be developed, verified by recognised theories and validated against large scale experiments.

There are a few publications on safety aspects of hydrogen–air detonations, e.g. Ref. [45]. LES models were previously used for hydrogen–air to simulate 3D deflagrations, e.g. Ref. [20], and DDT, e.g. in a channel with obstruction (0.92