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Sensitivity Analysis of Models for Particle Air Flames

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The objective of this study is to review the development of theories for computing the characteristics of laminar premixed particle-air flames. Unlike gaseous flames, where conduction, species diffusion, and chemical reaction are important processes, particle-laden flames such as coal-air systems involve additional processes such as devolatalization, particulate radiation, and conduction between gaseous and particulate phases. Development of four theories by Cassel et al. [1], Seshadri et al. [2], Goroshin et al. [3] and Bidabadi and Rahbari [4] are presented. A sensitivity analysis was performed and a discussion on the validity of models for use with coal is presented based on the controlling parameters of each model.

Nomenclature

A	parameter characterizing rate of vaporization of fuel particles [g/(m^2 K s]
a	absorption coefficient[1/m]
B	Arrhenius frequency factor [1/s]
b	scaled mass fraction of fuel at the boundary between reaction/convection zone [-]
C_9	correction factor >1, accounts for radiation of glowing combustion products [-]
c_p	specific heat [J/(kg K)]
D	diffusion coefficient at T_u [m^2/s]
E	activation energy of the reaction [J/mol]
F	geometrical view factor flame/reactants [-]
K_1	defined in Eq. 5
k	thermal conductivity [J/(s m K)]
M	oxygen equivalent of fuel, [kg_{fuel} / mol_O]
n	temperature exponent characterizing rate of vaporization of fuel particles [-]
n_u	particle number density [#/m^3]
p	average partial pressure of oxygen [-]
Q	heat of reaction [J/kg]
q	ratio of heat of vaporization/ heat release [-]
R	gas constant [J/mol K]
r	average particle radius [m]
S_i	sensitivity parameter [-]
S_L	laminar burning velocity [m/s]
T	temperature [K]
W	molecular weight [g/mol]
Y	mass fraction [-]
Y_{Ff}	defined in Eq. 4
Ze	Zeldovich number, defined in Eq. 4
α	thermal diffusivity ($k/(c_p\rho)$) [m^2/s]
δ	overall flame thickness [-]
ε	emissivity of fuel particles [-]
η	defined in Eq. 5
κ	defined in Eq. 5
μ	defined in Eq. 5
ν	heat capacity of the gas to solid phase at stoichiometric fuel concentration $c_{sBst}/c_{g\rho g}$
ν_f	stoichiometric coefficient [-]
ξ	defined in Eq. 5
ξ_b	defined in Eq. 6
ρ	density [kg/m3]
σ	Stefan-Boltzmann constant [W/(m^{2}K^4)]
τ	defined in Eq. 3
τ_c	combustion time of individual separated particle at initial oxygen concentration [s]
φ	equivalence ratio [-]
φ_ω	defined in Eq. 5
ω	dust concentration [g/m^3]
γ	defined in Eq. 4

Subscript meanings

a	average ambient gas property around a particle as it passes through reaction zone
b	property of burned material
F	gaseous fuel
FC	fuel in combustion zone
f	at the reaction zone / flame location
g	gas
i	at ignition point
mix	combined solid and gas
O	oxygen
s	solid fuel particles
st	stoichiometric
u	unburned mixture at x=-∞

1. Introduction

Dust explosions are recognized as a significant hazard to many industries including manufacturing, power generation, and food production and have been for over 150 years [5, 6]. To predict dust explosions and protect industries from this hazard, the burning characteristics of dust suspensions needs to be known. Being able to predict the burning characteristics is also important for other applications, such as, coal combustion and propulsion systems [3]. To be able to describe combustion behavior, equations are derived to predict parameters like the burning velocity, flame temperature, and radiative heat flux. Burning velocity is important in calculating the flame speed and pressure wave that a combustion wave will produce.

Models available in literature [7, 8] that have been developed to analyze the burning behavior of particle air flames. The goal of this study is to perform a sensitivity analysis of four primary models that are available in combustion literature to specifically evaluate the controlling parameters of the burning behavior of a dust cloud. The results of the study can be applied towards creating sub modes for numerical solvers [9] as well as better experimental design for fundamental studies on dust deflagrations such as those observed in coal mines.

2. Sensitivity Analysis

The structure of a premixed particle-air flame is different compared to a gas-air flame as shown in Fig. 1. An important differentiating parameter is the non-linear fuel vaporization rate which represents the rate at which fuel-vapor is evolved from the condensed phase particles and mixes with the oxidizer thereby allowing a gas phase reaction zone as shown in Fig 1. The primary controlling parameters that influence the vaporization rate are particle type, size, number density and shape. Combustion literature has several models which incorporate these parameters as well as the complex interaction of particle-gas phase combustion and a comprehensive review of these models is given by Smoot et al. [10]. However, validation of these models has not been possible mainly due to the lack of good experimental data. Only recently has some progress been made towards this direction [11].

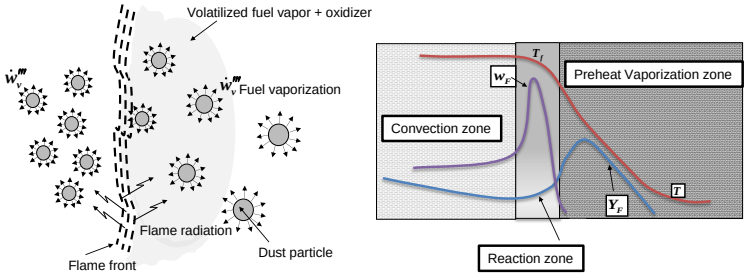

Figure 1: Schematic illustration of the structure of a dust-oxidizer flame. The fuel vaporization rate is given by $\dot{w}_v'''$ in units of mass of gaseous fuel vaporized per unit volume per second and the overall reaction rate is given by $\dot{w}_F'''$

All models presented in literature rely on some simplifications and assumptions which may be questionable. Further, it would be interesting to analyze which parameters influence the outcome of the model, especially when all the models are provided with the same input. To achieve this, a sensitivity analysis on four common premixed dust flame models [1-4] is performed. The influence of small changes in several input parameters (a detailed list is provided in Table 2) on the burning velocity (output) is analyzed using a sensitivity parameter S_i given by [12]:

$$S_i = \frac{\ln(y_1) - \ln(y_0)}{\ln(x_1) - \ln(x_0)} \quad , \tag{1}$$

where x_0 and x_1 are the initial and final value of the parameter to be examined, and y is the corresponding model solution in terms of laminar burning velocity. The normalized sensitivity parameter ($\bar{S}$) is calculated by dividing S_i value by the largest value ($S_{i,max}$) of the respective model. In the analysis presented below, the parameters listed in Table 2 were changed by +5% to arrive at the results below.

Brief Description of the Models

The first model presented is a pure gas phase (no dust) model by Semenov, Zel'dovich, and Frank-Kamenetsky [13] as shown in Table 1 (Eq. 1). Cassel et al. [1] presented two models. The first premixed dust-flame model is based on the Mallard and Le Chatelier [14] description of a combustion wave, (ambient gas in front raised to the ignition temperature by the conduction of heat from the burned to the unburned layers of the gas) but amended by an additional term to account for the effects of radiation (shown in Table 1 as Eq. 2). The second model developed by Cassel et al. [1] introduced burning time of a single particle and included the velocity of the burned mass relative to the flame front along with the ratio of densities of the unburned and burned gasses. These models consider the case in which oxygen diffusion governs the burning of individual particles.

The model presented by Sesahdri et al. [2] utilizes the low Mach number conservation equations of mass, energy, gaseous fuel species, and state. Through the use of assumptions and boundary conditions evaluated by splitting the flame structure into three zones (similar to that shown in Fig. 1) three coupled non-linear equations were derived (shown in Table 1 as Eq. 4). These equations require simultaneous numerical solution to calculate the laminar burning velocity, flame temperature, and the mass fraction of the fuel in the combustion zone. Seshadri et al. [2] assume all external forces, Soret and Dufour effects, and heat transport by radiation are negligible. It is further assumed that the particles do not vaporize completely prior to entering the reaction zone and the particle velocity equals gas velocity. The density of the fuel particle is also constant.

The model presented by Goroshin et al. [3] is based on a quasi one-dimensional approximation of the flame with conductive heat loss. Assuming a fuel controlled environment the equations are shown in Table 1 as Eq. 5. This model neglects radiative heat transfer from the flame to the preheat zone. Further, this model is mainly applicable to metal-dust flames where burning was assumed to occur heterogeneously in the flame front without formation of a continuous gas flame, as opposed to Cassel et al. [1] and Seshadri et al. [2], who assume a continuous flame front and no individual particle burning. Because of the excess oxygen in a fuel controlled flame, the burning time of a particle in the dust cloud is also assumed to be the same as a single particle.

The model presented by Bidabadi and Rahbari [4] (shown as Eq. 6 in table 1) includes a set of terms to describe heat transfer to particles. Bidabadi and Rahbari [4] rely on the same analytical formulation as Seshadri et al. [3] and hence similar assumption apply here as well.
As discussed earlier, the five models were compared with respect to each other using a sensitivity analysis. The base inputs used for the comparison are presented in Table 2 and the results obtained are discussed in the next section.

3. Results and Discussion

This study found that the assumptions used during model derivation had a significant influence on which input parameters have the largest effect on the output. In other words, each model is most accurate in the regime where model assumptions have the least impact. The gas phase model derived by Semenov, Zel'dovich, and Frank-Kamenetsky [13] uses an Arrhenius reaction rate assumption and the activation energy E is therefore most significant as shown in Fig. 2. Seshadri et al. [2], Goroshin et al. [3], and Bidabadi and Rahbari [4] include Arrhenius terms but none have the significance as compared to the gas phase model. The fundamental difference between the gas phase and dual phase models is the effects of thermal lag due to dust particle specific heat and the limitations of heat transfer to the particles. The thermal lag causes a delay in either the evaporation of the fuel vapors or surface reaction. A sensitivity analysis on the model by Cassel et al. [1] shows that the ignition and flame temperatures are most significant. This is also the only model presented here which includes the effect of particle radiation. Radiation is important when dealing with fuels such as coal which has a residual char. The model presented by Seshadri et al. [2] uses a vaporization kinetics model and *n*, the exponential term describing rate of fuel vaporization, is found to be the most important parameter as shown in Fig. 2. The model presented by Goroshin et al. [3] assumes diffusion as the primary controlling parameter and therefore the sensitivity analysis shows that thermal diffusivity α_{gu} is the most significant parameter. Further, as mentioned earlier, Goroshin et al. model [3] is mainly derived for fuels that burn with a heterogeneous flame with an individual flame around each particle. The model presented by Bidabadi and Rahbari [4] includes both vaporization kinetics and the temperature difference between the air and particles. Sensitivity analysis shows that the particle size is most significant which is mathematically shown by the multiplication of the exponent *n* by ξ which describes the thermal penetration depth normalized by the particle radius.

5. Conclusions

Premixed dust –air flame models are highly dependent on the assumptions associated with the initial derivation of the equations. Therefore, the choice of models is dependent on the expected behavior of the fuel in question. For example, in the case of coal dust particle–air flames, volatilization rate may be most significant thereby making the model by Seshadri et al. [2] most relevant. On the other hand with increased turbulence, radiation may be significant showing that Cassel et al. [1] or a combination of Cassel et al. [1] and Seshadri et al. [2] might be necessary to accurately estimate the burning rate.

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Table 1: Numerical Models Discussed in this Work

No.	Numerical Models
1	$$S_L = \left[\frac{2Q\alpha}{\rho c_p}\left(\frac{T_f}{T_f - T_0}\right)^2 \frac{R}{E} B \exp\left(\frac{-E}{RT_f}\right)\right]^{1/2}$$
2	$$S_L = \frac{k\frac{T_b - T_i}{\delta}}{\left(c_{p,g}\rho_g + c_{p,s}\omega\right)\left(T_i - T_u\right)} + \frac{\frac{\sigma\delta\omega\varepsilon C_9 F\left(T_b^4 - T_u^4\right)}{\rho_s r_u}}{\left(c_{p,g}\rho_g + c_{p,s}\omega\right)\left(T_i - T_u\right)}$$
3	$$S_L^2 = \frac{\alpha\rho_b}{\tau\rho_u}\frac{T_b - T_i}{T_i - T_u - \frac{\sigma\tau\omega\varepsilon C_9 F\rho_u\left(T_b^4 - T_u^4\right)}{\rho_s\rho_b r_u\left(c_{p,g}\rho_g - c_{p,s}\omega\right)}}, \tau = \frac{\rho_s {r_u}^2 R T_u^{3/2}}{2MDpT_a^{1/2}}, \alpha = \frac{k}{c_{p,g}\rho_g - c_{p,s}\omega}$$
4	$$S_L^2 = \frac{2(1+b)\nu_f k_u B\left(\frac{1}{Z_e}\right)^2}{\rho_u c_{p,mix}}\exp\left(-\frac{E}{RT_f}\right); y_{FC}Q = c_{p,mix}\left(T_F - T_u\right); 3a\alpha^{2/3} - 3a^2\alpha^{1/3} + a^3 - 1 = 0$$ $$a = \frac{\gamma}{3n}, b = \frac{y_{Ff}}{\frac{1}{Z_e}}, y_{Ff} = \frac{Y_F}{Y_{FC}}, Z_e = \frac{E\left(T_f - T_u\right)}{RT_f^2}, \gamma = \frac{4.836 An_u^{1/3} k_u\left(T_f - T_u\right)^n}{S_L^2\rho_u^{4/3} c_{p,mix} Y_{FC}^{1/3}\rho_s^{2/3}}$$
5	$$\frac{1}{\mu\phi} = \frac{\xi}{K_1(\xi + K_1)}\frac{1 - \exp(-K_1)}{\sqrt{1 + 4\frac{\eta}{\kappa^2}}}; K_1 = \frac{\kappa^2}{2}\left(1 + \sqrt{1 + 4\frac{\eta}{\kappa^2}}\right), \kappa^2 = \frac{{S_L}^2\tau_c}{k_{g,u}}, \eta = \frac{2\bar{\alpha}Nu\tau_c}{d^2}$$ $$\mu = \frac{\omega_{st}Q}{\rho_{gu}c_{p,g}\left(T_{si} - T_u\right)}, \xi = \frac{3\rho_{g,u}\alpha_{g,u}\tau_c c_{p,g}}{r_u^2\rho_s c_{p,s}}, \phi_\omega = \frac{\omega}{\omega_{st}}$$
6	$$S_L^2 = \frac{2(1+b)\nu_f k_{gu} B\left(\frac{1}{Z_e}\right)^2}{\left[\xi_b/(\xi_b + 1)\right]^2\rho_u c_{p,mix}}\exp\left(-\frac{E}{RT_f}\right); y_{FC}Q = c_{p,mix}\left(T_f - T_u\right)$$ $$3a\alpha^{2/3} - 3a^2\alpha^{1/3} + a^3 - \frac{\xi_b}{1 + \xi_b} = 0; a = \frac{\gamma}{3n}\frac{\xi_b}{\xi_b + 1}, b = \frac{y_{Ff}}{\frac{1}{Z_e}}$$ $$y_{Ff} = \frac{Y_F}{Y_{FC}}, Z_e = \frac{E\left(T_f - T_u\right)}{RT_f^2}, \xi_b = \frac{3k_{gu}k_s}{r^2\rho_u\nu_u c_{p,mix}\rho_s\nu_u c_s}$$

Table 2: Base model inputs varied in the sensitivity analysis

A	3.40E-02	[g/(m^2*K*s]		T_{si}	700	[K]
B	3.50E+06	[1/(mol*s)]		T_f	2.21E+03	[K]
E	1.21E+05	[J/mol]		α_{gu}	2.12E-05	[m^2/s]
F	0.5	[ ]		δ	0.05	[m]
n	1.33	[ ]		ε	0.8	[ ]
Q	5.49E+04	[J/g]		τ_c	4.76E-04	[s]
r	1.00E-05	[m]		φ	1	[ ]
T_b	1.20E+03	[K]		ω	100	[g/m^3]

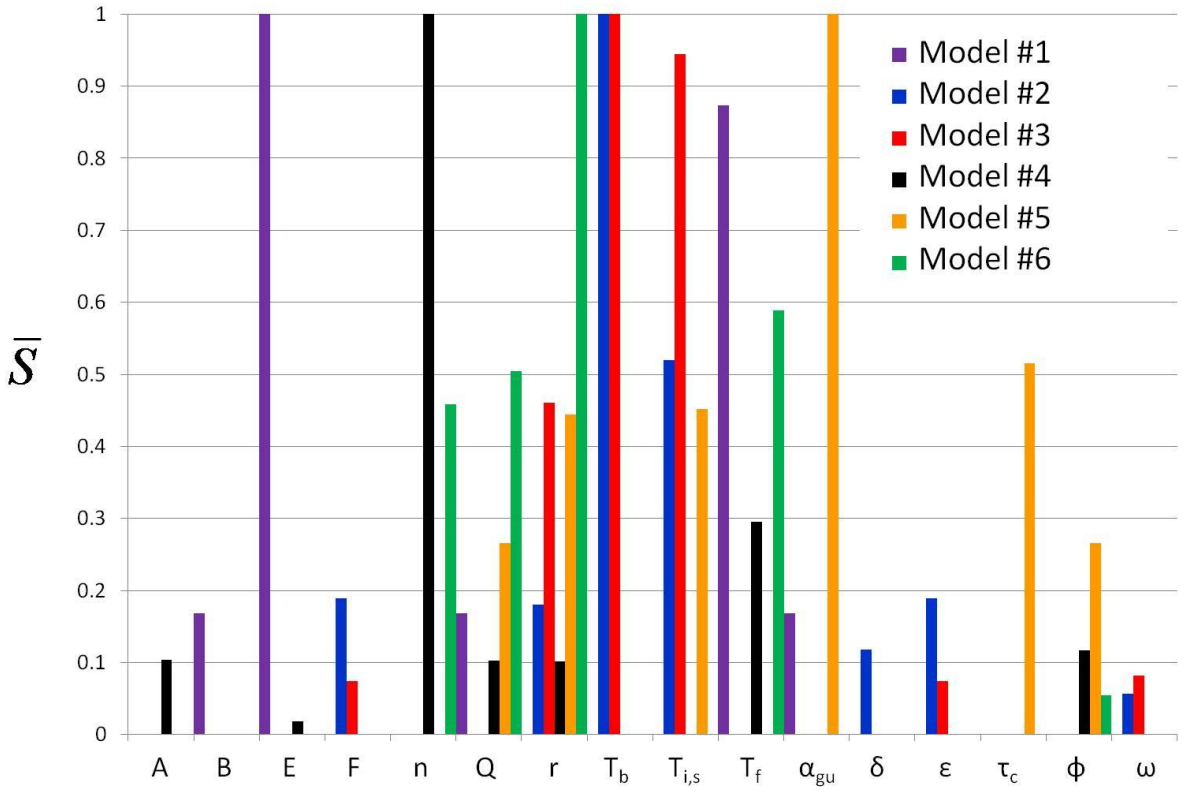

Figure 2: Normalized sensitivity parameter verses model inputs.

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