

Influence of Turbulence on the Deflagration to Detonation Transition in a Tube

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Formulation of the problem

One of the general mechanisms responsible for the transition to detonation of a flame is the turbulence generated by the tube wall, and probably by the flame itself. The focus of this study is the role of the turbulence and pressure waves in the acceleration of stoichiometric hydrogen-oxygen flame propagating in a tube and how it affects the transition processes.

The interaction between the wall and the flow behind the leading shock wave generates turbulence in the whole flowfield, starting at the wall and propagating toward the center. Correspondingly, as known from experimental data, the leading point of the turbulent flame is in the vicinity of the wall and this determines the flame velocity. Therefore, we consider the characteristics of the turbulence near the wall as the controlling factor of the whole turbulent combustion in the tube.

The present study of the problem is based on the assumption that the bulk flow in the detonation tube is one-dimensional. This is a simplified representation; in real situations a transverse propagation of pressure waves and their reflection from the wall are very important. But 2 or 3-D simulation of this phenomena is certainly difficult, at least time-consuming, and in this study the effects of the wall on the main flow were incorporated through boundary conditions, as well as by turbulence models for the mixing and reaction rates.

The predictions are based on numerical solutions of the Favre-averaged, one-dimensional, non-steady set of the conservation equations for individual species, mass, and total energy in the conservative form.

The turbulence model consists of two elements. The first is a simulation of diffusion processes by the wall and by flame generated turbulence using eddy viscosity formulation. The turbulent viscosity μ_t is computed using a $k-l$ model of turbulence $\mu_t = C_k \rho l \sqrt{k}$. The system of conservation equations is closed by including the balance equations for the turbulent kinetic energy k for the premixed flame [1].

The turbulence generated by the wall was incorporated through the turbulent production function by using the wall function and wall friction law. The turbulent length scale l is defined proportional to the boundary layer thickness

$$l = C_l \delta, \quad \delta = 0.4 x_d \text{Re}_x^{-0.2}, \quad \text{Re}_x = \frac{u x_d}{\nu},$$

where $x_d = x_l - x$, x_l is the position of leading pressure wave, $C_l = 0.025(1 + 30\alpha)$, $\alpha = \delta_r / \delta_e$, δ_r is the roughness height, and δ_e is the equilibrium layer thickness.

The second element of the simulation of the turbulence is a simulation of turbulence combustion.

The chemical model for premixed gases is a two-step model. The first step calculates the induction delay time; the second step calculates the heat release with a mean reaction rate. The mean reaction rate taken as [2]:

$$\dot{w} = C_w \frac{l}{\sqrt{k}} \left(\frac{u_L}{2/3k} + (1 + Da_t^{-2})^{-1/4} \right)^2 Y_f (1 - Y_f) \rho_0,$$

where Da_t is the Damkohler number.

Numerical technique and results

The numerical procedure for solving the set of equations is based on a two-step, time splitting technique for the different physical processes. In the first step, the shock wave propagation is found by solving Euler equations using an explicit TVD scheme with Roe's average [3]. At the second step, the diffusion processes is solved by a Cranck-Nicholson scheme and the kinetic terms are solved fully implicitly.

Simulation was performed for a tube $d = 10$ mm in diameter with various levels and types of roughness. At initial time the gas at rest with temperature $T = 300$ K and pressure $p = 10^5$ Pa. The boundary conditions are as follows: Non-flow, adiabatic condition at the left closed end of the tube ($x = 0$), and non-reflection conditions at the right open end ($x = L$). The tube wall is adiabatic. The properties of the wall were modeled by the wall friction law.

Figure 1 shows the typical isolines of (a) temperature, (b) pressure, and (c) Mach number, and its 3-D view in the (x,t) plane at the DDT for the case with $\alpha = 0.1$. We use the following labels: FF - flame front, IW - initial pressure wave generated during the ignition, LW - leading pressure wave generated by accelerating flame, Dt - detonation wave, Rt - retonation wave, Rf - wave reflected from wall.

Table 1 show the relation between transition time - t_d , transition distance - x_d/d , intensity of detonation wave just after DDT is occurring - P_d/P_0 , and the detonation velocity just after DDT - V_f , for the range of α values used in the simulation.

α	0.05	0.1	0.2	0.5
$t_d, [\mu s]$	1000	560	230	170
x_d/d	50	31	11	5
P_d/P_0	83	74	55	27
$V_f, [m/s]$ approx.	3500	3300	3100	3000

Table 1. Results of transition time, distance, intensity and flame velocity for various thickness ratios α .

Figure 2 shows the role of turbulence during the DDT. After first acceleration stage, the flame is decelerated because of low turbulence level ahead of flame, generated by the initial pressure wave (IW). The DDT occurred at the distance $x_d = 200$ mm and time $t = 380 \mu s$ after the leading pressure wave (LW) generated stronger turbulent flow. But the role of turbulence is, in general, the acceleration of flame front and it is not enough to explain the phenomenon of DDT just by the turbulence mechanism. At the final stage of the flame acceleration and just before DDT occurs, the flame propagation velocity is almost equal to the velocity of generating pressure waves. Both waves move almost together, and the magnitude of pressure increases at a fast rate (almost exponentially). This behavior of DDT is demonstrated clearly in Fig. 3, where the combustible mixture was ignited at some distance from the closed end of the tube. The first reflected pressure wave from the closed end accelerates the flame, but it is weak and DDT does not occur. When the stronger second wave reaches the flame front, then both waves move together for some time (about $50 \mu s$). This system of coupled waves is unstable and after a few pressure oscillations the DDT is achieved.

References

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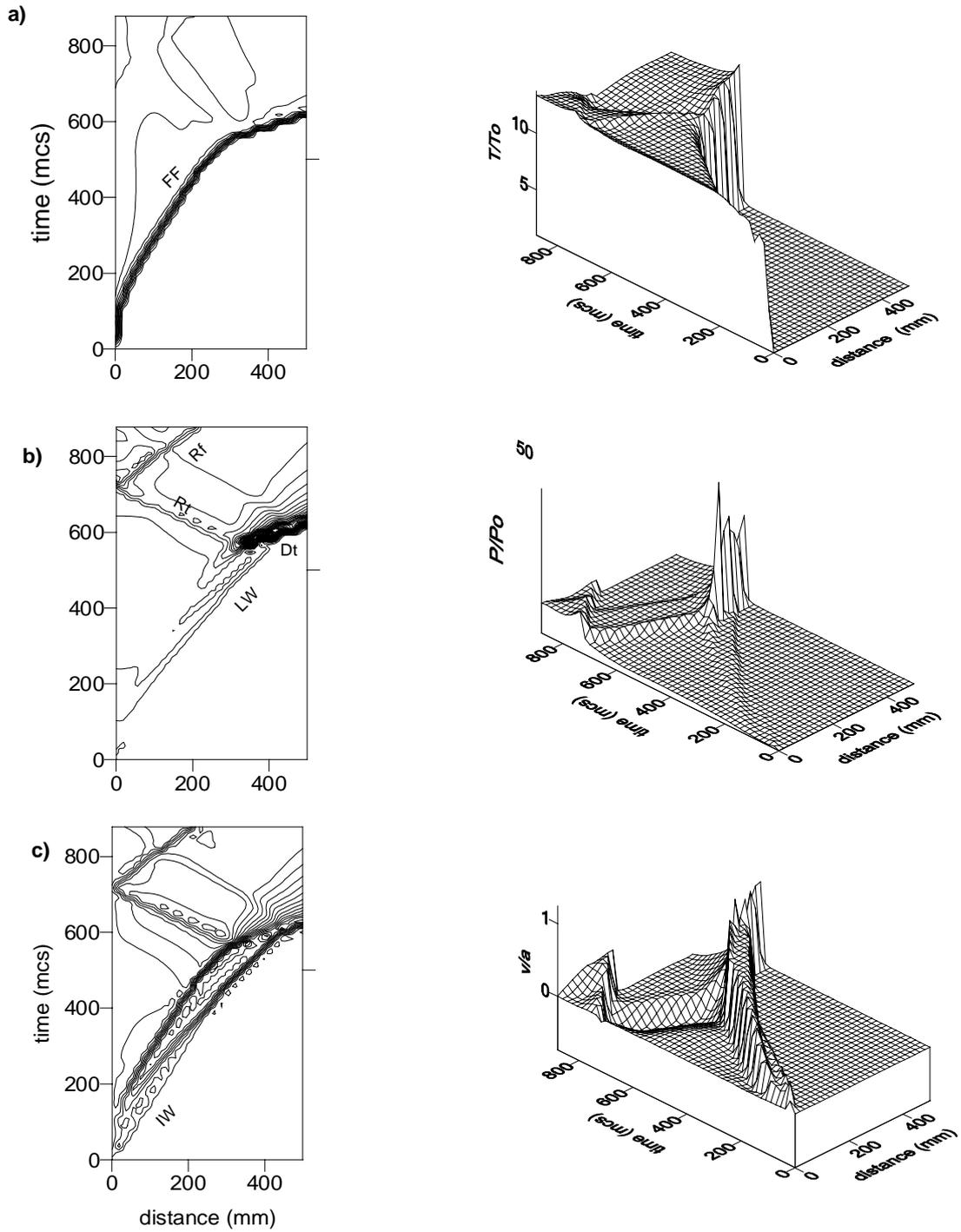


Figure 1. Plots of (a) Temperature, (b) Pressure, and (c) Mach number in the (x,t) plane for the DDT case with thickness ratio $\alpha = 0.1$ (ratio of wall roughness height to equilibrium layer thickness). Distance in millimeters, and time in microseconds. The temperature and pressure plots are non-dimensionalized to the initial values of $T_0 = 300$ K and $P_0 = 10^5$ Pa.

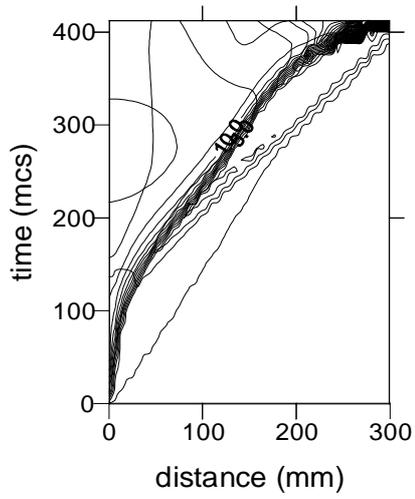


Figure 2

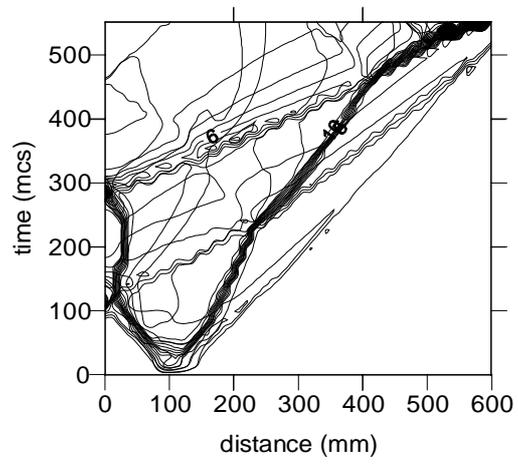


Figure 3

Figure 2. Plot of a DDT transition promoted by the stronger turbulence generated by the leading pressure waves from the flame front.

Figure 3. Plot of DDT transition when the igniter is located 10 cm from the closed end of the tube. The transition is promoted by the stronger waves reflected from the closed end.