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Modeling flame extinction and reignition in large eddy simulations with fast chemistry

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ABSTRACT

This work seeks to support the validation of large eddy simulation models used to simulate fire suppression. The emphasis in the present study is on the prediction of flame extinction and the prevention of spurious reignition using a fast chemistry, mixing-controlled combustion model applicable to realistic fire scenarios of engineering interest. The configuration provides a buoyant, turbulent methane diffusion flame within a controlled co-flowing oxidizer. The oxidizer allows for the supply of a mixture of air and nitrogen, including conditions for which oxygen-dilution in the oxidizer leads to flame extinction. Measurements to support model validation include local profiles of thermocouple temperature and oxygen mole fraction, global combustion efficiency, and the limiting oxygen index. The present study evaluates the performance of critical flame temperature based extinction and reignition models using the Fire Dynamics Simulator, an open-source fire dynamics solver. Alternate model cases are explored, each offering a unique treatment of extinction and reignition. Comparisons between simulated results and experimental measurements are used to evaluate the capability of these models to accurately describe flame extinction. Of the considered cases, those that include provisions to prevent spurious reignition show excellent agreement with measured data, whereas a baseline case lacking explicit reignition treatment fails to predict extinction.

1. Introduction

The numerical simulation of fire phenomena using classical computational fluid dynamics (CFD) methods has advanced significantly over recent years. This progress has led to an increasing demand for the use of CFD tools to analyze and predict the performance of fire protection systems. For fire suppression applications in particular, this demand remains largely unmet as modern CFD solvers have not yet been shown to adequately model fire suppression physics in configurations of practical interest, namely in the buoyant turbulent diffusion flames characteristic of most fire safety applications. This limitation is the result of the complex physical processes that govern turbulent fire suppression, comprising both localized extinction events and the potential reignition of unburned fuel following such extinction events. Neither of these phenomena are easily modeled. Further contributing to the issue is the general unavailability of detailed experimental data suitable for model validation, which also inhibits model development.

In recognition of these constraints, numerous experimental and computational studies have investigated the extinction behaviors of diffusion flames in various configurations. These works have successfully identified the primary physical mechanisms for extinction (thermal, aerodynamic, and kinetic quenching) [1–9], while others have made progress toward developing simple formulations to model flame extinction in cases applicable to realistic fire scenarios [10–15]. Additional studies have highlighted the primary features of flame reignition events, which may follow localized extinction in large-scale turbulent flames [16–21].

As noted in previous works, the primary difficulty associated with modeling flame extinction and reignition in fire applications is that both phenomena are controlled by small-scale quantities, including the flame temperature and the fuel-oxidizer mixing rate at the flame sheet, that cannot be resolved numerically in configurations of practical interest. In particular, the present study focuses on models that are specifically applicable to fire safety applications, i.e., models that are applicable to complex large-scale configurations where detailed fuel chemistry is typically unknown. Such models primarily comprise large eddy simulation (LES) approaches incorporating a combustion model based on the classical eddy-dissipation concept (EDC), wherein reactions are controlled by turbulent mixing and without regard for chemical kinetics. These modeling choices represent the most appro-

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Nomenclature

Symbols

C_u	model coefficient, (dimensionless)
C_v	model coefficient, (dimensionless)
h	mass-specific sensible enthalpy, (J/kg)
k	mass-specific kinetic energy, (m^2/s^2)
L_f	flame height, (m)
LOI	limiting oxygen index, (mol/mol)
$\dot{m}$	mass flow rate, (kg/s)
$\dot{m}'''$	mass reaction rate, ($kg/m^3/s$)
M	turbulence resolution criterion, (dimensionless)
Pr	Prandtl number, (dimensionless)
$\dot{Q}'''$	volumetric heat release rate, (W/m^3)
s	oxidizer to fuel mass ratio, (kg/kg)
Sc	Schmidt number, (dimensionless)
t	time, (s)
T	temperature, (K)
u	velocity, x-direction, (m/s)
v	velocity, y-direction, (m/s)
V	volume, (m^3)
w	velocity, z-direction, (m/s)
W	width, (m)
X	mole fraction, (mol/mol)
Y	mass fraction, (kg/kg)
Δ	LES filter width, (m)
Δh_{comb}	mass-specific enthalpy of combustion, (J/kg)
Δh_f°	mass-specific standard enthalpy of formation, (J/kg)
$[\Delta x,\ \Delta y,\ \Delta z]$	numerical grid resolution, (m)
η_{comb}	combustion efficiency, (dimensionless)
μ	dynamic viscosity, (kg/m/s)
ρ	mass density, (kg/m^3)
τ	time-averaging window, (s)
τ_{mix}	turbulent mixing time scale, (s)
χ_{rad}	radiative loss fraction, (dimensionless)

Scripts

∞	ambient property
b	burner
$crit$	critical
dil	diluent
ext	extinction
f	flame
$fuel$	fuel
ign	ignition/reignition
k	indexing variable (species)
ox	oxidizer
rms	root mean square
sgs	sub-grid scale
t	turbulent
tc	thermocouple

priate selections for simulating fire phenomena in practical engineering applications because alternative direct numerical simulations (DNS) cannot be applied to large-scale configurations of engineering interest, and the combustion of realistic fuel sources cannot be represented using detailed finite-rate chemical kinetics models. Available treatments for modeling flame extinction phenomena in these scenarios include models based on a critical flame temperature [10,11], or models based on a critical flame Damköhler number [6,7,12–15].

Critical flame temperature based models are often simpler and computationally less expensive, though such models do not consider the effect of chemical time scales. Such models are therefore incapable of modeling aerodynamic quenching effects and are unsuitable for configurations with high-strain flames [12]. By comparison, Damköhler number based extinction models incorporate additional physics to account for chemical time scales and aerodynamic quenching effects. For this reason, Damköhler number based extinction models may be expected to be more accurate [7,12,13]; however, critical flame temperature based models may also be expected to perform adequately in low-strain flame configurations where chemical time scale effects may be safely ignored [11].

While flame extinction modeling has achieved notable advancement over recent years, numerical studies focused on flame reignition phenomena are relatively few. As a result, available models for the treatment of flame reignition are presently limited to critical temperature based models [14,15]. This limitation is compounded by relatively unstudied issues concerning how the model should distinguish between piloted and non-piloted fuel sources, or between primary ignition at the fuel source and reignition occurring downstream of localized extinction events in the bulk flow. Such issues are particularly relevant to LES models incorporating EDC combustion because combustion is controlled by mixing and without regard for the initial temperature of the reactants. In such applications, careful consideration for reignition must be provided, otherwise spurious reignition may result, presently defined as the simulated reignition of previously extinguished combustible mixtures occurring at non-physical low temperatures.

The present work provides a detailed investigation of spurious reignition and its significance in affecting simulated extinction performance. The selected configuration includes recent experimental data for the suppression of a buoyant turbulent methane diffusion flame via nitrogen dilution of the oxidizer [22,23]. This simplified, but well-characterized configuration incorporates the essential features of a suppressed accidental fire (low-strain buoyancy-driven flow, turbulence, intense radiative emissions), while isolating the flame extinction physics of interest. In particular, simulations in the selected configuration highlight conditions for which localized flame extinction events may be followed by reignition events.

The present study utilizes the Fire Dynamics Simulator (FDS) [24], an open-source CFD solver that is widely used throughout the fire safety consulting and design industries. The selected numerical framework incorporates a LES approach utilizing the classical EDC treatment for mixing-controlled combustion. Selected models for flame extinction and reignition use the concept of a critical flame temperature, which should be viewed as an empirically-determined fuel-specific quantity approximating the flame temperature at the limits of flammability (considering heat losses) [25].

The present work follows a separate recent numerical study of the same configuration, but incorporating a robust Damköhler number based extinction model and a simple critical temperature based reignition model [15]. Results from that study suggest that simulated extinction performance in the present configuration is dominated by the reignition model and that the quality of the extinction model may therefore be of minor importance. The present work extends the study presented in Ref. [15] by evaluating whether a much-simplified critical flame temperature based extinction model can achieve similar performance in the selected low-strain configuration. The present investigation of spurious reignition then attempts to explain the dominance of the reignition model.

Results from the present work demonstrate the potential impairment that spurious reignition can cause to simulated extinction performance when its effects are not considered. To prevent such impairment, a pair of simple options for reignition modeling are developed and validated. The first is a novel concept featuring a