Combustion of particles, agglomerates, and suspensions – A basic thermophysical analysis

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A B S T R A C T

Ignition and combustion of single particles, particle agglomerates, and suspensions are analyzed using a simple thermophysical approach that considers ideal, non-volatile fuel particles undergoing heterogeneous reaction controlled by a combination of diffusion and kinetic rates. This approximation is useful to describe the combustion behavior in suspensions of refractory metal-fuel particles, where the lack of significant premixing of fuel vapor with oxidizer can lead to combustion in a diffusion micro-flame enveloping the particle. The transition from kinetic heterogeneous-fuel oxidation to diffusion-controlled combustion occurs via thermal runaway, customarily called particle *ignition*. There is, however, a critical particle size below which an individual particle cannot ignite at any temperature, and the combustion will be controlled by heterogeneous kinetics at a temperature close to that of the bulk gas. While individual particles may not be able to ignite, the *collective effect*, which results from the self-heating of particle suspensions to thermal runaway, can enable fast reaction in suspensions. Micron- and sub-micron-sized fuel particles are used for their high reactivity, but such particles often agglomerate before combustion. The ignition and combustion behavior of an agglomerate can be drastically different from its isolated constituent particles due to a large internal surface area inside of the agglomerate that is partially accessible to oxidizer, while only the external surface area of the agglomerate is available for heat loss. It is shown that the interplay between the thermal regimes of reaction, the collective effects of the suspension, and the collective effects of agglomeration can lead to a wide range of observed ignition and combustion phenomena that are independent of the material-specific fuel and oxide properties.

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1. Introduction

The study of heterogeneous combustion is motivated by a wide range of technical applications spanning from propulsion [1] and energetic materials [2] to clean energy carriers [3–6], or combustion mitigation for industrial safety [7]. Most practical scenarios of heterogeneous combustion involve burning suspensions of micron- and sub-micron-sized solid fuel particles. The high specific surface area of the small fuel particles in the suspension permits combustion rates comparable to those of more conventional gaseous hydrocarbon fuels [5].

The general combustion behavior of solid-fuel suspensions can be classified by the physical and chemical properties of the fuel. Plastics and many organic solid materials can easily volatilize

(evaporate or gasify) before combustion can occur. The gasified fuel premixes with the oxidizer leading to mostly homogeneous combustion phenomena as observed in flames of hydrocarbon sprays [8,9]. In suspensions of refractory materials, such as carbon, boron, and some metals, the fuel boiling point can exceed the flame temperature leading to combustion controlled by heterogeneous surface reactions [10]. Additionally, the reaction of metal vapors with some gaseous oxidizers are nearly non-activated [11,12]. As a result, vapors from metals even with relatively low boiling points, such as lithium or magnesium, cannot be premixed with the oxidizer and will burn either heterogeneously at the particle surface or in a diffusion micro-flame enveloping the particle [13]. Many practical fuels such as coal, organic solids, and metalized slurries volatilize only partially [14], forming a complex hybrid flame [15], with either overlapped or separated gaseous and heterogeneous combustion zones [16].

Historically, the majority of research on heterogeneous combustion has focused on experimental and theoretical studies of ignition and combustion of relatively large, isolated fuel particles in a

Nomenclature

Greek Symbols

Symbol	Description	Units
α	Thermal diffusivity of the gas	m^2/s
$\dot{\omega}$	Rate of oxidizer consumption per unit surface area	$kg/(s \cdot m^2)$
ϵ	Porosity of the agglomerate	-
ϵ_0	Initial porosity of the agglomerate	-
η	$\eta = 3B\lambda/(\rho_s H r_{p,0}^2)$	-
λ	Thermal conductivity of the gas	$W/(m \cdot K)$
Ω	Ratio of heat release to the activation energy $(q\upsilon C_{g,0}\mathcal{R}/\rho_g c_g E_a)$	-
ϕ	Fuel-to-oxidizer equivalence ratio	-
β	Mass transfer coefficient	m/s
β_{ag}	Mass transfer coefficient of an agglomerate	m/s
β_p	Mass transfer coefficient of a particle	m/s
κ	Pre-exponential factor of surface reaction rate	m/s
ρ_g	Bulk gas density	kg/m^3
ρ_s	Solid fuel density	kg/m^3
υ	Stoichiometric coefficient relating the mass of solid fuel consumed per mass of oxidizer in the reaction	-
τ	Combustion time	s

Roman Symbols

Symbol	Description	Units
$\mathcal{D}$	Mass diffusivity of oxidizer	m^2/s
$\mathcal{R}$	Universal gas constant	$J/(K \cdot mol)$
Da	Damhöhler number	-
Le	Lewis number	-
B	Total mass concentration of the solid fuel	kg/m^3
C	Oxidizer concentration within an agglomerate	kg/m^3
H	Heat transfer coefficient of a suspension	$W/(m^2 \cdot K)$
j	Oxidizer diffusion flux to the particle surface	$kg/(s \cdot m^2)$
k	Rate of surface reaction	m/s
q	Heat of reaction per unit mass of the solid fuel	J/kg
R	Radial coordinates within the agglomerate simulation domain	m or μm
t	Time	s
A_{ag}	Agglomerate surface area	m^2
A_p	Particle surface area	m^2
B_{ag}	Agglomerate mass concentration	kg/m^3
B_p	Particle mass concentration	kg/m^3
C_g	Oxidizer concentration in the bulk gas	kg/m^3
c_g	Specific heat capacity of the gas phase	$J/(kg \cdot K)$
C_0	Initial oxidizer concentration in the bulk gas	kg/m^3
c_s	Specific heat capacity of the solid phase	$J/(kg \cdot K)$
C_{ag}	Oxidizer concentration at the agglomerate surface	kg/m^3
C_p	Oxidizer concentration at the particle surface	kg/m^3
Da^*	Normalized Damhöhler number	-
E_a	Activation energy	J/mol
h_{ag}	Hear transfer coefficient of an agglomerate	$W/(m^2 \cdot K)$
h_p	Hear transfer coefficient of a particle	$W/(m^2 \cdot K)$
k_{eff}	Effective rate of reaction	m/s
m_{ag}	Agglomerate mass	kg
$m_{ag,0}$	Initial agglomerate mass	kg
$\dot{m}_{ox,tot}$	Total mass-consumption rate of oxidizer within the agglomerate	kg/s
m_p	Particle mass	kg
$m_{p,0}$	Initial particle mass	kg
N_{ag}	Number density of agglomerates	m^{-3}
N_p	Number density of particles	m^{-3}
$\dot{Q}_L$	Rate of heat loss per particle	J/s
$\dot{Q}_R$	Rate of heat production per particle	J/s
r_{ag}	Agglomerate radius	m or μm
$r_{ag,0}$	Initial agglomerate radius	m or μm
r_{cr}	Critical particle radiu for ignition	m or μm
l_c	Characteristic length scale for particle ignition $(l_c = \mathcal{D}/\kappa)$	m or μm
$r_{p,0}$	Initial particle radius	m or μm
r_p	Particle radius	m or μm
T_{ad}	Adiabatic flame temperature	K
T_{ag}	Agglomerate temperature	K
$T_{ag,0}$	Initial agglomerate temperature	K
T_g	Gas temperature	K
$T_{g,0}$	Initial gas temperature	K
T_{ig}	Ignition temperature	K
$T_{p,0}$	Initial particle temperature	K
T_p	Particle temperature	K
T_{stoich}	Adiabatic flame temperature of the stoichiometric mixture of particles and gas	K
V_{ag}	Agglomerate volume	m^3
$V_{ag,0}$	Initial agglomerate volume	m^3
V_p	Particle volume	m^3
$V_{p,0}$	Initial particle volume	m^3
V_{tot}	Total volume of the solid fuel within an agglomerate	m^3

Subscripts

Symbol	Description	Units
0	Initial	-
ad	Adiabatic	-
ag	Agglomerate	-
cr	Critical	-
c	Characteristics	-
eff	Effective	-
g	Gas phase	-
ig	Ignition	-
ox	Oxidizer	-
p	Particle	-
stoich	Stoichiometric	-
s	Solid phase	-
tot	Total quantity within an agglomerate	-