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Effects of radiation on large-scale spherical flame propagation

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ABSTRACT

One-dimensional numerical simulations are conducted for large-scale spherical flame propagation in near-stoichiometric methane/air mixture. With the help of adaptive mesh refinement, we simulate the spherical flame propagation up to a radius of 4 m inside an extremely large computational domain of 20 m. The emphasis is placed on quantifying the radiation effects on large-scale spherical flame propagation. Besides the adiabatic model neglecting radiative loss, two radiation models are used in simulation: one is the optically thin model considering only radiation emission and the other is the statistical narrow band model considering both radiation emission and absorption. The effects of radiative loss and radiation absorption on large-scale spherical flame propagation are quantified through comparison among results predicted by these three models. It is shown that for the near stoichiometric methane/air mixture, radiation has little influence on small-scale spherical flame propagation with radius below 4 cm; while radiative loss and radiation absorption both have great impact on large-scale spherical flame propagation with radius up to 4 m. Spherical flames without and with self-acceleration are both considered in 1D simulation. Radiation effects on the propagation speed and acceleration exponent of the large-scale self-accelerating spherical flame are assessed. It is found that radiation effects on acceleration exponent are exaggerated when radiation absorption is neglected. In experiments for large-scale spherical flame propagation, the acceleration exponent is not strongly affected by radiation due to radiation absorption.

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1. Introduction

Outwardly propagating spherical flames are popularly used to measure the laminar flame speed, especially at elevated pressures ([1, 2] and references therein). In experiments, radiation of H_2O and CO_2 in the burned gas cannot be avoided, and it affects the spherical flame propagation. Though there are many theoretical studies (e.g., [3–7]) on spherical flame propagation with radiation, it is difficult to quantify the influence of radiation on spherical flame propagation speed due to the nonlinearity and spectral dependence of radiation. Recently, many studies [1,2,8-17,41] have assessed the radiation effects on laminar flame speed measurement using propagating spherical flames. It was shown that radiation effects are important for near-flammability-limit and/or highly-diluted mixtures with relative low laminar flame speed [11,15]. On the other hand, the influence of radiation on spherical flame propagation was found to be negligible for near-stoichiometric mixtures [11,15]. In spherical flame experiments measuring the laminar flame speed, the flame radius is usually below 10 cm. Therefore, previous studies [1,2,8–17] only examined the radiation effects on small-scale spherical flame propagation with radius below 10 cm. It is not clear how radiation affects large-scale spherical flame propagation with radius above 1 m. Are radiation effects on large-scale spherical flame still negligible for near-stoichiometric mixtures? This motivates the present work, which aims to answer this question.

In fact, several groups conducted experiments for large-scale spherical flame propagation and investigated the self-acceleration caused by the Darrieus–Landau instability [18,19]. Gostintsev et al. [20] summarized the experimental data for spherical or hemispherical flames with radii in the range of 0.3–10 m and suggested a power-law between flame radius and time. Bradley et al. [21] conducted experiments in a large vented box structure with the dimensions of $10 \times 8.75 \times 6.25\,m^3$ and the large-scale spherical flame propagation in methane/air and propane/air mixtures was measured up to radii beyond 3 m. Bauwens et al. [22–24] Conducted experiments in an enclosure with internal dimensions of $4.6 \times 4.6 \times 3.0\,m^3$ and examined large-scale spherical methane/air, propane/air and hydrogen/air flames up to a radius of 0.6 m. Kim et al. [25–27] conducted large-scale spherical flame experiments in a cubic plastic tent with the volume of $27\,m^3$ and recorded spherical flames with radii above 1 m. Bradley et al. [20] mentioned that for large-scale spherical flames, radiation from the burned gas is important and it affects flame propagation speed. However, in these experiments [20–27], it is difficult to quantify the influence

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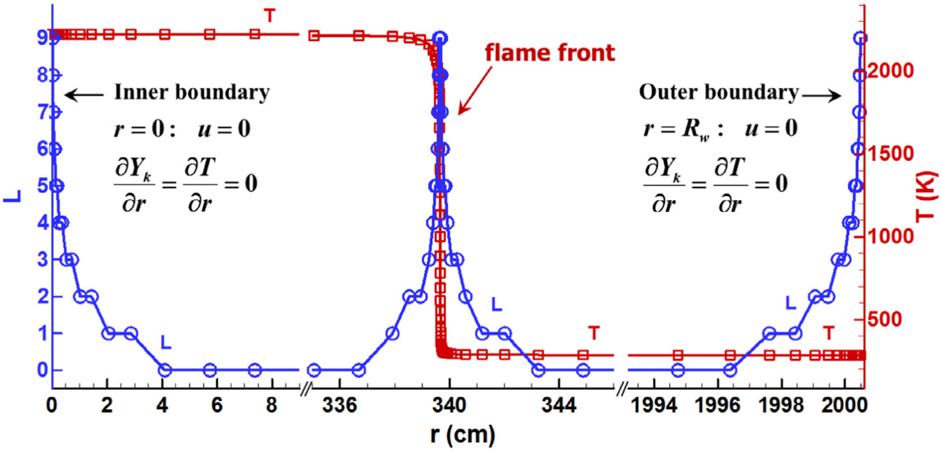

Fig. 1. Mesh level (L) and temperature (T) distributions on the computational domain of 0 ≤r≤R_w= 2000.4864 cm. The boundary conditions are shown. The mesh size for mesh level of L is equal to 16,384/2^L µm.

of radiation on the propagation and acceleration of large-scale spherical flames. Therefore, the influence of radiation on large-scale spherical flame propagation is still not well understood.

Based on the above-mentioned considerations, the objective of this study is to numerically quantify the radiation effects on large-scale spherical flame propagation in near-stoichiometric mixture. Specifically, one-dimensional numerical simulations are conducted for large-scale spherical flame with radius up to 4 m in methane/air mixture with the equivalence of $\phi=1.1$. We choose the same mixture as the one used in the experiments of Bradley et al. [21], so that the present simulation results can be compared with experimental data in [21] .The influence of radiative loss and radiation absorption is quantified through comparison among results predicted by different radiation models. Moreover, large-scale self-accelerating spherical flame is also considered. The radiation effects on both flame propagation speed and acceleration exponent are assessed.

2. Numerical methods and specifications

The code A-SURF [11,28,29] is used to simulate 1D large-scale spherical flame propagation. A-SURF solves the conservation equations for a multi-species reactive mixture using the finite volume method. The CHEMKIN packages [30] are incorporated into A-SURF to calculate the reaction rates as well as the temperature- and component-dependent thermodynamic and transport properties. The mixture-averaged model is used to evaluate the mass diffusivities. A-SURF has been successfully used in previous studies on flame and detonation propagation (e.g., [31–36]). The readers are referred to Refs. [11,28,29] for details on numerical schemes and code validation of A-SURF.

To compare with experimental data reported by Bradley *et al.* [21], we consider the large-scale spherical flame with radius up to 4 m in CH_4/air mixture. Same as the experiments [21], the equivalence ratio of CH_4/air is $\phi=1.1$, and the initial pressure and temperature are $P=1$ atm and $T_u=285$ K, respectively. The detailed chemical mechanism, GRI-Mech 3.0 [37], is used. Since we consider flame propagation in a confined spherical chamber and the flame radius reaches 4 m, a very large chamber radius of $R_w=20$ m is used in order to diminish the influence of pressure rise and wall confinement [11,38] (see Appendix B). The effects of instability and buoyancy are not included in 1D simulation. Therefore, only radiation effect appears and it can be readily quantified.

To efficiently resolve the flame propagation in an extremely large computational domain of 0 ≤r≤R_w=2000.4864 cm shown in Fig. 1, adaptive mesh refinement is used. There are 1221 base meshes with the size of 16,384 µm; and thereby $R_w=1221\times$ 16,384 µm = 2000.4864 cm. The maximum mesh level is 9 and thus the finest mesh size is $16{,}384/2^9=32$ µm. As shown in Fig. 1, the propagating flame front is always covered by the finest grids at the level of $L=9$. Furthermore, both boundaries are covered by the finest grids so that the boundary conditions shown in Fig. 1 are satisfied in simulation. The total mesh number is around 2000. As shown in Appendix A, grid convergence is achieved to ensure numerical accuracy.

Table 1
Three models for radiation.

Abbreviation	Model description
ADI	Adiabatic model without radiative loss
OTM	Optically thin model; only radiative emission is considered
SNB	Statistical narrow band model; radiative emission and absorption are considered

Similar to our previous studies [11,15,17], three models listed in Table 1 are used to quantify the radiation effects on large-scale spherical flame propagation. The adiabatic model (denoted by 'ADI') neglects radiation. The optically thin model (denoted by 'OTM') only considers radiation emission; while the statistical narrow band model (denoted by 'SNB') considers both radiation emission and absorption. For OTM, radiation emission from CO_2, H_2O, CO, and CH_4 is considered and the Planck mean absorption coefficients in [39] are used. For SNB, the radiative transport is calculated using a fitted statistical narrow-band correlated-*k* (FSNB-CK) method [9].

In simulation, the flame front, R_f, is defined as the location of the maximum heat release rate. The spherical flame propagation speed, $S=dR_f/dt$, is calculated through numerical differentiation.

3. Results and discussion

3.1. Stable and unstable spherical flames

One-dimensional simulation is suitable only for stable spherical flame propagation. However, in large-scale spherical flame experiments [21–27], the Darrieus–Landau instability induces significant flame acceleration. In 1D simulation, we can artificially modify the reaction rate so that flame acceleration occurs.

The following relationship between flame propagation speed S and flame radius R_f is obtained through fitting the present

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