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Modeling maximum flame speeds

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Abstract

A simple gold model for flame acceleration in tubes, caused by repeated obstacles, has been developed using a "boxcar" approach. The tube is assumed to consist of a series of chambers separated by obstacles. The feedback mechanism for flame acceleration is modeled by assuming that the effective burning velocity in the *n*th chamber depends on the same quantity in the $(n-1)$th chamber. The equation for flame propagation is shown to be a logical difference equation. The equation predicts the various experimentally observed end results of flame acceleration such as total flame extinguishment after a flame has reached a certain critical flame speed, subsonic steady-state flame propagation, and continuous flame acceleration leading to transition to detonation. This equation models flame acceleration phenomenologically by associating various terms with effects such as flame folding, fine-scale turbulence, quenching and gas dynamics. The predicted maximum flame speeds (subsonic flame propagation) for various mixture compositions, obstacle spacings, obstacle blockage ratios, and initial gas temperatures agree with the experimental results fairly well.

1. Introduction

A freely expanding flame is intrinsically unstable. It has been deomonstrated, both in laboratory-scale experiments (Wagner, 1981; Moen et al., 1980) and large-scale experiments (Hjertager et al., 1983; Moen et al., 1982), that obstacles located along the path of an expanding flame can cause rapid flame acceleration. Qualitatively, the mechanism for this flame acceleration is well understood. Thermal expansion of the hot combustion products produces movement in the unburned gas. If obstacles are present, turbulence can be generated in the combustion-induced flow. As a flame continues to propagate, large-scale turbulence in the flow field can enhance the overall burning rate in the reaction zone by causing a flame to "fold" and "stretch", resulting in an increase in the flame surface area. Small-scale turbulence increases the local burning rate by increasing the local mass and energy transport. An overall higher burning rate, in turn, produces a higher flow velocity in the unburned gas. This feedback loop results in a continuous acceleration of the propagating flame.

Turbulence induced by obstacles in the displacement flow does not always enhance the burning rate. Depending on the mixture sensitivity, high intensity turbulence can lower the overall burning rate by excessive flame stretching and by

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rapid mixing of the burned products and the cold unturned mixture. If the temperature of the reaction zone is lowered to a level that can no longer sustain continuous propagation of the flame, a flame can be extinguished locally. The quenching by turbulence becomes more significant as the velocity of the unburned gas velocity increases. For some insensitive mixtures, this can set a limit to the positive feedback mechanism. The weakening of the feedback mechanism eventually causes the flame to reach a steady-state velocity. Hence, both the rate of flame acceleration and the eventual steady-state velocity (also referred to as the maximum flame speed) depend on the competing effects of turbulence on combustion.

In an earlier study of flame propagation in tubes filled with obstacles (Lee et al., 1985) observed that obstacle-induced flame acceleration is a highly unstable phenomenon. Steady-state flame propagation with a uniform velocity is not always the end result of flame acceleration. Depending on the mixture sensitivity (burning velocity) and obstacle configuration, sometimes the flame may be quenched or extinguished abruptly after it has accelerated past a critical velocity. Alternatively, the flame may continue to accelerate until gas dynamic choking of the induced flow limits the maximum velocity or until a transition to detonation occurs. Even though the mechanism of flame propagation in these steady-state regimes (Lee et al., 1985) is fairly well understood, the mechanism that causes the manifestation of one regime or another is not. At the present time, models that can predict these end results of flame acceleration are not available.

This paper describes an approach to modeling flame acceleration due to repeated obstacles where details of the structures of the flow field and the reaction zone are ignored and flame acceleration is modeled phenomenologically using the effects of flame folding, fine -scale turbulence, quenching and gas dynamics. The predicted steady-state flame speeds are compared with the maximum flame speeds measured by Beauvais et al. (1993) of the Technical University of Munich.

2. Modeling turbulent flame acceleration

Because of the complex nature of turbulent flame acceleration, "brute-force" approaches that involve solving the three-dimensional turbulent flow field equations, together with detailed kinetics for the chemical reactions, are unlikely to produce useful results in the near future. In the past few years, many computer codes have been developed to model the problem of turbulent flame acceleration by repeated obstacles (Hjertager, 1982a; Ashurst and Barr, 1982; Chan et al., 1985). They all employ various degrees of simplification, such as small flame Mach numbers and no compressibility effects. For describing the initial phase of flame acceleration, these models have been found to be fairly successful. However, these codes do not include a damping term in the burning rate model to account for the quenching effects of turbulence on combustion. Thus, according to these codes, a flame can neither reach a steady-state velocity nor become quenched abruptly after it has accelerated past a critical velocity. The criterion for transition to detonation in these codes is usually chosen arbitrarily with no physical justification. Nevertheless, they all manage to reproduce the trend of the experimental results reasonably well. Hjertager (1982b) has attempted to incorporate the negative aspect of turbulence on combustion by comparing the chemical time and the fluid-dynamic time. If the former is longer, the burning rate is set to zero. This either "on" or "off" approach has been shown to be very successful in modeling flame acceleration. However, this approach still cannot predict the abrupt jump from one steady-state regime to another such as transition to detonation. To obtain better insight into the phenomenon, a new approach to model flame acceleration in channel or tube filled with obstacles is introduced in this paper.

To model flame propagation in tubes filled with repeated obstacles, the tube is assumed to consist of a series of chambers (or boxcars) separated by obstacles, as shown in Fig. 1. The flow properties, such as the turbulent intensity and the burning rate, are considered uniform everywhere in each chamber. One can define an effective burning velocity S_T for the combustion zone such that

$$S_T = \int S_l \, da/A = \frac{S_l A_f}{A} \quad (1)$$

where S_l is the local turbulent burning velocity (uniform along the flame front) da is the differential flame surface area, A_f is the total flame surface area and A is the cross-sectional area of the tube. Eq. (1) implies that the influence of turbulence on the effective burning velocity is the combined effect of turbulence on local burning velocity (via turbulent transport of heat and mass) and the flame surface area (via flame folding).

To model the feedback mechanism, the effective burning velocity S_{T_n} in the nth chamber is assumed to depend on the effective burning velocity in the $(n-1)$th chamber

$$S_{T_n} = f(S_{T_{n-1}})$$

where $f(S_{T_{n-1}})$ is assumed to be a function in the form of a polynomial.

$$S_{T_n} = A + BS_{T_{n-1}} + CS_{T_{n-1}}^2 + \dots \quad (2)$$

The present model also assumes that the enhancement of burning rate by turbulence, quenching by excessive stretching and gas-dynamic effects can be modeled independently by various terms in Eq. (2). On the basis of experimental observation and physical reasoning, an empirical equation of flame propagation can be expressed as

$$S_{T_n} = \alpha + \beta S_{T_{n-1}} - \gamma S_{T_{n-1}}^2 + \delta S_{T_{n-1}}^3 \quad (3)$$

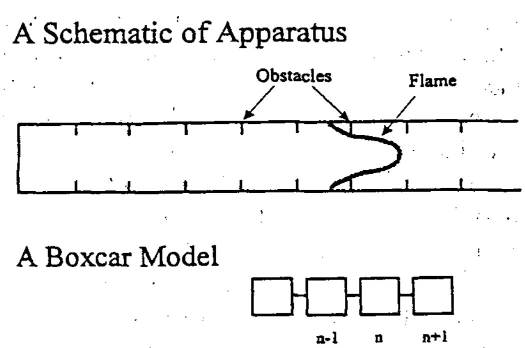

Fig. 1. A conceptual picture of the "boxcar" model.

The first two terms on the right-hand side represent an enhancement of the burning velocity by turbulence. Quenching by turbulence is assumed to be the only damping mechanism for flame acceleration and is represented by a second-order term. The gas dynamic effects (increase in burning rate by the pre-compression effects of the precursor shock) are represented by a third-order term. It is obvious that these effects cannot be fully described by individual terms in Eq. (3). However, a simple equation allows us to examine qualitatively the dynamic feature of an extremely complex phenomenon.

The parameter α, β, γ and δ in Eq. (3) are assumed to depend on the initial and boundary conditions of the system, such as the burning velocity of the mixture and the obstacle configuration. Other secondary effects such as heat loss to the wall and momentum loss due to obstacles are ignored. Eq. (3) has the form of a logistic difference equation. Logistic difference equations are intrinsically unstable, and unique steady-state solutions as n approaches infinity do not always exist. The convergence of the solution depends on the coefficients of the various terms. Logistic difference equations have been used to model complex phenomena that exhibit chaotic behavior (Kadanoff, 1983; May and Oster, 1976). It is proposed that the instability behavior of flame acceleration in an obstacles-filled tube can also be modeled using this type of equation.

Following the feedback mechanism as described earlier, it can be assumed that the burning velocity in one chamber is related to the burning velocity in the previous chamber. At the same time, the burning velocity in a chamber depends on the turbulent fluctuating velocity in the same chamber. Therefore the burning velocity in the nth chamber can be assumed to be related to the turbulent fluctuating velocity u' in the $(n-1)$th chamber.

$$S_{T_n} = f(S_{T_{n-1}}) = f'(u'_{n-1}) \quad (4)$$

The local turbulent fluctuating velocity can be assumed to be proportional to (i) the local mean flame velocity $(\rho_u/\rho_b)S_T$, where ρ_u and ρ_b are the densities of the unburned and burned gas respectively, (ii) the blockage ratio BR (equal to the blocked area divided by the total cross-sectional area) because any decrease in flow area causes an increase in the flow velocity and (iii) the spacing (or pitch) P of the obstacles because, depending on the spacing of the obstacle, obstacle-induced turbulence can decay substantially before further enhancement by the next occurs. As a result, the following phenomenological expression is assumed:

$$u' = \frac{K}{1-\mathrm{BR}}\frac{D}{P}\frac{\rho_u}{\rho_b}S_T$$

where D is the diameter of the tube and K is the arbitrary constant. In a non-dimensional form, Eq. (4) becomes

$$S_T = f\left(\frac{K}{1-\mathrm{BR}}\frac{D}{P}\frac{\rho_u}{\rho_b}S_T\right)$$

The equation of flame propagation becomes

$$S_{Tn} = S_L + B\left(\frac{K}{1-\mathrm{BR}}\frac{D}{P}\frac{\rho_u}{\rho_b}S_{Tn-1}\right) - C\left(\frac{K}{1-\mathrm{BR}}\frac{D}{P}\frac{\rho_u}{\rho_b}S_{Tn-1}\right)^2\frac{1}{S_L} + D\left(\frac{K}{1-\mathrm{BR}}\frac{D}{P}\frac{\rho_u}{\rho_b}S_{Tn-1}\right)^3\left(\frac{1}{S_L}\right)^2 \quad (5)$$

where S_L is the laminar burning velocity of the mixture and B, C and D are constants. The flame speed in the nth chamber is simply $(\rho_u/\rho_b)S_T$.

Eq. (3) (a general form of Eq. (5)) is a logistic difference equation. The dynamic behaviour of this equation has been discussed by Chan (1987). Depending on the coefficients of the equation, a stable long-term solution does not always exist. Four end results (as n approaches infinity) of flame acceleration are possible for Eq. (3). Depending on the coefficients, four end results are possible as n increases: S_T can abruptly acquire a negative value after an initial increase, S_T can reach a steady-state value, S_T can oscillate between two values, or S_T can continue to increase without bound. These end results are illustrated in Fig. 2. The values of the coefficients are chosen arbitrarily for illustration purpose. If a different set of coefficients were chosen, the width of the four regimes may change. Physically, these four end results can be interpreted as flame quenching

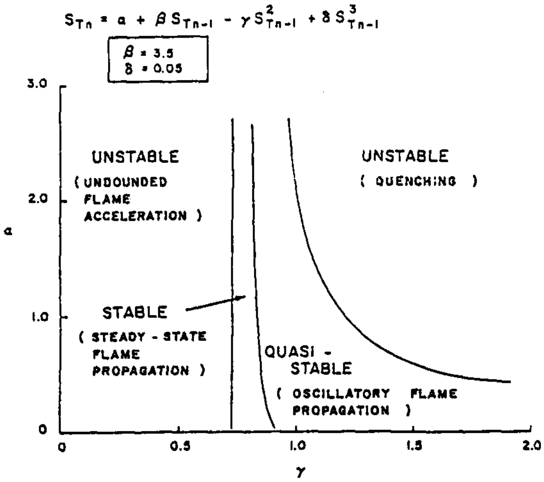

Fig. 2. Stability regimes for the equation of flame propagation (Eq. (3)).

after an initial acceleration, oscillatory flame propagation, steady-state flame propagation and continuous flame acceleration respectively. It should be pointed out that continuous flame acceleration will eventually lead to conditions that trigger the transition to detonation. This model does not predict transition to detonation directly. If transition to detonation is not possible owing to boundary limitation, the propagation velocity of the reaction front will be limited by the local gas-dynamic choking condition.

As shown in Fig. 2, the quenching regime and the unbounded flame acceleration regime are unstable regimes. Stable steady-state solutions are not possible. Steady solutions are possible for a certain range of γ. Furthermore, a single-valued long-term solution can be obtained for a narrow range of γ only. The long-term solution becomes unstable when γ is increased beyond a certain critical value. At this point, two other long-term solutions emerge. S_T oscillates between these two values indefinitely. This branching process is often referred to as bifurcation. As a result, this regime can only be considered as quasi-stable. Experimentally, this flame speed oscillation is difficult to detect because of limited spatial resolution of the detectors (photodetectors, thermal couples or pressure transducers). In most cases, only a mean value can be measured. As a result, the stable and quasi-stable regimes are often treated as a single regime. Qualitatively, these end results agree with experimental observation for flame propagation in tubes filled with obstacles (Lee et al., 1985). This phenomenological model has demonstrated that the existence of these end results of flame acceleration as well as the transition from one regime to another regime are caused by the inherent instability associated with the feedback mechanism.

3. Maximum flame speeds

The maximum flame speed (MFS) in the phenomenological model is defined as a steady-state flame speed or the average of the oscillatory flame speeds. Beauvais et al. (1993) at the Technical University of Munich examined flame propagation in a tube filled with repeated orifice obstacles. The steady-state velocity of the reaction wave (referred to as the MFS) for various H_2–air–steam mixtures were measured in their experiments. Their data included both subsonic deflagration speeds and supersonic detonation speeds. Parameters that were varied in their experiments included the blockage ratio, the steam concentration, the initial mixture temperature and the spacing of the obstacles.

To determine whether the above phenomenological model can predict these MFSs qualitatively, the parameters considered in the experiments of Beauvais et al. were varied in the model. The constants in Eq. (5) were chosen to achieve the best fit to experimental results. Typical values for the constants in Eq. (5) are shown as follows: S_L values taken from Liu and MacFarlane (1983); $S_{T0} = 0$ m s^{-1}; $B = 1.6$; $C = 0.001$; $D = 10^{-10}$ (i.e. gas-dynamic effects are ignored); $K = 30$; ρ_u/ρ_b values taken from equilibrium calculations using the data of Gordon (1971).

Figs. 3 and 4 show the MFSs for various hydrogen concentrations, obstacle spacings and obstacle blockage ratios (orifices). Within a certain range of conditions, the trend of the MFS predicted by the phenomenological model agrees with the experimental results fairly well. Outside this range, the predictions by this simple model are not as good. For example, the predicted values are much lower than the measured results for obstacle spacings below 200 mm. It is assumed in the model that the combustible mixture in the $(n-1)$th chamber is all consumed before a flame propagates into the nth chamber. It was observed in the experiment that, for obstacles very close together, a reaction zone can be stretched out, leaving behind pockets of unburned gas in the wakes of the obstacles. As a result, assuming that

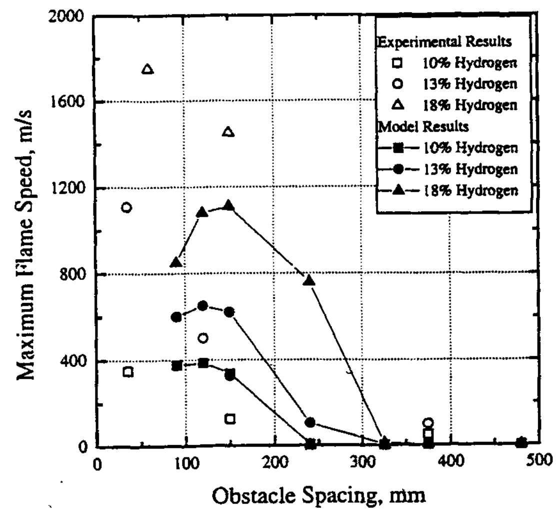

Fig. 3. MFS vs. obstacle spacing for flame propagation in a tube filled with oriifice obstacles (blockage ratio, 0.3).

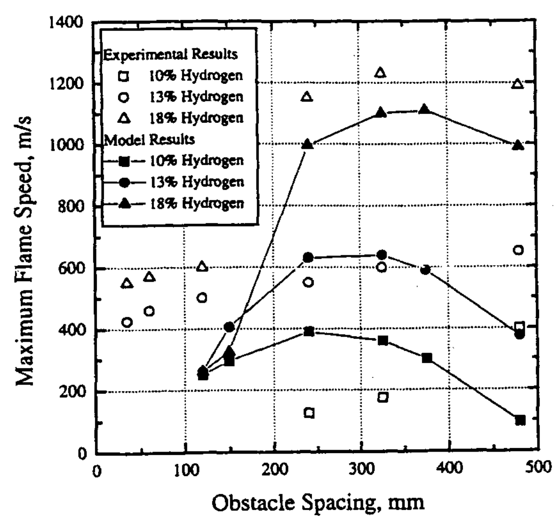

Fig. 4. MFS vs. obstacle spacing for flame propagation in a tube filled with orifice obstacles (blockage ratio, 0.7).

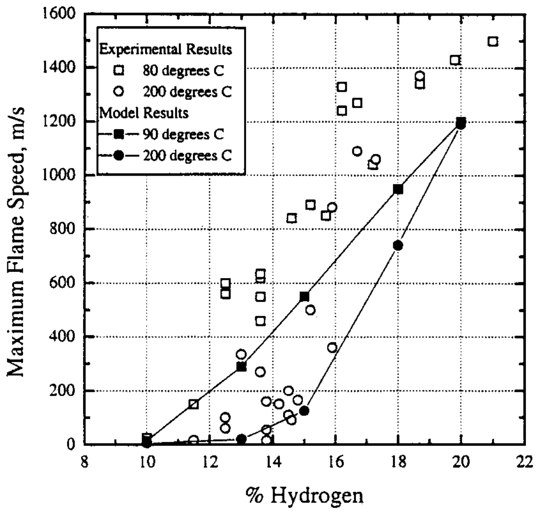

Fig. 5. MFS vs. hydrogen concentration for flame propagation in a tube filled with orifice obstacles (blockage ratio, 0.7; obstacle spacing, 500 mm; steam concentration, 0%).

burning can occur in only one chamber for all obstacle spacings is unrealistic. In reality, a flame can burn in several chambers at the same time. To modify the present model to account for multiple-chamber burning would make the model too complicated and is beyond the scope of the present study. It was also observed in the experiments of Beauvais et al. that, for sensitive mixtures (e.g. mixtures containing more than 18% of H_2), flame acceleration could lead to transition to detonation and MSFs over 1000 m s^{-1} (see Fig. 4). Since the present model does not simulate detonation, it cannot predict supersonic flame speeds. For those experiments in which transition to detonation had occurred, the MFSs would be severely underestimated by the model.

Figs. 5 and 6 show the effects of steam and initial temperatures on MFS. In these series of experiments, the obstacle spacing was 500 mm and the blockage ratio of the obstacles was 0.7. Both of these figures show good agreement between the predicted and the observed MFSs for insensitive mixtures at initial temperatures of 80 and 200 °C. However, for more sensitive mixtures (H_2 concentrations higher than 18%), the measured MFSs are higher than 1000 m s^{-1}, indicating that transition to detonation had occurred in these experiments. The present model again under predicts these values.

The above comparisons indicate that a simple phenomenological model can predict the eventual outcomes and the MFS with limited success. It is understood that the simple equation of flame propagation (Eq. (5)) is incapable of modeling the flame acceleration phenomenon in detail. For example, it cannot predict the MFS of stretched-out flames or detonation velocities. However, this equation does provide some new physical insights into the problem. It has demonstrated that the existence of various steady-state regimes is the result of the inherent instability associated to the feedback mechanism.

4. Summary

A simple global model for flame acceleration caused by repeated obstacles has been developed using a "boxcar" approach. The feedback mechanism for flame acceleration is modeled by assuming that the effective burning velocity in the nth chamber depends on the same quanitity in the $(n-1)$th chamber. The effects of turbulence in

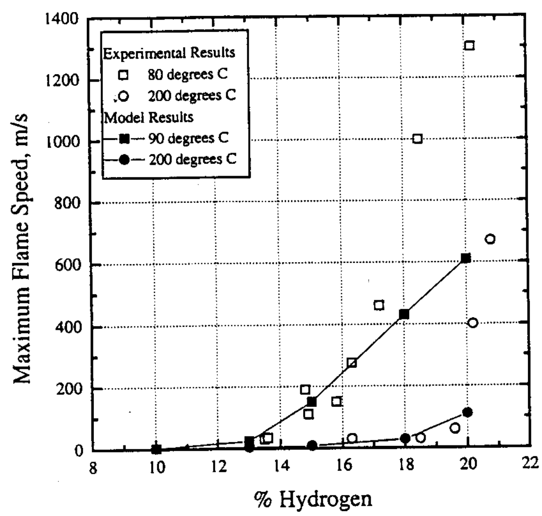

Fig. 6. MFS vs. Hydrogen concentration for flame propagation in a tube filled with orifice obstacles (blockage ratio, 0.7; obstacle spacing, 500 mm; steam concentration, 20%).

enhancing the burning rate and quenching are modeled by separate terms in the equation. The equation of flame propagation is shown to be a logistic difference equation. This model suggests that the unstable behaviour of flame acceleration is caused by the inherent instability of the feedback mechanism. The predicted MFSs were compared with the values obtained in experiments. For a certain range of experimental conditions, the model predicts the trend of the observed results fairly well.

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