Dimensional Scaling for Propagation in Particulate Clouds with Lateral and Volumetric Losses

Fredric Lam, XiaoCheng Mi, Andrew. J. Higgins
Department of Mechanical Engineering, McGill University
Montreal, Quebec, Canada

1 Introduction

The propagation behavior of reaction fronts is influenced by the nature and extent of losses that are present in the combustible systems. Losses in mass, momentum, and energy can result in a propagation velocity deficit and, upon reaching a critical extent, the failure of self-sustained propagation, or quenching [1, 2] . This critical extent of losses is known as the propagation limit, and it can be quantified by various parameters according to the nature of these losses. For example, the limit to flame propagation through quenching plates absorbing chemically released heat can be measured as the critical distance between the plates [3–5]; the propagation limit of detonations experiencing lateral expansion behind the shock front can be determined as the critical charge diameter or thickness [6–8]. The fundamental mechanism governing these propagation limits is the interaction between losses and the propagation dynamics of reaction fronts. Different regimes of propagation dynamics therefore result in different propagation criticalities.

In a reaction-diffusion system that consists of spatially discrete sources of energy (e.g., suspensions of fuel particulates [9], calcium waves in intercellular signaling [10], etc.), a regime of complex, stochastic propagation dynamics, distinct from those observed in continuum systems, arises when the characteristic source spacing is on a scale comparable to the flame thickness [11–15]. While the limits to flame propagation have been studied extensively in the continuum regime of combustion, the response of stochastic propagation dynamics to heat losses has not been placed under in-depth scrutiny.

In this study, the dependence of the critical dimension (i.e., the smallest possible diameter or thickness allowing propagation) of a three-dimensional domain containing point-like heat sources on various system parameters, such as the magnitude of losses, will be examined. The cylindrical and slab (i.e., prismatic with finite thickness) geometries will be explored, and the ratio between the critical dimensions of these geometries will be examined using a reaction-diffusion model of point sources implemented via a numerical construction of analytic solutions. Particulates are characterized by an ignition temperature and a reaction time, and losses through heat diffusion into the surrounding inert media and through a volumetric loss term will be considered.

Correspondence to: fredric.lam@mail.mcgill.ca

2 Model

Static point-like heat sources that release heat upon reaching an ignition temperature T_{ign} are considered. Sources are embedded in an inert medium, and are randomly distributed over a finite three-dimensional domain (cylinder and slab geometries are considered). An example of a cylindrical and a slab domain is shown in Figure 1.

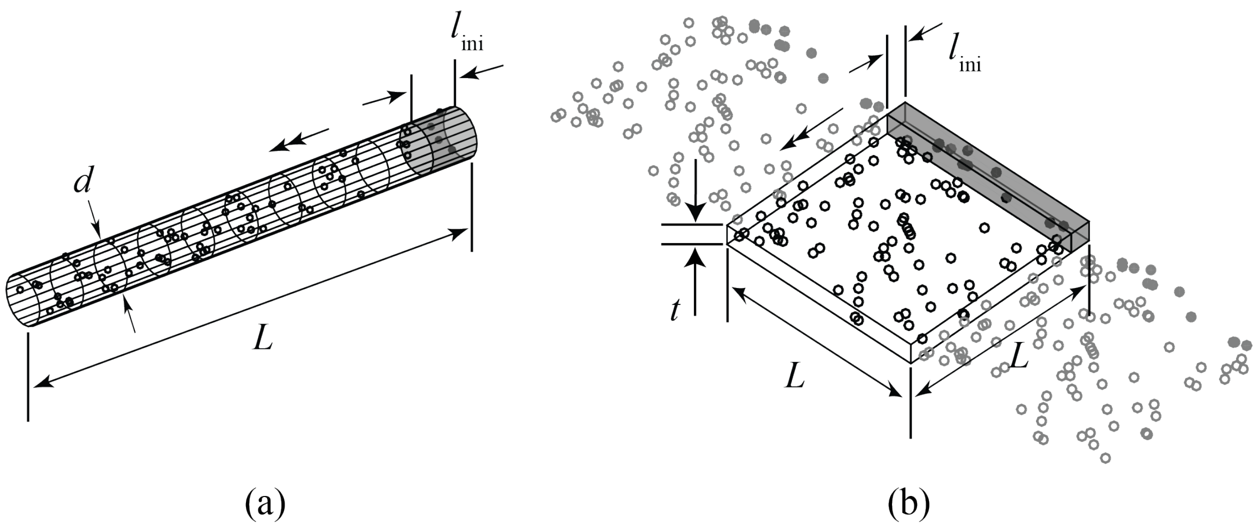

Figure 1: Schematic of domain with (a) cylindrical geometry with diameter d, and (b) slab geometry with thickness t at the initial time. Empty markers indicate unignited sources, and filled markers indicate ignited sources. Sources are forced to ignite simultaneously in the shaded region of length $l_{\text{ini}} = 0.1L$. The double arrow indicates the direction of propagation. The implementation of periodic boundary conditions via the method of images is shown in (b) as the sets of faded markers.

The domain is considered to be continuous with its surroundings, i.e., the inert medium extends to infinity, and heat diffuses throughout the medium. As such, heat is lost from the finite region containing discrete sources into the environment containing no sources. Additional losses can be introduced via a volumetric loss term; thus, the governing equation can be written as

$$\frac{\partial T}{\partial t} = \alpha \nabla^2 T + \frac{hA}{mc_p}(T - T_0) + \frac{qB}{\rho c_p} R \tag{1}$$

where α, ρ, c_p are the thermal diffusivity, density, and heat capacity of the medium in which heat sources are embedded, h is the heat transfer coefficient between the medium and an isothermal volumetric heat sink, m is the mass of the medium contained within the cylinder or slab boundaries, and T_0 is the initial temperature of the medium. The contribution of the discrete heat sources is characterized by heat release per unit mass q, fuel mass per unit volume B, and heat release rate R. In the case of constant heat release over reaction time t_{r}, the heat release rate can be written using the Heaviside function H in terms of the times of ignition of the i-th source $t_{\text{ign},i}$, i.e., $R = \frac{1}{t_{\text{r}}} \sum_i \delta(\mathbf{x} - \mathbf{x}_i) H(t - t_{\text{ign},i}) H(t_{\text{r}} - t + t_{\text{ign},i})$. In the limit of instantaneous reaction, the reaction rate becomes $R = \sum_i \delta(\mathbf{x} - \mathbf{x}_i)\delta(t - t_{\text{ign},i})$ Nondimensionalization of the equation using the average source spacing l, characteristic heat diffusion time scale $t_{\text{d}} = l^2/\alpha$, and adiabatic flame temperature T_{ad} gives rise to the nondimensional governing equation

$$\frac{\partial \theta}{\partial \tau} = \nabla^2 \theta + \nu \theta + \frac{1}{\tau_{\mathrm{c}}} H(\tau - \tau_{\mathrm{ign},i}) H(\tau_{\mathrm{c}} - \tau + \tau_{\mathrm{ign},i}) \tag{2}$$

where the key nondimensional parameters are identified as the discreteness parameter $\tau_{\mathrm{c}} = t_{\mathrm{r}}/t_{\mathrm{d}}$, the ignition temperature $\theta_{\mathrm{ign}} = \frac{T_{\mathrm{ign}} - T_0}{T_{\mathrm{ad}} - T_0}$, and the volumetric heat loss parameter $\nu = \frac{hV}{kA} \frac{l^2}{(V/A)^2}$. The flame is initiated by forcing all the sources in the first 10% of the domain length to ignite simultaneously at time $t = 0$. In the limit of instantaneous reaction ($\tau_{\mathrm{c}} = 0$), the analytic solution for the temperature field is given by linear superposition of the Green's functions for sources that have ignited; for $\tau_{\mathrm{c}} > 0$, the solution is given by the time-convolution of the Green's function. Source ignition times are computed by searching for ignition events in time using the analytic solution, and flame propagation is considered successful if there exists an ignited source in the last 10% of the domain length. For each set of parameters, a minimum of 40 runs for 20 values of diameter or thickness were used to obtain the critical dimension, i.e., the diameter d_{c} of the cylinder or the thickness t_{c} of the slab for which flame propagation is successful in 50% of the runs. The length of the domain (and the transverse dimension of the slab) was fixed at 10 times the diameter or thickness. Periodic boundary conditions in the transverse direction were implemented for the slab using images (copies of the domain).

3 Results and Discussion

The case with $\nu = 0$ is presented here for brevity; while volumetric heat loss is not considered, energy is lost through heat diffusion from the finite domain to the environment. Figure 2 shows the critical dimension (i.e., critical diameter and critical thickness) as a function of the discreteness parameter τ_{c} for values of ignition temperature θ_{ign} from 0.05 to 0.3.

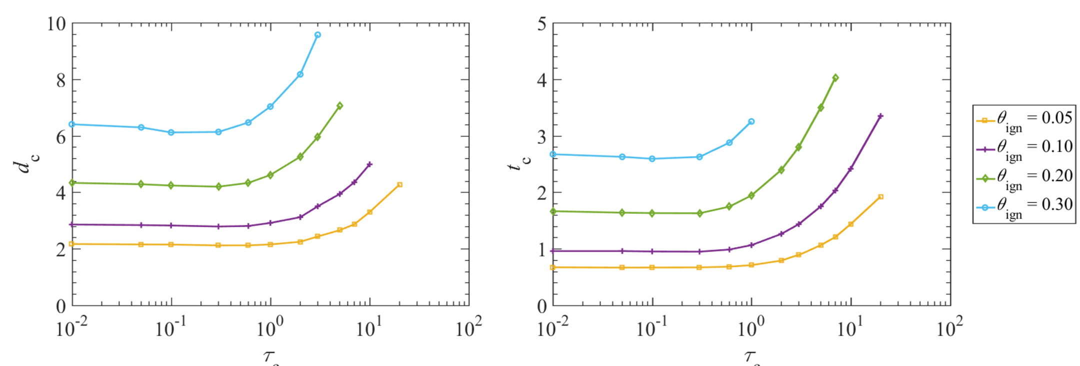

Figure 2: Critical dimension at which the flame propagates for 50% of runs for cylindrical (left) and slab (right) geometries, plotted as a function of discreteness parameter τ_{c} for values of the ignition temperature $\theta_{\mathrm{ign}} = 0.05$, $\theta_{\mathrm{ign}} = 0.10$, $\theta_{\mathrm{ign}} = 0.20$, $\theta_{\mathrm{ign}} = 0.30$, and with volumetric heat loss parameter $\nu = 0$ (i.e., heat loss is limited to heat diffusion across lateral faces of the cylinder and slab). The critical dimension is nondimensionalized by the average spacing between discrete sources, and temperature is nondimensionalized by the adiabatic flame temperature.

As depicted in Figure 2, the critical dimension for both the cylindrical and slab geometries increases with the discreteness parameter τ_{c}; that is, as the flame is made more continuum-like, more energy is required to sustain flame propagation under the influence of lateral heat losses. As τ_c approaches zero (i.e., in the discrete limit), the critical dimension approaches a plateau. Note that the critical thickness of the slab falls below unity; that is, a slab with thickness below one average source spacing in thickness can still allow propagation for sufficiently low ignition temperature. As the ignition temperature θ_ign is increased, the critical dimension increases in both geometries, i.e., propagation is only possible with a greater ratio of domain volume to surface area.

The ratio of the critical diameter to the critical thickness, or the scaling ratio, is plotted as a function of τ_c in Figure 3. In the discrete limit, the scaling ratio is a function of the ignition temperature, but not the discreteness parameter. In this limit, propagation is sustained by heat diffusing between neighboring sources, i.e., through a percolation-like mechanism.

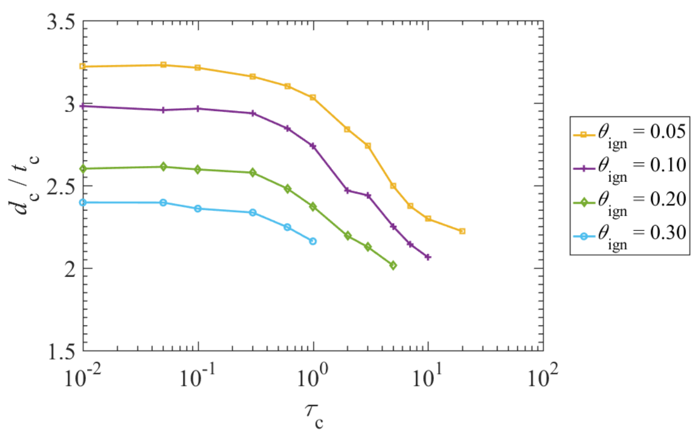

Figure 3: Scaling ratio of the critical diameter to the critical thickness as a function of the discreteness parameter τ_c for values of the ignition temperature $\theta_\mathrm{ign} = 0.05$, $\theta_\mathrm{ign} = 0.10$, $\theta_\mathrm{ign} = 0.20$, $\theta_\mathrm{ign} = 0.30$, considering only lateral losses. Scaling ratio plateaus at low τ_c, but remains a function of θ_ign. Scaling ratio begins to decrease from the plateau value in the continuum limit.

In the continuum limit, the heat release time of heat sources is large compared to the heat diffusion time, and the resulting flame structure is continuum-like, with many ignited sources contributing to the ignition of the next. As τ_c increases, the scaling ratio decreases, approaching a value in the neighbourhood of $2:1$. Flame propagation at high ignition temperatures requires contribution from multiple ignited sources, and is thus more continuum-like.

4 Conclusions

The propagation limits of a reaction-diffusion wave fueled by discrete sources was investigated via a simple three-dimensional model characterized by a discreteness parameter τ_c and an ignition temperature θ_ign. Heat losses due to lateral heat diffusion into an infinite inert medium and a volumetric heat loss term characterized by the heat loss parameter ν were considered. The scaling ratio, i.e., the ratio of the critical cylinder diameter to the critical slab thickness was found to depend on the discreteness parameter τ_c and the ignition temperature θ_ign. The percolation-like propagation in discrete systems explored in this work constitutes a regime of propagation that fails to be captured using classical homogenizing methods.

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