# Flame Propagation Limit in Solid Fuel Suspension without Heat Loss

François-David Tang, Andrew J. Higgins, Sam Goroshin

Department of Mechanical Engineering, McGill University, Montreal, Quebec, H3A 2K6 Canada

#### 1 Introduction

The thermal theory of premixed flame in homogeneous media [1] does not predict the existence of a fuel concentration limit at the absence of heat losses. Unlike earlier flame theories of Mallard and Le Châtelier, that postulated existence of a specific "ignition temperature" below which the reaction rate is negligible, premixed laminar flame models assume the combustion reaction is governed by Arrhenius kinetics at all temperatures. Accordingly, there is no specific fuel concentration at which a "cut-off" flame temperature can be defined, and thus a premixed flame can theoretically propagate at arbitrarily small fuel concentration, albeit at very low flame speed.

In contrast to homogeneous mixtures, the notion of an ignition temperature can be introduced for flames propagating through heterogeneous suspensions of non-volatile solid fuel particles in a gaseous oxidizer. In this case, the critical temperature marks a rapid transition (bifurcation) in the particle reaction rate from low intensity reaction governed by Arrhenius kinetics to fast, high-temperature combustion governed by oxygen diffusion to the particle's surface [2]. The particle ignition temperature in this case can be considered as a "cut-off" point below which the combustion rate is negligible. The fuel concentration limit for flame propagation  $B_L$ , associated with this "cut-off" temperature can be found from a simple balance equation:  $B_L = Q/(T_i - T_0)c\rho$ , where  $T_i$ and  $T_0$  are ignition and initial temperatures of the mixture, c and  $\rho$  are the specific heat and density of the mixture of particles and gas and Q is the heat of combustion. In accordance to a simple thermal theory of the flame propagation in such suspensions [3], the flame speed at the limit is zero and increases with an increase in fuel concentration above the concentration limit  $B_L$ .

The thermal theory of flame propagation in particle suspensions mentioned above is based on a quasihomogeneous description of the suspension media when each point in the flame is assumed to contain a great enough concentration of particles so that they can be treated as a continuum. Such a description is justified when characteristic flame width (the thicknesses of the combustion and preheat zones) is much larger than the average distance between particles in the suspension. In the opposite case, which is often encountered in practical situations, the flame width is comparable to the distance between particles and treatment of the discrete nature of the particles is necessary. An analytic model of quasi-steady flame propagation in particulate suspension was developed by Goroshin et al. [3] that treats the particles as point-like sources of heat. The model predicts a much weaker dependence of the flame speed on the fuel concentration than the dependence of the continuum model in the vicinity of  $B_{l}$ , but the model exhibits the same "thermodynamic" flame propagation limit  $B_L$  as the homogeneous approach. The present work analyzes the dynamics of the flame in the discrete heat source system by numerical simulations of the governing unsteady heat equation. In particular, the flame propagation limit in the system is investigated in comparison to the thermodynamic limit predicted by the continuous and quasisteady solutions.

## 2 The model

The model of the discrete source system proposed by Goroshin et al. consists of point sources of heat (spatial delta functions) that, upon being activated, release heat that diffuses into the surrounding inert medium. The heat release can be instantaneous or steady over a finite amount of time. As the heat conducts to neighboring unburned particles and raises their temperature to ignition, the new sources are activated. The moving boundary between unburned particles and particles that have been ignited can be considered a propagating flame front, as shown by figure 1.



Figure 1: Schematic representation of the discrete source system proposed by Goroshin et al.

In order to initiate a flame in the discrete source system, the domain of particles is divided into two regions: a constrained region where the propagation of the flame is prescribed via a fixed sequence of ignition, and an unconstrained region where the flame propagates by first raising the temperature of a particle to its ignition temperature and then diffusing the heat of the reaction. The ignition temperature used in the unconstrained region is defined by the temperature of the last particle in the constrained region at the moment it is activated. Thus, in a given simulation, a quasi-steady flame speed is assigned based on the specified ignition sequence and the ignition temperature. This ignition temperature is then assigned to the remaining particles in the unconstrained region, and the wave of particle ignitions is allowed to continue to propagate on its own.

The system is further simplified to a one-dimensional flame traveling through regular spaced particles (or planes of energy release). In the one-dimensional model, the absence of side boundary conditions implies a condition of no heat loss at the walls. In fact, it can be shown that the one-dimensional model is equivalent to a two and three dimensions system with infinite size.

To compute the temperature field from a group of reacting particles with known ignition time  $t_{ign,i}$  and location  $x_i$ , a function  $f(x_i)$  is introduced to describe the spatial distribution of the activated source *i*, which equals 1 if a particle has reacted or 0 otherwise. The temperature field is governed by the heat equation with a source term:

$$\rho c \frac{\partial T}{\partial t} = \lambda \nabla^2 T + \frac{BQ}{t_c} f(\mathbf{x}_i)$$
(1)

where  $\lambda$  is the thermal conductivity of the inert gas, *B* is the mass concentration of the fuel, *Q* is the heat of reaction and  $t_c$  is the reaction time of a particle. The system is linear, so the solution to equation 1 can be obtained by the superposition of Green's functions, each function  $G_i$  describing by itself the solution of the temperature field due a single reacting particle. Assuming that a group *A* of particle has reacted, the temperature at location *x* and at time *t*, T(x,t) can be formally expressed as:

$$T(\mathbf{x},t) = \sum_{i \in A} G_i(\mathbf{x}|\mathbf{x}_i,t|t_{ign,i})$$
<sup>(2)</sup>

In the present study, the flammability limit is determined by solving the unsteady heat propagation and examining if the flame is able to continue to propagate through the unconstrained region.

#### **3** Results

Results are presented in terms of dimensionless time  $\tau = t\alpha l^2$  and temperature  $\theta = c_p \rho (T - T_0) / (BQ)$ , where  $\alpha$  is the thermal diffusivity and l is the characteristic distance between neighboring particles. The dimensionless ignition temperature  $\theta_{ign}$  is defined when  $T = T_{ign}$ . The case where the  $\theta_{ign} = 1$  describes a mixture containing a fuel concentration equal to  $B_l$ , while the other limiting case of  $\theta_{ign} = 0$  represents the case of infinite heat release from the reaction. Based on the normalization of time, the dimensionless combustion time is defined as  $\chi = t_c \alpha / l^2$ .

Flame propagation in the constrained region is prescribed by specifying  $\delta \tau$ , the delay time between the ignition of two neighboring particles occurring up to some  $n^{\text{th}}$  particle. Based on  $\delta \tau$ , the ignition time  $t_{ign,i}$  (*i*=0,1,...,*n*) of all the particles in the constrained region can be determine from the particle location *i* by the linear relationship  $t_{ign,i} = i \delta \tau$ . Figure 2 presents the relationship between  $\delta \tau$  and the temperature at the  $n^{\text{th}}$  particle  $\theta_n$  at the time of ignition  $t_{ign,n}$  for various values of the combustion time  $\chi$ .



Figure 2: Dependence of the ignition temperature  $\theta_n(t_{ign,n})$  as a function of the delay time  $\delta \tau$  between particles.

For a longer delay time between particles, the heat released from earlier particles can diffuse further and contribute to heating the next unreacted particle, permitting the flame to propagate with a larger ignition temperature. Thus, as shown in figure 2,  $\theta_n(t_{ign,n})$  increases monotonically with the delay time  $\delta \tau$  for any value of  $\chi$  and in the limit of  $d\tau \rightarrow \infty$ ,  $\theta_n(t_{ign,n}) \rightarrow 1$ . From here,  $\theta_n(t_{ign,n})$  is then assigned to the ignition temperature  $\theta_{ign}$ . By defining the flame speed  $\eta=1/\delta \tau$ , this result implies that a combustion front could theoretically travel at zero flame speed for a mixture with a concentration equal to  $B_l$  or equivalently  $\theta_{ign}=1$ . If the latter is true, the flame should, once initiated, be able to sustain propagate into the unconstrained region for any value of  $B > B_l$ .

When the transient heat equation is solve for the unconstrained region, the flame is able to continue propagating in the unconstraint system at the same speed that had been specified in the prescribed region for values of  $\theta_{ign} < 0.5$ . Indeed, flame propagation in this region can be shown to reach the same steady-state average velocity as predicted by the analytic model of Goroshin et al., regardless of the means of initiation. For example, rather than initiating the flame via the prescribed propagation in the constrained regime, the entire prescribed region can be activated simultaneously (constant volume explosion) and the heat diffusion into the unconstrained regime will initiate a flame that continues to propagate. The flame will, after a transient period, reach the same terminal velocity.

For  $\theta_{ign} \ge 0.5$ , initiation of the flame becomes more difficult in the simulations. The significance of the  $\theta_{ign} = 0.5$  value is that, at this condition, a semi-infinite region that undergoes constant volume explosion is unable to raise the temperature of the other half of the domain to ignition. In this case, the flame must be "overdriven" or initiated via a traveling wave in order to ignite particles from the unconstraint domain.

Figure 3 presents the time-temperature dependence of the first particle of the unconstraint region (i.e.  $\theta_{n+1}$ ) for different values of  $\theta_{ign}$  and for the specific case of  $\chi=0$ . Since the *x* and *y*-axis have been normalized with respect to  $\theta_{ign}$  and  $\delta\tau$ , the temperature profiles interest at the same point (1,1) for all  $\theta_{ign}$ . This agrees with the prescribed initiation of the flame where  $\theta_{n+1}$  reaches  $\theta_{ign}$  at time  $\tau_r = \delta\tau$ , where  $\tau_r$  is the time relative to  $t_{ign,n}$ .



Figure 3: Temperature  $\theta$  of the first particle in the unconstrained region normalized with  $\theta_{ign}$  as a function of  $\tau_r$  normalized with  $\delta \tau$  for various  $\theta_{ign}$ . The thin line represents the case where  $\theta_{ign} = 0.1, 0.2, ..., 0.7$ , while the dashed thick line corresponds to  $\theta_{ign} = \theta_{lim}$ . The dots indicate where the ignition temperature is achieved earlier than the prescribed time.

For  $\theta_{ign} \leq \theta_{lim}$ , the particle ignition is consistent with the constraint region, where in the particular case of  $\chi=0$ , we find  $\theta_{lim}\approx0.568$ . For  $\theta_{ign} > \theta_{lim}$ , propagation of a flame is no longer possible. As shown on figure 3, a second solution  $\delta \tau_2$  arises where  $\theta/\theta_{ign}=1$  at some time prior to  $\tau_r=\delta\tau$  and the time of ignition is no longer in phase with that of the prescribed ignition. For the model to be physically meaningful, ignition should occur during a period of increasing temperature (i.e.  $dT/d\tau>0$ ). The sudden change of the ignition sequence from  $\delta\tau$  to  $\delta\tau_2$  leads to the inability of the next particle to reach the ignition temperature, and the flame promptly quenches in the simulations. Thus, in the simulations, a limiting temperature  $\theta_{lim}$  occurs at a much lower ignition temperature than predicted by a quasi-homogeneous model, namely  $\theta_{ign}=1$ . A consequence of  $\theta_{lim}$  different from unity is that the minimum flame speed  $\eta$  is non-zero at the quenching condition. Further simulations for  $\chi$  non-zero show that  $\theta_{lim}$  approaches 1 when  $\chi$  increases, and thus the quasi-homogeneous limit is recovered for  $\chi$  sufficiently large.

#### 4 Conclusion

The propagation limit in an idealized heterogeneous mixture is shown to be different of that of an equivalent homogeneous mixture predicted by thermodynamic considerations, even in the absence of heat loss. The value of ignition temperature at which this new limit is encountered is almost twice that predicted by homogeneous theory. Furthermore, the minimum flame speed at the quenching condition is non-zero. Both the limiting concentration and the minimum flame speed cannot be predicted *a priory* from the energy balance, but stem from the structural dynamics of the flame. However, it can be shown that the solution converges toward the homogeneous solution when the combustion time  $\chi$  approaches infinity.

### References

- [1] Zel'dovich YaB et al. (1985). The mathematical theory of combustion and explosions. Plenum Publishing Corporation
- [2] Vulis, LA (1961). Thermal regime of combustion. McGraw-Hill, NY
- [3] Goroshin S, Lee JHS, Shoshin Y (1998). Effect of the discrete nature of heat sources on flame propagation in particulate suspension. 27th Symposium (International) on Combustion, The Combustion Institute, pp. 743-749