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.

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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

28 fuel-oxidizer mixing rate at the flame sheet, that cannot be resolved numer-
29 ically in configurations of practical interest. In particular, the present study
30 focuses on models that are specifically applicable to fire safety applications, *i.e.*
31 models that are applicable to complex large-scale configurations where detailed
32 fuel chemistry is typically unknown. Such models primarily comprise large eddy
33 simulation (LES) approaches incorporating a combustion model based on the
34 classical eddy-dissipation concept (EDC), wherein reactions are controlled by
35 turbulent mixing and without regard for chemical kinetics. These modeling
36 choices represent the most appropriate selections for simulating fire phenom-
37 ena in practical engineering applications because alternative direct numerical
38 simulations (DNS) cannot be applied to large-scale configurations of engineer-
39 ing interest, and the combustion of realistic fuel sources cannot be represented
40 using detailed finite-rate chemical kinetics models. Available treatments for
41 modeling flame extinction phenomena in these scenarios include models based
42 on a critical flame temperature [10, 11] or models based on a critical flame
43 Damköhler number [6, 7, 12–15].

44 Critical flame temperature based models are often simpler and computa-
45 tionally less expensive, though such models do not consider the effect of chem-
46 ical time scales. Such models are therefore incapable of modeling aerodynamic
47 quenching effects and are unsuitable for configurations with high-strain flames
48 [12]. By comparison, Damköhler number based extinction models incorporate
49 additional physics to account for chemical time scales and aerodynamic quench-
50 ing effects. For this reason, Damköhler number based extinction models may
51 be expected to be more accurate [7, 12, 13]; however, critical flame temperature
52 based models may also be expected to perform adequately in low-strain flame
53 configurations where chemical time scale effects may be safely ignored [11].

54 While flame extinction modeling has achieved notable advancement over
55 recent years, numerical studies focused on flame reignition phenomena are rel-
56 atively few. As a result, available models for the treatment of flame reignition
57 are presently limited to critical temperature based models [14, 15]. This limi-
58 tation is compounded by relatively unstudied issues concerning how the model

59 should distinguish between piloted and non-piloted fuel sources, or between
60 primary ignition at the fuel source and reignition occurring downstream of lo-
61 calized extinction events in the bulk flow. Such issues are particularly relevant
62 to LES models incorporating EDC combustion because combustion is controlled
63 by mixing and without regard for the initial temperature of the reactants. In
64 such applications, careful consideration for reignition must be provided, other-
65 wise spurious reignition may result, presently defined as the simulated reignition
66 of previously extinguished combustible mixtures occurring at non-physical low
67 temperatures.

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

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

86 The present work follows a separate recent numerical study of the same
87 configuration, but incorporating a robust Damköhler number based extinction
88 model and a simple critical temperature based reignition model [15]. Results
89 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 [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 spatially variable reignition criterion that permits fuel sources to be explicitly defined as either piloted or non-piloted. The second is an adaptation of the tiered reaction concept proposed in [15], which permits separation of ignition, extinction, and reignition via a split reaction mechanism. The present work additionally provides a validation study for the combination of these reignition treatments with the existing critical flame temperature based extinction model provided in the FDS solver.

2. Modeling Approach

2.1. Solver

The Fire Dynamics Simulator (FDS) provides a variable density, low Mach-number Navier-Stokes solver tuned for buoyancy-driven flows with heat release. FDS features a block-structured, Cartesian staggered grid and a parallel computing capability using MPI and OpenMP protocols. The numerics are generally second-order accurate with explicit time integration. Combustion is first-order accurate and time-split from transport, consistent with the classical eddy-dissipation concept (EDC) model [26, 27]. As applied in the present work, combustion is treated with a single-step, global reaction involving lumped species for the fuel, oxidizer, and products [28].

118 A large eddy simulation (LES) framework is employed for subgrid-scale tur-
 119 bulence modeling, where the LES residual stress and transport terms are closed
 120 via gradient diffusion coupled with a modified version of the Deardorff eddy-
 121 viscosity model [29], using an algebraic model for the subgrid kinetic energy
 122 based on scale similarity [30], and constant values for the turbulent Schmidt
 123 and Prandtl numbers.

124 FDS models thermal radiation via the radiative transfer equation using a
 125 discrete-ordinates, finite-volume method with gray absorption properties [31].
 126 In the present study, the description of thermal radiation is further simplified
 127 by modeling flame emission using the concept of a global radiative loss fraction
 128 (χ_{rad}); where χ_{rad} is prescribed in the simulations a priori from experimental
 129 measurements.

For a comprehensive discussion detailing the mathematical models employed
 in the FDS solver, the reader is referred to the FDS technical reference guide
 [32–34]. Particularly relevant to the present work, the local volumetric heat
 release rate due to combustion, $\dot{Q}'''$, is given by

$$\dot{Q}''' = - \sum_k \dot{m}_k''' \Delta h_{f,k}^\circ, \quad (1)$$

where $\dot{m}_k'''$ is the volumetric mass reaction rate and $\Delta h_{f,k}^\circ$ the mass-specific
 standard enthalpy of formation for each species, k , present in the prescribed
 combustion reaction. The volumetric mass reaction rate of fuel, $\dot{m}_{fuel}'''$, is eval-
 uated as

$$\dot{m}_{fuel}''' = -\bar{\rho} \frac{\min(\tilde{Y}_{fuel}, \tilde{Y}_{ox}/s)}{\tau_{mix}}, \quad (2)$$

130 where $\bar{\rho}$ is the local mass density, $\tilde{Y}_{fuel}$ and $\tilde{Y}_{ox}$ are the local mass fractions of
 131 fuel and oxidizer, and s is the stoichiometric oxidizer-to-fuel mass ratio. Other
 132 $\dot{m}_k'''$ are then determined from $\dot{m}_{fuel}'''$ based on prescribed stoichiometric reaction
 133 coefficients.

In Eq. 2, τ_{mix} is a modeled characteristic mixing time-scale with alternate
 definitions based on the resolution of the flow-field [35]. For all numerical reso-
 lutions considered in the present study, τ_{mix} is governed by turbulent advection

and defined as

$$\tau_{mix} = \frac{C_u \Delta}{\sqrt{(2/3) k_{sgs}}}, \quad (3)$$

where $C_u = 0.4$ is a model coefficient calibrated to match experimental flame height measurements [34], $\Delta = (\Delta x \Delta y \Delta z)^{1/3}$ is the LES filter width defined by the local grid resolution $(\Delta x, \Delta y, \Delta z)$, and k_{sgs} is the modeled subgrid turbulent kinetic energy derived from the turbulence sub-model.

Using the Deardorff model [29], the turbulent viscosity, μ_t , is given by

$$\mu_t = \bar{\rho} C_v \Delta \sqrt{k_{sgs}}, \quad (4)$$

where $C_v = 0.1$ is a model coefficient set to match a value reported in the literature [36]. Turbulent transport coefficients for mass and energy are then derived from μ_t via constant Schmidt and Prandtl numbers, $Sc_t = Pr_t = 0.5$.

The subgrid turbulent kinetic energy is evaluated as

$$k_{sgs} = \frac{1}{2} \left([\tilde{u} - \hat{u}]^2 + [\tilde{v} - \hat{v}]^2 + [\tilde{w} - \hat{w}]^2 \right), \quad (5)$$

where $[\tilde{u}, \tilde{v}, \tilde{w}]$ are the cell-mean values of the x , y , and z -components of the local velocity field, and $[\hat{u}, \hat{v}, \hat{w}]$ are weighted averages of their respective cell-mean counterparts over the adjacent computational cells (representing a test-filtered velocity field over length scale 2Δ) [30, 32].

2.2. Configuration

The configuration for the present study follows the experimental facility developed by White *et al.*, illustrated in Fig. 1 [22, 23]. This configuration provides the suppression of a buoyant, turbulent, methane diffusion flame via nitrogen dilution of the oxidizer. Flames are stabilized above a 5-cm-wide by 50-cm-long slot burner surrounded by a 50-cm-wide by 75-cm-long co-flowing oxidizer. Surrounding the fuel port is a thin 5-cm-wide strip of ceramic fiberboard, which encourages horizontally directed entrainment at the flame base and promotes transition to fully turbulent conditions within the flame. Methane flows at a fixed rate of 1.0 g/s to yield a flame with an unsuppressed total heat release rate of 50 kW.

Figure 1: (a) Diagram of experimental facility. (b) Plan-view of fuel/oxidizer port surface.

156 The co-flowing oxidizer is supplied at a fixed rate of 85 g/s, including a vari-
 157 able flow of nitrogen gas mixed into the oxidizer to provide controlled flame
 158 suppression. Suppression potential is monitored via the oxygen mole-fraction in
 159 the oxidizer stream ($X_{O_2}^{ox}$), measured using a sampling probe connected to a Ser-
 160 vomex 540E paramagnetic oxygen analyzer (uncertainty ± 1250 ppm; response
 161 time ± 5 s). The flow rate of nitrogen supplied to the oxidizer varies between
 162 0–40 g/s yielding changes in $X_{O_2}^{ox}$ from the ambient $X_{O_2}^{ox} = 0.21$ to as low as
 163 $X_{O_2}^{ox} = 0.11$, a value sufficient to achieve global flame extinguishment.

164 Available measurement data to support model validation include local ther-

Figure 2: Illustration of the numerical configuration; a 50 kW methane diffusion flame is visualized where the local volumetric heat release rate exceeds 200 kW/m^3 .

165 mocouple temperatures, measured via exposed-junction 1.0 mm bead-diameter
 166 K-type thermocouple probes (uncertainty $\pm 2 \text{ K}$; response time $\pm 3 \text{ s}$); local oxy-
 167 gen mole fractions, measured using a sampling probe connected to the aforemen-
 168 tioned oxygen analyzer; global radiative loss fraction, measured via heat flux
 169 transducer combined with infrared flame imaging and an analytical multipoint
 170 radiation source model [22]; global combustion efficiency, measured via carbon
 171 dioxide generation calorimetry [23]; and the value of $X_{O_2}^{ox}$ at extinction, termed
 172 the limiting oxygen index (*LOI*).

173 The numerical configuration is depicted in Fig. 2, which visualizes the simu-
 174 lated flame at ambient condition ($X_{O_2}^{ox} = 0.21$). The computational domain is a
 175 0.8-m-wide by 1.0-m-long by 1.0-m-tall box ($x \times y \times z$), which is large enough to
 176 prevent excessive boundary-condition effects on the simulated flame. The base-
 177 line numerical grid features a uniform resolution in each coordinate direction
 178 with $\Delta x = \Delta y = \Delta z = 5.0 \text{ mm}$. The total number of computational cells is 6.4
 179 million.

180 All edges of the computational domain feature an open, passive-flow bound-
 181 ary condition, with a background species of ambient air. The boundary con-
 182 ditions at the fuel and oxidizer ports utilize a prescribed mass-flux boundary
 183 condition (accounting for both convective and diffusive components), with values

184 specified to match the experiment (fuel mass flow, $\dot{m}_{fuel} = 1.0$ g/s, and oxidizer
185 mass flow, $\dot{m}_{ox} = 85$ g/s). The fuel and oxidizer, as well as any ambient en-
186 trainment, enter the domain with a constant temperature of $T_\infty = 293$ K. All
187 solid surfaces within the domain, comprising the structural rim of the oxidizer
188 port and the ceramic fiberboard around the fuel port, are described as inert,
189 isothermal objects with constant temperature, $T_\infty = 293$ K, and with zero-flow
190 boundary condition. At initial condition, the interior of the domain includes a
191 uniform composition of air at $T_\infty = 293$ K with ambient relative humidity of
192 40%.

193 The value of $X_{O_2}^{ox}$ at the oxidizer-port boundary is varied by controlling the
194 relative mass fluxes of air and nitrogen leaving the oxidizer-port, which are
195 balanced to maintain a constant total oxidizer flow rate, $\dot{m}_{ox} = 85$ g/s. At
196 the start of each simulation ($t = 0$ s), $X_{O_2}^{ox} = 0.21$, remaining constant at this
197 value for the first 5 s of simulation time, a duration sufficient to achieve steady
198 conditions in the flame and oxidizer flow fields.

199 After $t = 5$ s, the value of $X_{O_2}^{ox}$ is steadily decreased at a rate of $dX_{O_2}^{ox}/dt =$
200 0.002 s^{-1} . Simulations are conducted for a total duration of 60 s so that $X_{O_2}^{ox} =$
201 0.10 at the end of the simulation, a value sufficient to achieve global flame
202 extinction. Simultaneous with the reduction in $X_{O_2}^{ox}$, the value of χ_{rad} also
203 steadily decreases over the course of the simulation, with a prescribed trend
204 matching experimental data [22].

205 In addition to transient simulations, which feature continuously variable
206 $X_{O_2}^{ox}$, alternative steady-state simulations are conducted to provide converged
207 turbulence statistics at discrete $X_{O_2}^{ox}$ conditions. For such simulations, $X_{O_2}^{ox} =$
208 0.21 again for the first 5 s of the simulation to establish a stabilized ambient
209 flaming condition. After $t = 5$ s, $X_{O_2}^{ox}$ is decreased rapidly over a 3 s duration
210 to a final specified value, which is then held constant for the remainder of the
211 simulation.

212 Simulations are conducted using 40 processors on the University of Maryland
213 Deepthought2 high-performance computing cluster. Typical simulations require
214 roughly 2500 CPU hours using Intel Ivy Bridge E5-2680v2 2.80 GHz processors.

Table 1: Run-time characteristics for simulations with varying grid resolution.

Δx (mm)	# Cells (-)	# Cores (-)	CPU Time (hr)
20.0	356,000	2	22
10.0	1,056,000	5	111
5.0	6,400,000	40	1,085
2.5	51,200,000	320	30,655

2.3. Resolution

To evaluate grid sensitivity in the present configuration, a series of simulations have been conducted featuring uniform grid resolution corresponding to $\Delta x = 20.0$ mm, 10.0 mm, 5.0 mm, and 2.5 mm. These simulations are conducted with constant $X_{O_2}^{ox} = 0.21$ (no suppression) for a duration of 30 s. Simulated diagnostics include vertical centerline (z -direction), and lateral cross-flame profiles (x -direction) of various locally computed quantities including gas-phase temperature, z -component of flow velocity, and the resolved and subgrid turbulent kinetic energies. Time-mean and root-mean-square (rms) statistics for each quantity are gathered over the final 25 s of each simulation, during a period when the flow is statistically stationary. Run-time characteristics for these simulations are summarized in Table 1, comparing the total number of cells, processors, and computational cost applicable to each resolution case.

Figure 3 presents comparisons of vertical centerline and cross-flame profiles of the time-mean and rms gas temperature, T , among each resolution case. As shown, adequate grid convergence with a mean relative deviation less than 5% is observed for $\Delta x \leq 5.0$ mm in the mean temperature field. However, T_{rms} is under-predicted on the order of 50-100 K compared to the finest resolved case at $\Delta x = 2.5$ mm. These results indicate that there remain unresolved turbulent fluctuations in the temperature field for $\Delta x \geq 2.5$ mm, though these fluctuations negligibly impact the mean field. The simulated peak mean value of $T \approx 1200$ K closely resembles a value of 1191 K predicted by an empirical

Figure 3: Simulated gas temperature (T) at selected grid resolutions; (a) mean z -profile, (b) rms z -profile, (c) mean x -profile at $z = 0.25$ m, (d) rms x -profile at $z = 0.25$ m.

correlation developed for line-fire geometries from corresponding experimental measurements in a similar configuration [37].

Figure 4 presents similar resolution comparisons of the time-mean and rms velocity component magnitude, w . As shown, adequate grid convergence (mean relative deviation less than 5%) is observed for $\Delta x \leq 5.0$ mm in both the mean and rms values. As with the results for temperature, the simulated far-field value of $w \approx 2.8$ m/s agrees well with a value of 2.88 m/s predicted by empirical correlation [37].

The mean turbulent kinetic energy resolved by the numerical grid, k_t , may be approximated as

$$k_t = \frac{1}{2} (u_{rms}^2 + v_{rms}^2 + w_{rms}^2), \quad (6)$$

where u_{rms} , v_{rms} , and w_{rms} , are respectively the root-mean-square statistics

Figure 4: Simulated z -velocity magnitude (w) at selected grid resolutions; (a) mean z -profile, (b) rms z -profile, (c) mean x -profile at $z = 0.25$ m, (d) rms x -profile at $z = 0.25$ m.

for the x , y , and z components of the flow velocity. The unresolved subgrid
turbulent kinetic energy, k_{sgs} , may then be retrieved from the turbulence model
(see Eq. 5).

From these diagnostics, and following the conventions given in previous work
[38], a characteristic resolution criterion, M , may be defined as

$$M = \frac{k_t}{k_t + k_{sgs}}, \quad (7)$$

where this ratio indicates the fraction of the modeled turbulent kinetic energy
that is resolved by the numerical grid, taking a value of unity when k_{sgs} is
negligible and decreasing toward zero as k_{sgs} begins to dominate k_t . Note that
 k_{sgs} is a modeled quantity and should not be expected to represent the true
turbulent fluctuations in the unresolved flow. As a result, $M = 1$ does *not* imply

Figure 5: Simulated turbulence resolution criterion (M) at selected grid resolutions; (a) mean z -profile, (b) mean x -profile at $z = 0.25$ m.

that 100% of the turbulence in the flow is resolved by the grid. This criterion merely indicates the degree of influence that the turbulence model has on the flow field. Following established recommendations [36, 38], $M \geq 0.8$ satisfies reasonably well-resolved LES. Vertical centerline and cross-flame profiles of M are presented in Fig. 5.

As shown in Fig. 5, for $\Delta x \leq 5.0$ mm, $M \geq 0.8$ for all z along the flame centerline and for all x along a representative cross-flame profile, though there is a small region very near to the fuel port for which $M < 0.8$. This downward peak near $z = 0.01$ m is attributed to the laminar-turbulent transition that occurs at the flame base.

The limiting **integral** length scale of interest in the present configuration is the flame width (W_f , approximated as the burner width, $W_b = 5$ cm). For the baseline resolution of $\Delta x = 5.0$ mm, $W_b/\Delta x = 10$, indicating that this length scale is resolved over ten computational cells. In consideration of the previous results, this resolution may be considered marginal in the near-field region of the flame base (where $W_f \approx W_b$), but adequate in the intermediate and far-field regions within and above the bulk of the flame (where W_f increases with elevation so that $W_f > 10$ cm and $W_f/\Delta x > 20$ above mid-flame height, $z > 0.25$ m). While it is questionable whether the $\Delta x = 5.0$ mm resolution accurately captures the transition from laminar to turbulent flow near the flame

base, this resolution is deemed adequate and most cost-effective for the aims of the present study.

2.4. Flame Extinction & Reignition

The fundamental limitation of any mixing-controlled combustion scheme (as presented in Eqs. 1–5), is that combustion is guaranteed to occur anywhere fuel and oxidizer are mixing, regardless of local conditions for temperature or fuel/oxidizer dilution. This represents the characteristic ‘mixed-is-burned’ treatment adopted by the EDC combustion framework and has the advantage that detailed heat transfer and chemical kinetics treatments are not necessary to model primary ignition at the fuel source (there is no need to specify a pilot in order for ignition to occur). As a result however, additional modeling provisions must be considered in order to account for flame extinction and prevent spurious reignition, each respectively addressed in the following sections.

2.4.1. Extinction

The baseline flame extinction algorithm available in FDS uses the concept of a critical flame temperature [11], which accounts for the thermal quenching mechanism, but neglects the aerodynamic and kinetic quenching mechanisms. For extinction via nitrogen dilution of the oxidizer in the present low-strain configuration, thermal quenching acts as the dominant mode of extinction; therefore a critical flame temperature based extinction model is sufficient in the present configuration.

The criterion for flame extinction in FDS incorporates an enthalpy balance where in order for combustion to occur, the potential heat release due to combustion must be sufficient to increase the mean temperature of the reactant mixture above a critical value, T_{ext} , defined as the critical flame temperature [11, 25]. Combustion is allowed to proceed if the inequality given by

$$\hat{Y}_{fuel}(h_{fuel}(\tilde{T}) + \Delta h_{comb}) + \hat{Y}_{ox}h_{ox}(\tilde{T}) + \hat{Y}_{dil}h_{dil}(\tilde{T}) > \hat{Y}_{fuel}h_{fuel}(T_{ext}) + \hat{Y}_{ox}h_{ox}(T_{ext}) + \hat{Y}_{dil}h_{dil}(T_{ext}), \quad (8)$$

295 is satisfied, where $[\hat{Y}_{fuel}, \hat{Y}_{ox}, \hat{Y}_{dil}]$ and $[h_{fuel}, h_{ox}, h_{dil}]$ are the mass fractions
 296 and mass-specific sensible enthalpies of the fuel, oxidizer (defined as air for the
 297 present study), and diluent (defined as any non-reactant species, including any
 298 inert agents or products of combustion) present in the reactant mixture, $\tilde{T}$ is the
 299 initial cell temperature, and Δh_{comb} is the mass-specific enthalpy of combustion
 300 of the fuel. Note that Eq. 8 considers only the initial composition of the reactant
 301 mixture at the beginning of the combustion time step (after transport, but
 302 prior to any reaction). Extinction occurs if the local concentrations of fuel and
 303 oxidizer and/or the local cell temperature are too low to support combustion
 304 (thermal quenching). For further discussion of Eq. 8, the reader is referred to
 305 [11] and [32].

The reactant mixture referred in Eq. 8 represents the portion of the com-
 putational cell that is subject to potential combustion. The composition of the
 reactant mixture is defined relative to the composition of the host computational
 cell via the following,

$$\hat{Y}_{fuel} = \min \left(\tilde{Y}_{fuel}, \tilde{Y}_{ox}/s \right), \quad (9)$$

$$\hat{Y}_{ox} = s \hat{Y}_{fuel}, \quad (10)$$

$$\hat{Y}_{dil} = \left(\tilde{Y}_{ox}/\tilde{Y}_{ox} \right) \left(\tilde{Y}_{fuel} - \hat{Y}_{fuel} + \tilde{Y}_{dil} \right), \quad (11)$$

306 where $[\tilde{Y}_{fuel}, \tilde{Y}_{ox}, \tilde{Y}_{dil}]$ are the local mass fractions of the fuel, oxidizer, and
 307 diluent in the computational cell.

308 By Eqs. 9–11, the reactant mixture comprises a stoichiometric combination
 309 of fuel and oxidizer, with additional diluent included such that the ratio of dilu-
 310 ent to oxidizer in the reactant mixture matches that in the host computational
 311 cell ($\hat{Y}_k$ is the mass of species k in the stoichiometric reactant mixture divided
 312 by the total mass of the computational cell). These definitions (Eqs. 9–11) have
 313 the effect that excess fuel is treated as a diluent but excess oxidizer is not. As a
 314 result of this convention, combustion is likely to occur in a cell having a small
 315 amount of fuel in excess oxidizer, but is likely to be suppressed in a cell having a
 316 small amount of oxidizer in excess fuel. This treatment accommodates reason-

able combustion and extinction performance in relatively coarse computational cells, as are frequently used in simulations of practical-scale fire configurations. For further discussion of Eqs. 9–11, the reader is referred to [11] and [32].

The critical flame temperature used in the present study, $T_{ext} = 1600$ K, is representative of typical hydrocarbon fuels [25]. If the criterion specified in Eq. 8 fails, combustion is suppressed and the reaction source terms for species generation/consumption and heat release are set to zero for that computational cell, at that time step ($\dot{Q}''' = \dot{m}_k''' = 0$ in Eqs. 1 and 2).

2.4.2. Reignition

By inspection of the combustion scheme presented in Eqs. 1–5, it is apparent that spurious reignition may be an issue anywhere fuel and oxidizer mix downstream of a localized extinction event. Including consideration for the previously defined extinction criterion (Eq. 8), reignition may occur as long as fuel and oxidizer are locally present in sufficient quantities to satisfy Eq. 8, which is possible even for low initial cell temperatures near ambient condition. An example of this fact is the initial ignition of primary combustion at the start of a simulation, which desirably does not require any specification for a pilot or other ignition heat source. Still, any non-physical, low-temperature reignition of previously extinguished fuel can significantly degrade the performance of the extinction model. These issues apply not only to the scheme presented in Eqs. 1–5, but more broadly to EDC combustion models in general, which are widely used in LES fire modeling applications. For applications in which flame extinction is the primary modeling interest, spurious reignition must be prevented.

Restricting available solutions, any reignition or extinction criterion that is implemented to prevent spurious reignition cannot be globally applied in the model without also suppressing primary ignition at the fuel source. In particular, preliminary simulations in the present configuration have found that simple pilots or transient heat sources are incapable of achieving self-sustained primary combustion of the fuel when a global reignition criterion is applied in

the model. This issue may be circumvented by fully modeling primary ignition, though this would require an explicit ignition source coupled with detailed reaction kinetics and a highly-resolved treatment for heat transfer at the fuel source. Such an option is generally unavailable in fire applications which often include fuel sources that cannot be described with detailed reaction kinetics and complex configurations for which resolved heat transfer at the fuel source would require prohibitive computational cost. Despite these challenges, recent works have made notable progress in modeling and distinguishing ignition, extinction, and reignition processes in LES applications [14, 15].

Simulations in the present configuration highlight the noted issues surrounding spurious reignition, including conditions for which flame extinction leads directly to non-physical reignition if explicit treatment preventing such reignition is not provided in the model. As a preliminary modeling attempt, and following the convention of the critical flame temperature employed by the extinction criterion, a simple temperature based reignition criterion may be written as

$$\tilde{T} > T_{ign}, \quad (12)$$

where $\tilde{T}$ is the initial temperature of the computational cell (before the combustion time step) and T_{ign} is a critical temperature for reignition. As with the extinction criterion, if the inequality in Eq. 12 is unsatisfied, combustion is suppressed and the reaction source terms for species generation/consumption and heat release are set to zero for that cell, at that time step ($\dot{Q}''' = \dot{m}_k''' = 0$ in Eqs. 1 and 2). It should be noted that while Eq. 12 is relatively crude, its present use emphasizes the need for an explicit treatment of reignition and reflects the limited physical insight available to inform modeling choices for reignition phenomena. Equation 12 should be viewed as a preliminary modeling attempt that should be expected to improve with future research efforts.

As previously discussed, Eq. 12 cannot be generally applied in the solver without requiring an explicit treatment for primary ignition at the fuel source. To avoid this complication, implementations with selective application of Eq. 12 that still permit spontaneous primary ignition are explored in the following.

370 Three simple modeling cases, respectively denoted M1, M2, and M3, and each
 371 utilizing Eqs. 8 and 12 to treat extinction and reignition in various capacities,
 372 are summarized as follows.

In each of the following cases, the baseline single-step global reaction scheme employed for primary combustion follows the EDC treatment and is defined as

373 where reaction R1 is allowed to proceed only if the inequalities in both Eqs. 8
 374 and 12 are satisfied, subject to the respective temperature criteria T_{ext} and T_{ign} .

375 The first case, M1, represents the standard EDC behavior for which $T_{ext} =$
 376 1600 K and $T_{ign} = 0$ K everywhere in the computational domain. Here, Eq. 12
 377 is universally satisfied such that M1 includes no provision to prevent spurious
 378 reignition. As previously stated, spurious reignition may occur if, downstream
 379 of a region where Eq. 8 is unsatisfied (and therefore reaction R1 is suppressed),
 380 the resulting unburned fuel propagates to a region where Eq. 8 is satisfied such
 381 that reaction R1 then spontaneously proceeds (potentially at non-physically low
 382 ignition temperatures).

383 The second case, M2, provides a novel development consisting of a simple
 384 extension of M1, but including a small prescribed ignition zone near the fuel
 385 source within which $T_{ign} = 0$ K. Elsewhere in the domain, $T_{ign} = 900$ K, a value
 386 approximately equal to an experimentally measured auto-ignition temperature
 387 for methane fuel [39]. Everywhere in the domain, $T_{ext} = 1600$ K, consistent with
 388 M1. The ignition zone is defined within a region that extends 5 mm below, 5 mm
 389 around, and 2 cm above the surface of the fuel port. A diagram illustrating the
 390 bounds of the ignition zone is provided in Fig. 6.

391 The spatially-variable application of T_{ign} employed by M2 effectively elimi-
 392 nates the issue of spurious reignition. Reignition is allowed to occur, but only if
 393 the local cell temperature is high enough to support such a process (via Eq. 12).
 394 M2 additionally provides the framework necessary to distinguish between pi-
 395 loted and non-piloted fuel sources, where for non-piloted applications, the igni-
 396 tion zone may be located remotely from the fuel source to model spontaneous

397 ignition of a fuel leakage away from the leakage source.

398 The confined region of the ignition zone permits the convenience and sim-
 399 plicity of spontaneous primary ignition, but does so without subjecting the bulk
 400 of the computational domain to this convention. Despite these advantages, the
 401 specification of this zone is somewhat arbitrary and guidelines for its size and
 402 location do not yet exist. These are subjects of interest in the present work.

The third case, M3, follows conventions developed in recent affiliated works
 [14, 15], separating ignition and reignition using a tiered reaction mechanism.
 Including the primary reaction, R1, two additional reactions are introduced as

403 where Fuel* is a secondary fuel species representing unburned fuel that has
 404 had the opportunity to react, but has been suppressed by Eq. 8. Here, reac-
 405 tion R2 acts as a mutually-exclusive alternate reaction pathway to reaction R1,
 406 transforming the primary Fuel into Fuel* if, and only if, R1 is suppressed. Reac-
 407 tion R3 then provides for the reignition of Fuel*, where the reignition criterion
 408 in Eq. 12 may be independently applied to R3 without affecting primary ignition
 409 in R1 (different T_{ign} may be separately applied to each reaction).

410 In M3, T_{ext} and T_{ign} apply uniformly throughout the domain, with reaction-
 411 specific values defined as follows. For reaction R1, $T_{ext} = 1600 \text{ K}$ and $T_{ign} = 0 \text{ K}$,
 412 equivalent to the treatment in M1. For reaction R2, $T_{ext} = 0 \text{ K}$ and $T_{ign} =$
 413 0 K , signifying that R2 is always unrestricted whenever R1 is suppressed. For

Figure 6: Diagram of the ignition zone applied in modeling case M2.

Table 2: Critical temperature parameters for model cases M1, M2, and M3.

Case	Reaction	T_{ext} (K)	T_{ign} (K)
M1	R1	1600	0
M2	R1	1600	900
	R1	1600	0
M3	R2	0	0
	R3	1600	900

reaction R3, $T_{ext} = 1600$ K and $T_{ign} = 900$ K, matching the treatment in M2 (outside the ignition zone).

A summary of the critical temperature parameters, T_{ext} and T_{ign} , as applied in cases M1, M2, and M3 is displayed in Table 2. For M1 and M2, the extinction and reignition criteria (Eqs. 8 and 12) are each applied only to reaction R1, whereas for M3, Eqs. 8 and 12 are each applied to R1, R2, and R3 independently. If either criterion fails, the applicable reaction source terms for species generation/consumption and heat release are set to zero for that computational cell, at that time step ($\dot{Q}''' = 0$ $\dot{m}_k''' = 0$ in Eqs. 1 and 2).

The tiered reaction mechanism adopted in case M3 is advantageous in that it does not require an arbitrarily specified ignition zone. To its disadvantage however, M3 requires the additional complexity of reactions R2 and R3 and the computational expense of transporting an additional reacting species in Fuel*.

It is also important to recognize the implications of the stoichiometric requirement for air in the fuel transformation reaction, R2. This convention is necessary for the system of reactions R1–R3 to reduce back to the classical EDC treatment (R1) in cases of zero or total extinction; however, in situations where reaction R1 is extinguished and there is insufficient air to support reaction R2, fuel transformation will fail, permitting the persistence of the primary fuel in conditions of extinction, and providing the potential for spurious reignition to later occur (as visualized in the results that follow). While technically permissi-

ble, this issue is limited to cases of extreme oxidizer dilution and in the majority of practical applications, M3 effectively eliminates spurious reignition.

3. Results and Discussion

3.1. Model Validation

A preliminary validation of each modeling case (M1, M2, and M3) against measured thermocouple temperatures (T_{tc}) and local oxygen mole fractions (X_{O_2}) is presented in Fig. 7. Measured and simulated data are reported as lateral cross-flame profiles (x -direction) at selected elevations corresponding to $z = 12.5$ cm ($\sim L_f/4$) and $z = 25.0$ cm ($\sim L_f/2$) above the fuel port, for a partially-diluted oxidizer condition of $X_{O_2}^{ox} = 0.18$. This validation condition serves to evaluate the influence that each extinction and reignition treatment may have on the flame structure for a partially suppressed condition where complete combustion is still expected.

As shown in Fig. 7, simulated T_{tc} and X_{O_2} for all three cases agree reasonably well with the measured values. In particular, peak T_{tc} at both $z = 12.5$ cm and $z = 25.0$ cm show good agreement, though the simulated profiles are slightly wider than measured at both elevations. Agreement for X_{O_2} at $z = 12.5$ cm is also good, though the simulated trends at $z = 25.0$ cm are slightly sharper than measured. These results validate that each case yields mean temperature and mixing fields that resemble those measured in the experiment, confirming that the simulated flame structure is not unreasonably skewed by the extinction and reignition treatments.

A preliminary verification test to evaluate the capacity for spurious reignition in each case is depicted in Fig. 8, which visualizes each simulated flame at $X_{O_2}^{ox} = 0$ (pure nitrogen co-flow). For this condition, total flame extinction is definitively expected with no possibility of reignition, corresponding to a simulated combustion efficiency of $\eta_{comb} = 0$. Here, the simulated combustion efficiency is defined as

$$\eta_{comb} = \frac{1}{\tau \dot{m}_{fuel} \Delta h_{comb}} \int_{\tau} \int_V \dot{Q}''' dV dt, \quad (13)$$

Figure 7: Simulated and measured mean x -profiles of local thermocouple temperature (T_{tc}) and oxygen mole fraction (X_{O_2}) at selected elevations above the fuel port, and for $X_{O_2}^{ox} = 0.18$; (a) T_{tc} at $z = 12.5$ cm, (b) T_{tc} at $z = 25.0$ cm, (c) X_{O_2} at $z = 12.5$ cm, (d) X_{O_2} at $z = 25.0$ cm.

where $\dot{Q}'''$ is the local volumetric heat release rate in each computational cell, $\dot{m}_{fuel}$ is the mass flow rate of primary fuel from the fuel port, V is the volume of the computational domain, and τ is a time-averaging window.

For case M1 in Fig. 8(a), as expected, there is significant spurious reignition and $\eta_{comb} = 0.69$. As shown, extinction is correctly predicted within the region of influence of the diluted oxidizer; however, as soon as the plume of unburned fuel mixes with sufficient air from the surrounding ambient (roughly 1 m above the fuel port) the inequality in Eq. (8) is satisfied and combustion proceeds spontaneously.

For case M2 in Fig. 8(b), there is no spurious reignition and $\eta_{comb} = 0$. For

467 M3 however, in Fig. 8(c), there is a nearly negligible, but still finite occurrence
 468 of spurious reignition ($\eta_{comb} = 0.01$). This is due to the tiered reaction scheme
 469 implemented in M3, where the fuel transformation reaction (R2) includes a
 470 stoichiometric requirement for air. As there is no air present in the oxidizer at
 471 $X_{O_2}^{ox} = 0$, reaction R2 fails within the diluted oxidizer, allowing the extinguished
 472 primary fuel to persist within the domain. Upon initial mixing with air in
 473 the ambient, most but not all of this primary fuel is eventually transformed to
 474 secondary fuel (via the extinction model). Spurious reignition in case M3 is thus
 475 significantly reduced compared to M1, though it is not as thoroughly eliminated
 476 as in M2.

477 Figure 9 presents simulated η_{comb} for each case plotted versus $X_{O_2}^{ox}$ and
 478 compared against experimental data [23], which depict a plateau of constant

Figure 8: Spurious reignition in each modeling case for $X_{O_2}^{ox} = 0$; (a) M1 suffers significant
 spurious reignition ($\eta_{comb} = 0.69$), (b) M2 thoroughly eliminates spurious reignition ($\eta_{comb} =$
 0), (c) M3 suffers slight, but nearly negligible spurious reignition ($\eta_{comb} = 0.01$).

Figure 9: Simulated and measured combustion efficiency (η_{comb}) plotted versus $X_{O_2}^{ox}$; M1, which permits spurious reignition, fails to match the measured trend, while M2 and M3, which include provisions to prevent spurious reignition, match the measured data well.

479 $\eta_{comb} \approx 1$ for $X_{O_2}^{ox} > 0.14$. Between $X_{O_2}^{ox} = 0.14$ and $X_{O_2}^{ox} = 0.125$, a sharp drop
 480 in η_{comb} occurs, tapering briefly before global extinction ($\eta_{comb} = 0$), occurring
 481 at $X_{O_2}^{ox} \approx 0.12$. Compared to the measured data, all simulated cases match the
 482 initial plateau in η_{comb} for $X_{O_2}^{ox} > 0.14$. For $X_{O_2}^{ox} < 0.14$, M1 fails to follow the
 483 experimental trend and significantly over-predicts η_{comb} , primarily due to the
 484 occurrence of spurious reignition, as illustrated in Fig. 8(a). Notably, M1 does
 485 not predict deviation from $\eta_{comb} \approx 1$ until $X_{O_2}^{ox} < 0.12$, where the experimental
 486 data (and M2 and M3) show global extinction. Also noteworthy, M1 fails to
 487 ever predict extinguishment.

488 As shown in Fig. 9, cases M2 and M3 follow the experimental η_{comb} trend
 489 very well, falling within measurement uncertainty (± 0.04), and matching the
 490 extinction limit at $LOI \approx 0.12$. Despite their different approaches at address-
 491 ing spurious reignition (M2 via spatially defined ignition zone, and M3 via tiered
 492 reaction mechanism), the two cases also agree with one another remarkably well.
 493 In both cases, this agreement is achieved using relatively simple temperature-
 494 based extinction and reignition treatments, with physically-relatable critical
 495 temperature values ($T_{ext} = 1600$ K and $T_{ign} = 900$ K). The results in Fig. 9

Figure 10: Simulated and measured combustion efficiency (η_{comb}) among tiered reactions in modeling case M3; reaction R1 represents primary combustion, while reaction R3 represents reignition.

clearly demonstrate the significance of adequately preventing spurious reignition in simulations with localized flame extinction.

With its tiered reaction mechanism, case M3 permits additional detailed diagnostics to compare the relative contributions of heat release from either primary combustion (reaction R1) or reignition (reaction R3). These results are presented in Fig. 10. As shown, combustion is initially dominated by R1 at ambient $X_{O_2}^{ox}$, though there is considerable reignition heat release from R3 ($\sim 30\%$), indicating that even at ambient conditions, M3 predicts localized extinction (though later reignition satisfies total $\eta_{comb} \approx 1$). As $X_{O_2}^{ox}$ is reduced, $\eta_{comb, R1}$ steadily and monotonically decreases while $\eta_{comb, R3}$ gradually increases. For $X_{O_2}^{ox} > 0.14$, these trends offset, resulting in constant total simulated $\eta_{comb} \approx 1$. Near $X_{O_2}^{ox} \approx 0.135$, $\eta_{comb, R3}$ attains a peak value of roughly 80%, dropping off abruptly with further declining $X_{O_2}^{ox}$. Along with the continuous decline in $\eta_{comb, R1}$, total η_{comb} also decreases, tapering once $\eta_{comb, R3}$ drops to zero, occurring just before global extinction.

In agreement with the results of recent affiliated work [15], these trends clearly demonstrate that reignition treatment can dominate simulated suppres-

513 sion performance, where $\eta_{comb, R3}$ is maximized and significantly greater than
 514 $\eta_{comb, R1}$ throughout the region of rapidly declining η_{comb} in advance of the
 515 extinction limit. The simulated result that $\eta_{comb, R3} > 0$ at ambient $X_{O_2}^{ox}$ ad-
 516 ditionally suggests that local extinction and reignition events may be prevalent
 517 in turbulent fires, even for unsuppressed conditions. While these insights are
 518 interesting, it must be noted that no experimental measurements presently exist
 519 which could corroborate any distribution of total heat release amongst primary
 520 combustion and reignition. The present results are then useful to evaluate model
 521 performance, but should not be construed to represent actual flame behaviors
 522 until supporting measurements are made available.

523 3.2. Model Sensitivity

524 The sensitivity of modeling cases M1, M2, and M3 to variations in input
 525 parameters is examined in Fig. 11, which primarily compares simulated η_{comb}
 526 trends for each case among T_{ext} between 1500–1700 K, and T_{ign} between 800–
 527 1000 K. Specific to case M2, an additional sensitivity study considering the
 528 influence of the size of the prescribed ignition zone has also been performed.

529 Shown in Figs. 11(a), (c), and (e), respectively for cases M1, M2, and M3,
 530 a shift of T_{ext} by 100 K in either direction produces a corresponding shift in
 531 LOI by roughly 0.015. The same also results in a shift in the value of $X_{O_2}^{ox}$ at
 532 the inflection point of η_{comb} decline ($X_{O_2, crit}^{ox}$) by roughly 0.015, such that the
 533 entire η_{comb} trend is synchronously shifted to higher or lower $X_{O_2}^{ox}$ with variation
 534 in T_{ext} . Similarly shown in Figs. 11(d) and (f), respectively for cases M2 and
 535 M3, a shift of T_{ign} by 100 K in either direction results in a negligible change in
 536 LOI , but a shift in $X_{O_2, crit}^{ox}$ of roughly 0.01 (with M2 slightly more sensitive
 537 to variation in T_{ign} than M3). Shown in Fig. 11(b) (case M2), variations in
 538 ignition-zone elevation between 1.0–4.0 cm lead to a negligible change in LOI ,
 539 with changes in $X_{O_2, crit}^{ox}$ of less than 0.005. Simulated suppression performance
 540 in each case is then most sensitive to T_{ext} , less sensitive to T_{ign} , and for M2,
 541 even less sensitive to ignition zone size.

542 Note that while simulated suppression performance for case M2 is relatively

Figure 11: Sensitivity of simulated combustion efficiency (η_{comb}) to varying model parameters; (a) M1 T_{ext} sensitivity, (b) M2 ignition-zone size sensitivity, (c) M2 T_{ext} sensitivity, (d) M2 T_{ign} sensitivity, (e) M3 T_{ext} sensitivity, (f) M3 T_{ign} sensitivity.

insensitive to increasing size of the ignition zone, as shown in Fig. 11(b), there does exist a minimum effective size for the ignition zone below which spontaneous primary ignition is not achieved. For the present configuration, this ineffectiveness limit corresponds to an ignition zone one computational-cell high, extending 5 mm above the fuel port. This minimum size is likely to depend on the configuration of the fuel source, the selected value for T_{ign} , and the grid resolution (see Fig. 12 below), though no numerical or theoretical basis for its recommendation has yet been determined. A maximum size for the ignition zone however, may be discerned relative to the mean flame volume at ambient condition, where it would be desirable to limit the size of the ignition zone to be less than some small fraction of the mean flame volume.

The sensitivity of each modeling case to variations in grid resolution is explored in Fig. 12, including comparisons between the baseline resolution, $\Delta x = 5.0$ mm, and coarsened resolutions, $\Delta x = 10.0$ mm and $\Delta x = 20.0$ mm (the refined resolution of $\Delta x = 2.5$ mm is deemed prohibitively expensive for the present analysis, with an estimated computational cost of greater than 100,000 processor-hours per simulation).

As depicted in Fig. 12(a), grid sensitivity in case M1 is relatively negligible, attributed to the dominance of non-physical spurious reignition over extinction within the domain. Comparatively, grid sensitivity in cases M2 and M3 is significant, respectively shown in Figs. 12(b) and (c). In both cases, grid coarsening leads to an over-prediction of suppression, attributed to the inherent grid sensitivity of the gas-phase cell temperature on which the reignition criterion is solely based and which tends to be under-predicted in coarse grids. Grid sensitivity is greatest in case M2, attributed to the bounds of the specified ignition zone, whose size does not scale with the underlying grid resolution so that for coarse grids, the relative size of the ignition zone becomes too small (contains too few cells) to support primary ignition.

Overall, the relatively high grid sensitivity of cases M2 and M3 is to be expected because the simplistic reignition treatment used in these cases relies on the grid-resolved gas-phase cell temperatures, which are also highly grid sensi-

Figure 12: Sensitivity of simulated combustion efficiency (η_{comb}) to varying grid resolution;
(a) case M1, (b) case M2, (c) case M3.

574 tive. As a result of this sensitivity, the proposed critical temperature parameters
 575 used in the extinction and reignition models, T_{ext} and T_{ign} , should not be viewed
 576 as generally applicable fuel properties. Instead, the performance of the extinc-
 577 tion and reignition models, and therefore the appropriate choices for T_{ext} and
 578 T_{ign} , are inexorably linked to the applicable configuration (T_{ext} and T_{ign} are
 579 dependent on the flow condition because strain related extinction effects are
 580 neglected) and to the selected grid resolution (clearly shown in Fig. 12).

581 While it must be recognized that such grid sensitivity is a significant detri-
 582 ment to the utility of the proposed reignition treatments, it must also be pointed
 583 out that superior alternative treatments applicable to LES simulations incor-
 584 porating EDC combustion models have not yet been developed. The present
 585 models are therefore useful in light of lacking alternatives; however, improve-
 586 ment to the sensitivity of the proposed models or the development of superior
 587 alternatives should be a primary focus for future research.

588 3.3. Model Performance

589 Drawing from the present simulation results, a set of target objectives for ex-
 590 tinction and reignition models applicable to fire safety engineering applications
 591 could include the following.

- 592 1. Primary fuel should be allowed to ignite spontaneously without the need
 593 to model complex ignition physics.
- 594 2. Combustion should be extinguished wherever extinction conditions are
 595 encountered, as determined by the chosen extinction model.
- 596 3. Following extinction events, fuel should not spuriously reignite once non
 597 extinction conditions are encountered elsewhere in the computational do-
 598 main.
- 599 4. The model should ideally be free of arbitrary user input.
- 600 5. When desirable, the model should accommodate non-piloted fuel sources,
 601 such as fuel leakages.

602 Here, objective (1) is necessary for reasons described in Sec. 2.4.2, where the
 603 modeling of primary ignition is generally unavailable in fire applications, which

often include fuels that cannot be described with detailed reaction kinetics and complex configurations for which resolved heat transfer at the fuel source would require prohibitive computational cost. The current state-of-the-art solution to objective (1) in the classical EDC combustion treatment is to completely neglect ignition, where fuel burns spontaneously upon mixing with oxidizer. This convention then necessitates objectives (2) and (3), respectively for the provision of flame extinction and the prevention of spurious reignition, where the significance of objective (3) is readily demonstrated in the simulation results presented in Sec. 3.1.

Objective (4) recognizes the desire for a model that requires no arbitrary or configuration-dependent user input, while objective (5) accommodates potential specialized applications whose interests may include the modeling of fuel transport through a domain with spontaneous ignition occurring at a specified location other than the location of fuel injection. Note that objectives (4) and (5) are likely to conflict with one another, as user input is sure to be necessary to distinguish between a fuel source where spontaneous ignition is desired and a fuel leakage, where spontaneous ignition may be undesirable.

Of the modeling cases considered in the present study, all incorporate EDC mixing-controlled combustion, by which objective (1) is satisfied. Each case additionally includes a simple extinction criterion based on the concept of a critical flame temperature (see Sec. 2.4.1), satisfying objective (2). As discussed in Sec. 2.4.2 (and demonstrated in Sec. 3.1), this combination of EDC combustion treatment with simplistic extinction modeling unfortunately leads to spurious reignition and thus the failure of objective (3) in case M1.

While case M2 passes objective (3), it does so with the requirement that a prescribed ignition region be explicitly specified within the computational domain. While a prescribed ignition zone may be desirable in some applications (as recognized in objective (5), which only M2 passes), its requirement will be undesirable in many more cases where the appropriate spatial bounds of the ignition zone are not easily discernible. In general, the size and shape of the ignition zone must relate to the physical configuration of the fuel source

Table 3: Summary of objective performance for model cases M1, M2, and M3.

Objective	M1	M2	M3
(1)	✓	✓	✓
(2)	✓	✓	✓
(3)	×	✓	O
(4)	✓	×	✓
(5)	×	✓	×

and therefore no one-size-fits-all approach may be advised. Additional model sensitivities to the size of the ignition region and its performance dependency on grid resolution must also be considered (see Sec. 3.2). For these reasons, case M2 fails objective (4).

Case M3 addresses objective (3) using a tiered reaction mechanism (see Sec. 2.4.2), which avoids the constraint of arbitrary user input and therefore passes objective (4). Still, case M3 does require the added computational expense associated with the solution of an additional transport equation for the secondary fuel species. Additionally, though M3 adequately prevents spurious reignition in most situations, there are cases for which it fails to do so (see Fig. 8(c)). For this reason, M3 only qualifies objective (3).

The performance of each of the presently investigated extinction/reignition cases with respect to the stated modeling objectives is summarized in Table 3, where ✓, ×, and O respectively indicate a passed, failed, or qualified objective.

From Table 3, it is readily apparent that a simple and generally applicable approach to achieve accurate modeling of extinction and reignition within the limitations of the EDC combustion framework has not yet been developed. In the present configuration, for which objective (3) has been shown to be paramount to achieve reasonable simulated extinction performance, cases M2 and M3 (which pass or qualify this objective) are shown to yield accurate results when compared to measured global combustion efficiency data (see Fig. 9).

656 While the reignition treatments adopted in these cases are simplistic and suffer
657 from sensitivity issues (see Figs. 11 and 12), they produce significant improve-
658 ments in model performance with manageable added complexity and computa-
659 tional cost.

660 The present results offer incentive to open new dialogues regarding the issue
661 of spurious reignition in EDC combustion models, which until this investigation,
662 has received limited or no attention in the broader research community, with
663 all existing focus paid exclusively to extinction. The present results highlight
664 that extinction modeling, while key to model performance, can be significantly
665 affected and potentially dominated by reignition.

666 4. Conclusions

667 The present work provides a validation study to evaluate the capability
668 of the Fire Dynamics Simulator (FDS), a large eddy simulation (LES)-based
669 fire dynamics solver incorporating a mixing-controlled, eddy-dissipation concept
670 (EDC) combustion framework to accurately describe flame response in a range
671 of diluted oxidizer conditions, including a transition from complete combustion
672 to total flame extinguishment. Three alternative cases for the implementation
673 of critical flame temperature based extinction and reignition models are con-
674 sidered, including a baseline case without explicit reignition treatment (M1), a
675 case including a novel spatially-variable reignition criterion (M2), and a case
676 incorporating a tiered combustion mechanism with separate treatment of igni-
677 tion, extinction, and reignition (M3). The extinction performance of these cases
678 are compared against available experimental measurements, including local pro-
679 files of thermocouple temperature and oxygen mole fraction, as well as global
680 combustion efficiency. Sensitivity studies for model input parameters and grid
681 resolution are also provided.

682 In agreement with previous works, the present study reinforces the result
683 that simulated extinction performance can be dominated by reignition. Com-
684 parisons of simulated results highlight the necessity for explicit treatment of

reignition in mixing-controlled combustion models, where cases M2 and M3, which include provisions to prevent spurious reignition, yield extinction results that closely match the experimental data, while case M1, which does not restrict spurious reignition, fails to adequately predict flame extinction. While the reignition treatments adopted in cases M2 and M3 are relatively crude and suffer issues with grid sensitivity, they are shown to produce significant improvements in modeled extinction performance in the present configuration with manageable parametric sensitivity, added complexity, and computational expense. Future research endeavors are necessary to improve the present limitations of these types of models.

In comparing the extinction performance provided by each case, it is apparent that no simple and generally applicable approach is yet available to accurately model both extinction and reignition in LES models with mixing-controlled EDC combustion. As a result, the requirement for configuration-dependent user input is currently inevitable for certain applications using these types of models. In particular, additional in-flame experimental measurements are necessary to provide insight into the development of superior models and to better differentiate and determine which of the available models may best represent both extinction and reignition phenomena in general applications.

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Nomenclature

Symbols

C_u	model coefficient	(-)
C_v	model coefficient	(-)
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	(-)
Pr	Prandtl number	(-)
$\dot{Q}'''$	volumetric heat release rate	(W/m ³)
⁷¹² s	oxidizer to fuel mass ratio	(kg/kg)
Sc	Schmidt number	(-)
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	(-)
η_{comb}	combustion efficiency	(-)
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	(-)

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

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