7th US National Technical Meeting
of the Combustion Institute
Hosted by the Georgia Institute of Technology, Atlanta, GA
March 20-23, 2011

Review of Theoretical Expressions for Laminar Burning Velocity of Particle-Air Flames

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The objective of this study was 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 devolatilization, particulate and gaseous 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] were presented. Sensitivity analysis describing the most influential parameters was also presented.

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_8	defined in Eq. 4
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 [-]
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	u	unburned mixture at x=-∞
st	stoichiometric		

1. Introduction (present tense)

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 of a combustion wave and the pressure change that a combustion wave will produce. There are many different analytic and numeric expressions for calculating the burning velocity of a suspended dust cloud. This is largely due to the various types of fuels used and not knowing the specific content of fuels such as coal used in experiments. Results have been found to be effected by experiment design, but by distinguishing the key parameters, experiments can be designed to control the most important parameters [7]. By analyzing the sensitivity of a model to its input parameters effort can be made in finding the most important inputs to optimize the accuracy of the model. In addition, experimenters will be able to focus on characterizing these parameters of the fuels they use when generating experimental data.

2. Models (past tense)

Most models were either derived from the fundamental conservation of mass, energy, and species equations, and assumptions were made to simplify the expressions or a fundamental process was believed to govern the physical behavior. Then this behavior was described mathematically.

For comparison purposes, the first model presented is a gas phase model derived by Semenov, Zel'dovich, and Frank-Kamenetsky [8] which was presented as

$$S_L = \left[\frac{2Q\alpha}{\rho c_p} \left(\frac{T_F}{T_F - T_0} \right)^2 \frac{R}{E} B \exp\left(\frac{-E}{RT_F} \right) \right]^{1/2} . \quad (1)$$

Cassel et al. [1] presented two models. The first model was based on the historic Mallard and Le Chatelier [9] description of a combustion wave, which was based on the idea that the cold gas in front of the flame is raised to the ignition temperature by the conduction of heat from the burned to the unburned layers of the gas [10], but amended by an additional term to account for the effects of radiation. This equation assumed the form

$$S_L = \frac{k \frac{T_b - T_i}{\delta}}{\left(c_{p,g}\rho_g + c_{p,s}\omega\right)\left(T_i - T_u\right)} + \frac{\frac{\sigma\delta\omega\varepsilon C_9 F\left(T_b^4 - T_u^4\right)}{\rho_s r_u}}{\left(c_{p,g}\rho_g + c_{p,s}\omega\right)\left(T_i - T_u\right)} . \quad (2)$$

The second model presented 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. This model ignores the possibility that a slow

surface reaction rate is the determining factor and only considers the case in which oxygen diffusion governs the burning of individual particles and was written as

$$S_L^2 = \frac{\alpha\rho_b}{\tau\rho_u}\frac{T_b - T_i}{T_i - T_u - \dfrac{\sigma\tau\omega\varepsilon C_9 F\rho_u\left(T_b^4 - T_u^4\right)}{\rho_s\rho_b r_u\left(c_{p,g}\rho_g - c_{p,s}\omega\right)}}, \tau = \frac{\rho_s {r_u}^2 RT_u^{3/2}}{2MDpT_a^{1/2}}, \alpha = \frac{k}{c_{p,g}\rho_g - c_{p,s}\omega} \quad . \tag{3}$$

The model presented by Sesahdri et al. [2] started with the low Mach number flow fundamental conservation equations of mass, energy, gaseous fuel species, and state. Through the use of assumptions and evaluation at boundary conditions, the following set of three coupled non-linear equations was derived:

$$\begin{gathered} S_L^2 = \frac{2(1+b)\nu_f k_u B C_8^2}{\rho_u c_{p,mix}}\exp\left(-\frac{E}{RT_f}\right); y_{FC}Q = c_{p,mix}\left(T_F - T_u\right); 3a\alpha^{2/3} - 3a^2\alpha^{1/3} + a^3 - 1 = 0 \\ a = \frac{\gamma}{3n}, b = \frac{y_{Ff}}{C_8}, y_{Ff} = \frac{Y_F}{Y_{FC}}, C_8 = \frac{1}{Z_e}, Z_e = \frac{E\left(T_f - T_u\right)}{RT_f^2}, \gamma = \frac{4.836An_u^{1/3}k_u\left(T_f - T_u\right)^n}{S_L^2\rho_u^{4/3}c_{p,mix}Y_{FC}^{1/3}\rho_s^{2/3}} \end{gathered} \quad . \tag{4}$$

These equations were solved simultaneously to calculate the laminar burning velocity, flame temperature, and the mass fraction of the fuel in the combustion zone. This model assumed all external forces, the diffusion caused by pressure gradients, the Soret and Dufour effects, and heat transport by radiation were negligible. This analysis was valid only for solid state equivalence ratios greater than 0.7. It was assumed that the particles do not vaporize completely prior to entering the reaction zone and the particle velocity was equal to the gas velocity. In dealing with the low Mach number governing equations, it was assumed that the mean molecular weight does not vary, the thermal conductivity of the mixture is proportional to temperature, and the diffusion coefficient was proportional to the temperature squared. The density of the fuel particle was presumed to be constant. The diffusion was neglected when defining the mass fraction of the particles and the effect of heat loss was not considered in zones of flame propagation.

The model presented by Goroshin et al. [3] was based on a quasi one-dimensional approximation of the flame with conductive heat loss. For lean concentrations of fuel and air, the following equation was derived:

$$\begin{gathered} \frac{1}{\mu\phi} = \frac{\xi}{K_1\left(\xi + K_1\right)}\frac{1 - \exp\left(-K_1\right)}{\sqrt{1 + 4\dfrac{\eta}{\kappa^2}}}; K_1 = \frac{\kappa^2}{2}\left(1 + \sqrt{1 + 4\frac{\eta}{\kappa^2}}\right), \kappa^2 = \frac{{S_L}^2\tau_c}{k_{g,u}}, \eta = \frac{2\bar{\alpha}Nu\,\tau_c}{d^2} \\ \mu = \frac{\omega_{st}Q}{\rho_{gu}c_{p,g}\left(T_{si} - T_u\right)}, \xi = \frac{3\rho_{g,u}\alpha_{g,u}\tau_c c_{p,g}}{r_u^2\rho_s c_{p,s}}, \phi_\omega = \frac{\omega}{\omega_{st}} \end{gathered} \quad . \tag{5}$$

This model derivation assumed that radiative heat transfer from the flame to the preheat zone was negligible. The aluminum burned heterogeneously in the flame front without formation of a continuous gas flame, as opposed to Seshadri et al. [2], who assumed a continuous flame front and no individual particle burning. Because of the excess oxygen in a lean flame, the burning time of a particle in the dust cloud was assumed to be the same as a single particle.

The model presented by Bidabadi and Rahbari [4] used the same type of analysis as Seshadri et al. [2] but included a set of terms to describe heat transfer to particles. This derivation became the equations:

$$S_L^2 = \frac{2(1+b)\nu_f k_{gu} B C_8^2}{\left[\xi_b/(\xi_b+1)\right]^2 \rho_u c_{p,mix}} \exp\left(-\frac{E}{RT_f}\right); y_{FC} Q = c_{p,mix}(T_F - T_u)$$

$$3a\alpha^{2/3} - 3a^2\alpha^{1/3} + a^3 - \frac{\xi_b}{1+\xi_b} = 0; a = \frac{\gamma}{3n}\frac{\xi_b}{\xi_b+1}, b = \frac{y_{Ff}}{C_8} \quad . \tag{6}$$

$$y_{Ff} = \frac{Y_F}{Y_{FC}}, C_8 = \frac{1}{Z_e}, Z_e = \frac{E(T_f - T_u)}{RT_f^2}, \xi_b = \frac{3k_{gu}k_s}{r^2 \rho_u \nu_u c_{p,mix} \rho_s \nu_u c_s}$$

This model used the same assumptions as the model proposed by Seshadri et al. [2], but also ignored *q*, the ratio of the heat required to vaporize the fuel particles to the overall heat release. The Biot number was assumed to be small so that the particle temperature was constant over the particle radius.

3. Results (past tense)

To find the most important parameters in the models presented above, a sensitivity analysis was performed. Sensitivity analysis is the study of how the variation in the output of a model can be broken up into different sources of variation and how the model depends on the information fed into it. The value of the sensitivity parameter S_i was calculated using [11]

$$S_i = \frac{\ln(y_1) - \ln(y_0)}{\ln(x_1) - \ln(x_0)} \quad , \tag{7}$$

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 S_i value was normalized by dividing the calculated S_i value by $S_{i,max}$, the largest value calculated for the model. In the analysis presented below, the parameters listed in table 1 were changed by +5% to arrive at the results below. Figure 1 shows the normalized sensitivity parameter for the six models presented above.

Table 1: Base input parameters varied in 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]

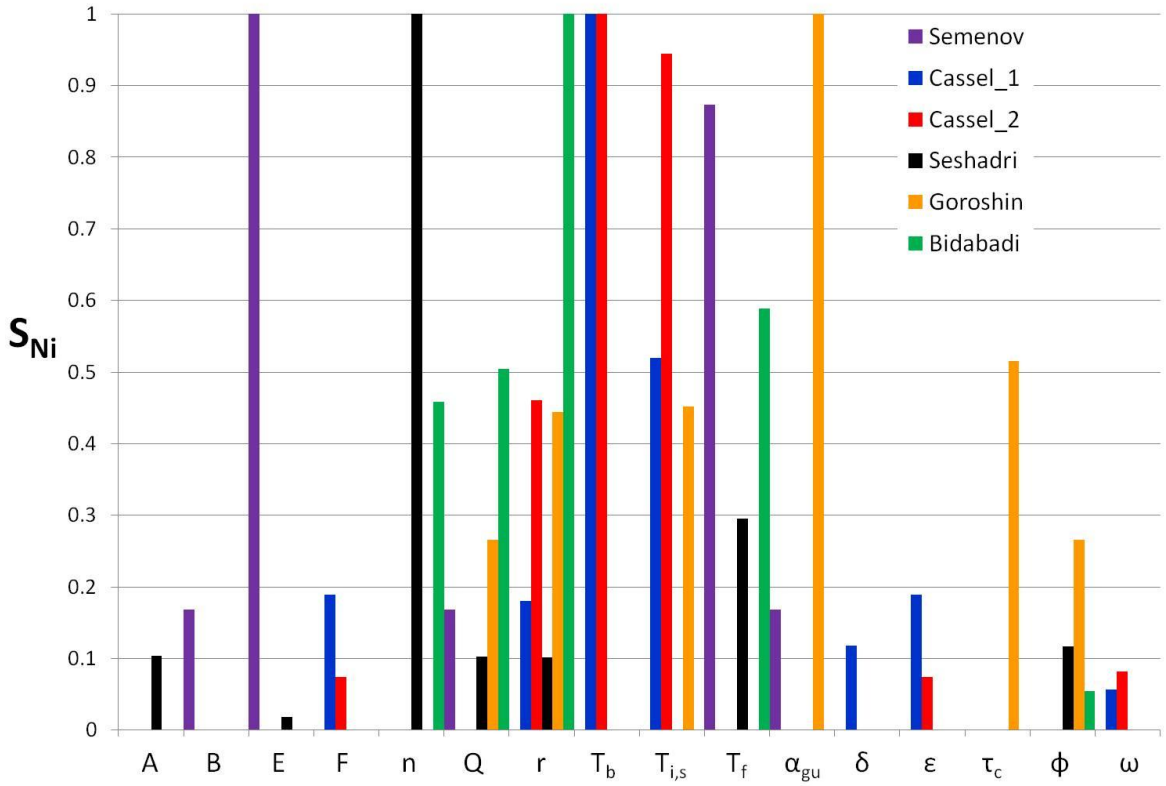

Figure 1: Normalized sensitivity analysis verses parameter

4. Discussion (present tense)

The sensitivity analysis presented above relates to the overall dust deflagration problem because a comprehensive theory for dust combustion is difficult due to the diversity of fuel properties, as discussed by Tang et al. [12]. This study found that the assumptions made when deriving the presented models determined which input parameters have the largest effect on the output. Thus each model is most accurate in the regimes in which the assumptions made in deriving the model have the least impact. The gas phase model derived by Semenov, Zel'dovich, and Frank-Kamenetsky [8] uses an Arrhenius reaction rate assumption and the activation energy E is most significant. It is of note that 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. The model presented by Cassel et al. [1] uses a thermal wave assumption and has the ignition temperature and burning temperature as the most significant parameters. The flame temperature, burned gas temperature, and dust ignition temperature all play a large role in the models that they appear in due to the assumption that the processes occur at a given temperature where in reality they occur over a range of temperatures. 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

the most important parameter. This model would be less accurate for fuels which burn mostly in the condensed phase, such as, iron dust. The model presented by Goroshin et al. [3] assumes diffusion to control burning and has the thermal diffusivity α_{gu} as the most significant parameter. This model is specifically derived for fuels that burn with a heterogeneous flame with an individual flame around each particle, thus it will be less accurate for fuels in which evaporation and combustion of gaseous fuel vapors are the controlling mechanisms [12], such as, with PMMA or other organic dusts which create a homogeneous flame. The model presented by Bidabadi and Rahbari [4] includes both vaporization kinetics and the temperature difference between the air and particles. In this model *n* is of less importance and the particle size plays the largest role. The significance of the particle size is due to *n* being multiplied by ξ which describes the thermal penetration depth normalized by the particle radius. The dust concentration played a relatively small role in burning velocity as seen in the experimental results presented by Smoot and Horton [13]. To create a model to use on a significant portion of possible dust fuels, vaporization kinetics, gas phase reaction rates, solid phase reaction rates, gas verses particle temperature variation, and radiation should be included to better capture the physics of what is occurring in a dust cloud flame.

To continue this work, analysis of liquid spray flame models and models which include multiple types of fuels and combinations of multiple sizes of fuels by Goroshin et al. [14] and Huang et al. [15] along with comparison of model output to experimental data.

Acknowledgements
The authors would like to thank Kulbhushan Joshi for his thoughts and advice and the National Science Foundation Graduate Research Fellowship Program for partial funding of this work.

References

1. **Cassel, H.M., et al., Third Symposium on Combustion, Flame and Explosion Phenomena, 1949: p. 185-190.**
2. **Seshadri, K., et al., Combustion and Flame, 1992. 89: p. 333-342.**
3. **Goroshin, S., et al., Combustion and Flame, 1996. 105: p. 147-160.**
4. **Bidabadi, M., et al., Combustion, Explosion, and Shock Waves, 2009. 45(3): p. 278-285.**
5. **Eckhoff, R.K., *Explosion Hazards in the Process Industries*. 2005, Houston, TX.**
6. **Eckhoff, R.K., *Dust Explosions in the Process Industries, Third Edition*. Third ed. 2003, Boston: Gulf Professional Publishing.**
7. **Kolbe, M., in *Mechanical Engineering*. 2001, Concordia University Montreal: Quebec, Canada.**
8. **Kuo, K.D.-y., *Principles of Combustion*. 1986, New York: John Wiley & Sons.**
9. **Mallard, E., et al., Annals des Mines, 1883. 4.**
10. **Warner, W.E., Transactions of the Faraday Society, 1926.**
11. **Saltelli, A., et al., *Sensitivity Analysis*. 2000: John Wiley & Sons, LTD.**
12. **Tang, F.-D., et al., Proceedings of the Combustion Institute, 2009. 32: p. 1905-1912.**
13. **Smoot, D., et al., Prog. Energy Combustion Science, 1977.**
14. **Goroshin, S., et al., Proc. Combust. Inst, 2000. 28: p. 2811-2817.**
15. **Huang, Y., et al., Proceedings of the Combustion Institute, 2007. 31: p. 2001-2009.**