Performance and calibration of two subgrid extinction models for turbulent diffusion combustion in an under-ventilated enclosure fire

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ABSTRACT

The fast-chemistry eddy dissipation combustion model fails to predict abrupt flame self-extinguishment when the oxygen content falls below the critical threshold. To overcome this limitation without recourse to the highly resolved simulations with the detailed chemical mechanisms, the bespoke subgrid extinction model is required. In this work, two subgrid extinction models are implemented in ANSYS Fluent and applied. The first extinction model utilizes conventional critical flame temperature concept, and the second one is the Damköhler number-based approach. The model formulation is used as derived earlier from the perfectly stirred reactor model, with the finite-rate reaction kinetics and radiative heat losses from the unresolved reaction zone.

To evaluate model performance and to select optimum model parameters, the burner fire with the constant fuel supply rate (corresponding to the nominal heat release rate 400 kW in complete combustion) is considered in 4x6x4.5 m compartment with the 0.3 m diameter lower air inlet connected to the ambient atmosphere. Conjugate heat transfer at the compartment walls and transient thermal conductivity in the compartment structures are accounted for.

Provided that the model parameters are optimized, both extinction models enable prediction of flame self-extinguishing, and the predicted times for flame to extinguish are similar to those recorded in the experiments. For the CFT model, best agreement with the experimental time to flame extinguishment is obtained if the critical flame temperature is set to 1900 K. For the Damköhler number-based approach, the optimum value of 0.25 is found for the model constant in the proportionality relationship between the resolved strain rate and the residence time in the reaction zone, which is not resolved in the simulations.

In spite of the similar performance of the two extinction models in the experimental scenario with weakly strained flame, the Damköhler number-based model is expected to be applicable in a wider range of scenarios including highly strained flames such as those affected by strong jets, sprays, and cross-winds.

KEYWORDS:

Extinction, under-ventilated combustion, CFD fire modeling
INTRODUCTION

Extinction in under-ventilated fires is observed as soon as the oxygen concentration decreases below a critical threshold. Comprehensive modeling of extinction and ignition phenomena can only be performed by using the detailed chemical mechanisms. This methodology appears impractical in fire modeling since the reaction zones of the flamelets are not spatially resolved, and the chemical composition of fuels is often unknown. The eddy-dissipation combustion model (most widely used in fire modeling) implies infinitely fast chemistry and assumes that fuel burning rate is solely controlled by subgrid mixing. Combustion is predicted by this model if fuel and oxygen are available at any concentration, regardless of the temperature. Extinction cannot, therefore, be predicted by the fast chemistry and mixing-controlled combustion model. As such, additional submodel is required to allow for the abrupt flame extinction observed in experiments.

To date, two distinct approaches have been developed to model local flame extinction:

1. Critical flame temperature concept (see Refs. [1], [2] etc.) – very simple approach, good for vitiated flames at low strain. It is this approach which is used in the open source specialized CFD code FDS for fire modeling [3]. It has been, however, demonstrated in Refs. [4], that this approach fails to predict extinction at high strain (blow-off, suppression by sprays).

2. Damköhler number-based modeling (Refs. [5], [6], [4], [7] among others) – allows for finite-rate chemistry, kinetic parameters must be calibrated. Note, that the perfectly stirred reactor (PSR) subgrid model investigated in Ref. [7] also reveals applicability of the properly formulated Damköhler number as a unified extinction criterion (incorporating both high-strain blow-off and low-strain radiative limits). The advantage of this approach is that it is suitable for highly strained flames.

More recently, the reactive volume fraction approach has also been proposed (see Ref. [8]) based on the heat balance in an eddy containing the fuel-air mixture.

Existing CFD modeling experience of flame extinction covers simulations of unconfined flames [2] and enclosure fires. The latter were mainly considered at small spatial scale [1, 2], while simulations of large-scale compartments remain limited. No subgrid models of local flame extinction are available in ANSYS Fluent for joint use with the eddy dissipation model. In this work, we implement and compare two of the above-listed approaches (critical flame temperature and Damköhler number-based extinction models) by simulating self-extinguishment of the 400 kW methane flame in an under-ventilated large-scale enclosure [9].

SUBGRID EXTINCTION MODELING

Critical flame temperature extinction model

Critical flame temperature (CFT) extinction model utilizes the assumption that the flame can only exist if the temperature in the reaction zone, \( T_r \), exceeds the critical value, \( T_{cr} \). In this model, the finite rate reaction is not allowed, and the temperature in the reaction zone, \( T_r = \hat{Y}_o \Delta h_{o1}/\hat{c}_r \), corresponds to that after complete burn-out of the stoichiometric mixture having oxygen mass fraction \( \hat{Y}_o \). In the above equality \( \hat{Y}_o \) and \( \hat{T} \) are the resolved oxygen mass fraction and temperature, \( \Delta h_{o1} \) is the heat of combustion per 1 kg \( O_2 \) consumed (known to be about 13 MJ/kg for many fuels), \( \hat{c}_r \) is the mixture specific heat, which should allow for the specific heat of combustion products and heat consumed in its dissociation. In case of presence of inert diluents, its specific heat should also be accounted for in evaluating \( \hat{c}_r \). Note, that proper assignment of the \( \hat{c}_r \) value is an approximation to the formulation of the extinction condition in terms of enthalpies as is done in FDS 6. Thus, extinction is predicted if \( \Delta h_{o1} \hat{Y}_o \hat{T}_r < \hat{c}_r (T_{cr} - \hat{T}) \); the burning rate is set to zero in the grid cells where this inequality is obeyed. To obtain the best agreement with different experiments, different CFT values might be recommended. For example, in Ref. [10] best agreement of flame extinction by FDS were obtained with the critical flame temperature 1773 K.

The inherent assumption of the CFT extinction model is that the heat is released immediately, regardless of the residence time characteristic of the reactants in the reaction zone which is affected by the local velocity strain. In highly strained flows local residence time is too low, and the heat required to rise temperature up to \( T_r \) would not be completely released. The model is therefore suitable for the low-strain flames with a low probability of strain-induced blow-off.
**Damköhler number-based extinction model**

This model is designed to overcome the abovementioned limitation of the CFT extinction model. Here we apply the approach developed in Ref. [7] where perfectly stirred reactor model is utilized to predict the state of the reaction zone of the diffusion flamelet occupying a small fraction of grid cell volume. It has been shown in Ref. [7] that the extinction condition can be formulated as that of sufficiently low Damköhler number, $Da < Da_{cr}$, which is defined as a product,

$$Da = \dot{r}_{f,cr} \tau_{res},$$

(1)

of the reaction rate, $\dot{r}_{f,cr}$, and the residence time, $\tau_{res}$, both are evaluated as explained below.

Evaluation of the reaction rate utilizes the single-step global reaction model,

$$\dot{r}_{f,cr} = A(M_{f,cr}/\rho)(\tilde{Y}_{f,cr} p/M_{f,cr})^{\nu_{f,cr}} \left(\tilde{Y}_{O_2} p/M_{O_2}\right)^{\nu_{O_2}} \exp\left(-\left(E_a/kT_f\right)\right).$$

(2)

The temperature in the reaction zone, $T_f$, obeys the equation,

$$T_f = T + \left(\tilde{Y}_{O_2} \Delta h_{f,cr}/\tilde{c_p}\right)/\left(1 + \tau_{res}/\tau_{max}(T_f)\right) + \Delta T_{f,\tau} + \Delta T_{f,\tau}^{\text{adi}},$$

(3)

which allows for the radiative heat losses, the rate of which is quantified by the characteristic time scale,$$
\tau_{max}(T_f) = \tilde{c}_p/\left(4\kappa\sigma(T_f^4 + \tilde{T}^4)(T_f + \tilde{T})\right),$$

where $\kappa$ is the local effective absorption coefficient, $\sigma = 5.67 \times 10^{-8}$ W/(m$^2$·K$^4$) is the Stefan-Boltzmann constant. Iterations are required to solve Eq. (3) for $T_f$.

Consistent with the CFT model, the assumption of stoichiometry, $\tilde{Y}_{f,cr} = \tilde{Y}_{O_2} / \left(\nu_{O_2} M_{O_2}/M_{f,cr}\right)$ (where $\nu_{O_2}$ is the stoichiometric mole oxygen to fuel ratio), is implied in evaluating temperature in the reaction zone and is also used to rewrite Eq. (2) as

$$\dot{r}_{f,cr} = A(M_{f,cr}/\rho)(\tilde{Y}_{f,cr} p/M_{f,cr})^{\nu_{f,cr}} \left(\tilde{Y}_{O_2} p/M_{O_2}\right)^{\nu_{O_2}} \exp\left(-\left(E_a/kT_f\right)\right).$$

(4)

The residence time is evaluated as $\tau_{res} = C_{SGS} \tilde{S}^{-1}$, where $\tilde{S}$ is the resolved strain rate, and $C_{SGS}$ is the model constant to be calibrated. We assume that the volume occupied by the reaction zone is much smaller than that of the grid cell, and therefore the resolved temperature $\tilde{T}$ and oxygen mass fraction $\tilde{Y}_{O_2}$ represent the environment for the reaction zone.

In the simulations presented below, we use the following kinetic parameters derived in Refs. [4, 7] for extinction of counter-flow methane-$O_2$-$N_2$ flames: $E_a = 121$ kJ/mol, $A = 8.883 \times 10^7$ (m·mol·s)$^{-1}$, $n_{O_2} = 1.13$, $n_{f,cr} = 0.56$, $Da_{cr} = 2$. For methane fuel $M_{f,cr} = 0.016$ kg/mol, $\Delta h_{f,cr} = 12.54$ MJ/kg, $\nu_{O_2} = 2$. To obey the equilibrium adiabatic flame temperature $T_{ad} = 2226$ K in the stoichiometric methane-air mixture at initial temperature of 300 K, specific heat of combustion products is set $\tilde{c}_p = Y_{f,cr,\text{ad}} \Delta h_f / (T_{ad} - T_0) = 1400$ J/(kg·K).

Fig. 1. The extinction domain predicted by the critical flame temperature model (at $T_{f,cr} = 1600$ K) and by the Damköhler number-based model ($n_{f,cr} = 1$, $n_{O_2} = 0$, $\kappa = 0$) at different values of $\delta$.
Comparison of the two extinction models is best illustrated for the special case when $n_{\text{fuel}} = 1$, $n_{O_2} = 0$, $\kappa = 0$ (first-order reaction, no radiative losses). Critical condition for extinction, $Da = Da_{cr}$, takes the form

$$\delta^{-1} = \left(\tilde{Y}_{O_2}/\left(\nu_{O_2}M_{O_2}/M_{\text{fuel}}\right)\right)\exp\left(-\left((E_a/R)/(\tilde{T} + \tilde{Y}_{O_2}(\Delta h_{\text{fuel}}/c_p))\right)\right),$$

where $\delta = \tau_{\text{str}}A/\text{Da}_{cr}$ is the dimensionless quantity inversely proportional to the local strain, $\tilde{S} \sim 1/\tau_{\text{str}}$. The dependence $\tilde{Y}_{O_2}(\tilde{T})$ at extinction boundary is shown in Fig. 1 for different values of $\delta$, and therefore local strain. It can be seen that the higher is the strain rate, the larger is the extinction domain. Depending on the strain, it may be either larger or smaller than that predicted by the critical flame temperature model.

The Damköhler number-based model allows for the finite reaction rate in and the radiative heat losses from the reaction zone. As such, two distinct extinction mechanisms are captured, strain-induced blow-off and radiative quenching; both are affected by the oxygen and diluent availability.

CASE DESCRIPTION AND MODEL SETUP

Under-ventilated fire scenario

Enclosure fire tests performed in the Lawrence Livermore National Laboratory (LLNL) in 1986, see Ref. [9], are considered. In this series of tests, the rectangular enclosure with the horizontal dimensions 4x6 m, 4.5 height was utilized (see Fig. 2 and Fig. 4). Centrally located 0.57 m diameter circular burner elevated 0.23 m above the floor level is used to supply gaseous fuel (methane) at a constant flow rate. Air injection occurs through the lower of two air inlets (0.3 m diameter circular pipes). Walls, floor, and ceiling are 10 cm thick. The outlet duct designed for the fan-driven exhaust ventilation is closed in the scenario considered here.

Model setup

Simulations were performed using ANSYS Fluent 16.2. Large eddy simulation approach (LES) is applied to predict gaseous flow with the Smagorinsky-Lilly subgrid model. Eddy-dissipation model (EDM) is applied to allow for the turbulence-reaction interaction. The single-step irreversible reaction of complete fuel oxidation is considered. Soot and thermal radiation modeling are performed as explained in Ref. [11].

Block-structured hexahedral meshes are used both in fluid and solid domains. Simulation results shown below were obtained with the mesh, having the following amounts of grid cells: fluid: 344 701, walls 99 888, floor and ceiling 36 296. The total amount of grid cells is 480 885. Cubic cells in the flame zone above the burner are of 3x3x3 cm size. The effect of mesh refinement was examined with both coarser and finer meshes in which the cell size above the burner was varied from 1.5 to 5 cm; simulation results were weakly affected. The coupled scheme was used for pressure-velocity coupling. Spatial discretization was set as follows: gradients – least squares cell based; pressure – second order; momentum – bounded central differences; energy, soot, species – second order upwind; transient formulation – bounded second order implicit.

The extinguished fuel is assumed to re-ignite as soon as the reactants in a grid cell do not obey the extinction condition. This implies overestimated ignitability of the reactants and might delay predicted flame extinguishment if the probability of the re-ignition is significant.

SIMULATION RESULTS

Here we consider enclosure configuration with no false ceiling, no fan-driven exhaust (the outlet duct is closed), open lower air inlet and closed upper air inlet (case TL-3 in Ref. [9]). Open air inlet prevents pressure growth as the temperature increases. Methane fuel is continuously supplied to the burner at the rate of 8 g/s corresponding to the nominal heat release rate of 400 kW. Conjugate heat transfer at the compartment walls and transient thermal conductivity in the compartment structures are accounted for.

In the experimental scenario replicated in this work flame was self-extinguished in 300 s after ignition. Dissimilar to the experimental observation steady burning with constant 400 kW heat release rate and slowly reduced peak temperature is predicted in the simulations without extinction model, at least for 500 s. The two-layer stratification is predicted, with the horizontal interface between the lower and upper layers located just above the burner. The air is entrained to the flame from the lower layer which is fed by the lower air inlet. The
flow through the lower layer inlet oscillates in time, ejecting vitiated gas and sucking the fresh air. Combustion is predicted at any non-zero oxygen concentration.

**Damköhler number-based extinction model**

After the fuel supply is turned on, turbulent flame develops above the burner, and the fire plume impinges the ceiling. Simulations replicate formation of a hot upper layer with gradually reduced oxygen concentration, eventually causing flame extinguishment. Flame (which is visualized by 500 °C resolved temperature iso-surface) disappears shortly after 300 s, which agrees with the experimental observations. As soon as the flame disappears, heat release ceases, and temperature decreases due to the heat transfer to the structures. Simulated temperature and velocity distributions, oxygen mass fractions and reaction rates are presented in Fig. 2.

![Fig. 2. Instantaneous resolved temperature and velocity, oxygen mass fraction and reaction rate distributions (left to right) in scenario 3-TL [9], time 250 s. Damköhler number-based extinction model, \( C_{SGS} = 0.25 \).](image)

The effect of the model constant, \( C_{SGS} \), on predicted dynamics of integral heat release rate (left) and peak resolved temperature (right). Scenario 3-TL [9], Damköhler number-based extinction model

The effect of critical flame temperature value on predicted dynamics of integral heat release rate and peak resolved temperature is shown in Fig. 5. Integral heat release rate exhibits slow and smooth decay, while the
peak flame temperature drops abruptly when the last pieces of flame disappear. With this criterion of flame self-
extinguishment, Fig. 5 shows that the value of 1900 K is best suited to replicate the experimental time of
extinction close to 300 s.

![Image](image_url)

Fig. 5. The effect of critical flame temperature value on predicted dynamics of integral heat release rate (left)
and peak resolved temperature (right). Scenario 3-TL [9], critical flame temperature extinction model

**CONCLUSIONS**

Provided that the model parameters are optimized, both extinction models enable prediction of flame self-
extinguishing, and the predicted times for flame to extinguish are similar to those recorded in the experiments.
The Damköhler number-based model is expected to be applicable in a wider range of scenarios including highly
strained flames such as those affected by strong jets, sprays, and cross-winds.

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