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Perfectly stirred reactor model to evaluate extinction of diffusion flame

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ABSTRACT

The paper focuses on developing and justification of the flame extinction model for large eddy simulations of under-resolved turbulent diffusion flames. The model is based on the perfectly stirred reactor (PSR) concept, in which the residence time is coupled with the local strain rate, and the radiative losses from the reaction zone are taken into account. The single-step global reaction of fuel oxidation is considered. A possible way to calibrate the kinetic parameters is that by fitting measured values of flame temperature and strain rate at diffusive extinction (blow-off). By comparing the simulation results with experimental data available for methane-air and heptane-air flames and with the published predictions made by the activation energy asymptotics for the ethylene-air flame, it is demonstrated that the PSR model is capable of evaluating flammability bounds of the diffusion flame, including high-strain blow-off and low-strain quenching (i.e., diffusive and radiative extinction). The confluence of these bounds is shown to produce the minimum extinguishing concentration of an inert diluent. For the flames diluted by nitrogen, carbon dioxide, water vapor, or argon, the minimum extinguishing concentrations predicted in this way by the non-adiabatic PSR model are shown to agree with the measured values. Possibility of formulating a unified extinction criterion, the Damköhler number, is confirmed.

1. Introduction

Extinction of a diffusion flamelet could be driven by either high strain (blow-off) or by excessive heat losses form the reaction zone (quenching). To designate these extinction mechanisms, we will use the bracketed terms bearing in mind that they are often termed as diffusive and radiative, respectively. Both phenomena have been thoroughly examined in a number of theoretical and experimental studies, albeit the blow-off phenomenon has attracted more attention, probably because of its higher relevance to industrial applications. Approximate analytical treatment of extinction is normally based on asymptotic approaches, which either assume a single-step global reaction with the high activation energy or consider reduced multistep chemistry [1]. The former approach is known as the activation energy asymptotics (AEA), that justifies separate consideration of reactive "inner" and inert "outer" zones in the strained laminar diffusion flamelet, and expansion of the inner variables in terms of the inverse Zeldovich number, which is assumed to be small. The examples of the AEA approach can be found in Refs. [2–4], which are essentially based on the seminal work by Liñán [5]. Consideration of three- or four-step reduced mechanisms provides the basis for the rate-ratio asymptotic analysis (RRA) [1], which further specifies the reaction zone structure as that composed of a thin inner layer and a broader oxidation layer. An important difference between both asymptotic analyses is in predicting of either oxygen or fuel leakage through the reaction zone as extinction is approached [6]. It is worthy of note, however, that when the overall kinetic rate parameters are deduced from the experiments, detailed simulations or RRA results, it appears that critical conditions of flame extinction can be approximated to an accuracy, that is acceptable for many practical applications. Based on this observation, this work is focused on a single-step global reaction, and a variety of data including both detailed simulations and measurements is used to validate such an approximation.

Alternative approach to model extinction stems from the "fine structure" concept [7,8], which suggests that reaction zone is not resolved by the computational mesh, and its volume is much smaller than that of the grid cell. As such, the reaction zone is treated as a perfectly stirred reactor (PSR) fed by the fuel and oxidizer streams, and the streams have compositions and temperatures related to the local resolved (cell-average) data. Both AEA and PSR approaches lead to the subgrid flame extinction model based on critical Damköhler number. Its advantage over the simplified flame extinction model based on the critical flame temperature concept [9] is that the strain rate effects are taken into account.

Beyond the subgrid extinction modeling, both AEA and PSR approaches can also be used to evaluate extinction of diffusion flames

Abbreviations: AEA, activation energy asymptotics; LES, large eddy simulation; LOC, limiting oxygen concentration; LOI, limiting oxygen index; MEC, minimum extinguishing concentration; RRA, rate-ratio asymptotics; SGS, subgrid scale.

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Nomenclature

A	pre-exponential factor $((\mathrm{mol/m^3})^{1-n}/\mathrm{s})$
A_*	modified pre-exponential factor (1/s)
c_P	constant pressure specific heat (J/kg K)
Da	Damköhler number (-)
E	activation energy (J/mol)
f_V	soot volume fraction (-)
h	enthalpy (J/kg)
h_f^0	enthalpy of formation (J/kg)
Δh_c	heat of combustion per 1 kg fuel (J/kg)
l_T	turbulent integral scale (m)
M	molecular weight (kg/mol)
n	reaction order (-)
P	pressure (Pa, atm)
$\dot{q}_{loss}$	heat loss rate (W/kg)
$\dot{r}_{fuel}$	reaction rate (1/s)
$\mathscr{R}$	universal gas constant (J/mol K)
s_i	mass stoichiometric coefficient for i-th specie (-)
S	strain rate (1/s)
T	temperature (K)
X	mole fraction (-)
Y	mass fraction (-)
Z	mixture fraction (-)
Ze	Zeldovich number (-)

Greek symbols

η_K	Kolmogorov length scale (m)
φ	fraction of the cell volume occupied by the reaction zone (-)
χ_C, χ_{CO}	fraction of the carbon atoms in the fuel molecule converted to soot and CO (-)
κ	absorption coefficient (1/m)
ν	stoichiometric coefficient (-)
ν_i', ν_i''	reactant/product stoichiometric coefficient (-)
ρ	density $(\mathrm{kg/m^3})$
σ	Stefan-Boltzmann constant $(\mathrm{W/m^2\ K^4})$
τ	time scale (1/s)

Subscripts

ad	adiabatic
air	air
bl	blow-off
ch	chemical
cr	critical
dil	diluent
eff	effective
ext	extinction
fuel	fuel
loss	heat losses
mix	mixture
max	maximum value
ox	oxidizer
rad	radiative
res	residence time
soot	soot
st	stoichiometric
0	inflow value
1	fuel stream
2	oxidizer stream
$\bar{}$	temperature-averaged
$\tilde{}$	resolved cell-averaged value

in bench scale tests, i.e., to predict fundamental extinction limits – limiting oxygen index (LOI) and minimum extinguisher concentration (MEC).

Unlike the AEA approach for the diffusion flamelet, the PSR extinction model is formulated for arbitrary activation energies and heats of combustion thereby avoiding possible effect of either parameter being not high enough in case of vitiated and/or hot reactants. It is also worthy of note that no separate fuel and oxygen streams could be identified at subgrid scale.

Validity of the PSR approach to model diffusion combustion is based on the analogy between extinction of premixed and diffusion flames. Despite the fundamental differences between premixed and diffusion flames, some of their characteristics do exhibit remarkable similarity. As an example, adiabatic flame temperature of the stoichiometric mixture also characterizes maximum temperature in the adiabatic diffusion flame, provided the reaction is infinitely fast. The RRA analysis shows that both in premixed and diffusion flames the characteristic temperature in the inner layer corresponds to the cross-over of the rates of chain-branching and chain-breaking reactions, and is therefore similar in both cases [1]. Furthermore, correspondence has been established between the fuel-rich/lean parts of the diffusion flame and upstream/downstream parts of the premixed flame, both separated by the similar fuel consumption layer [6]. It has been found that the extinction conditions in premixed and diffusion flames could also be similar. Indeed, in Ref. [10], the limiting oxygen index in diffusion flame was shown to be close to the corresponding value evaluated from the extinguishing concentrations of nitrogen in stoichiometric premixed flame. Zeldovich [11] and later Spalding [12] demonstrated that, at the extinction limit in adiabatic conditions, the mass burning rate in the diffusion flame approaches its maximum value, which is close to that in a steady premixed flame. Peters [13] has shown that the critical scalar dissipation rate at extinction of diffusion flame is related to the propagation speed of a premixed flame as $\chi_{ext} = (S_L^2/a)Z_{st}^2(1-Z_{st})^2$, where S_L, a and Z_{st} are, respectively, the laminar burning velocity, thermal diffusivity and stoichiometric mixture fraction.

More recent experimental [14–16] as well as computational and theoretical [3,4,17–20] works on diluent-induced flame extinction demonstrate that, similar to the critical extinguishing concentration in premixed flames, a fundamental concentration limit also exists in diffusion flames; when the diluent concentration exceeds such a limit, steady diffusion flame fails to exist at any strain rate. The fundamental limit arises as a merging point of two extinction limits governed by essentially different mechanisms, high strain blow-off and radiative quenching. The same phenomenon of dual extinction boundaries has been demonstrated for combustion of a motionless droplet in Ref. [2]. Two distinct extinction mechanisms (driven either by reactant leakage through the flame sheet or by excessive radiative losses) dominated, respectively, for sufficiently small and large droplets, and confluence of both limits made combustion impossible for all droplet sizes. Radiative extinction of the diffusion flame produced by large vaporizing droplets was observed in microgravity experiments and in detailed simulations as shown, for example, in Ref. [21]. It is worthy of note, that radiative extinction occurs at very low strain rates which are easier to achieve in microgravity conditions not affected by buoyancy.

The above indications of fundamental similarity of critical phenomena in diffusion and premixed flames justify further attempts to predict extinction of a diffusion flame using the PSR model. The perfectly stirred reaction model has been recently applied in Ref. [22] to predict extinction of the diffusion flame in the high-strain limit (blow-off). The single-step global reaction was considered, and calibration of the kinetic parameters was performed to replicate measured or computed (with detailed mechanisms) values of flame temperature and strain rate at blow-off. It was demonstrated that after such a calibration, the PSR model is capable of predicting the critical

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