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Visualizing turbulent flames using flamelet libraries

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A R T I C L E I N F O

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A B S T R A C T

This paper presents a ray tracing visualization technique to generate realistic images of turbulent non-sooting hydrocarbon flames. The method uses flamelet libraries to reconstruct the flame structure in physical space, calculating the light emitted in the visual range of light emitting radicals present in the flame. The generated visualizations clearly convey the complex structure of turbulent flames and provide a vehicle for presenting complex simulations of turbulent flames to the general public.

1. Introduction

Turbulent flames typically exhibit highly complex topologies. Using advanced large eddy simulation (LES) combustion methods, for example, a wide range of topology scales can be resolved, making detailed analysis of the instantaneous turbulent flame structure difficult. Traditionally, the results of such simulations are presented in the form of two-dimensional contour plots and one-dimensional line plots. While this is an efficient presentation of data for quantitative analysis, it is often difficult to fully grasp at-once the complex structure of the turbulent flame that a simple high speed shutter photograph of the real flame might convey. It is thus desirable to present simulation results in a more realistic visual manner, i.e., in the way a flame would be seen in person or captured by a photo camera. Such presentations of simulation results also provide an avenue to more effectively present scientific results to the non-expert for outreach efforts. Furthermore, they can enable a way to test optical analysis/post-processing tools used in experimental research, since using the visualized flame as a captured image of a real flame, the outcome of the post-processing analysis can be compared to the full three-dimensional data set of the simulation for quantitative benchmarking.

In this paper, a volume rendering ray tracing technique is described that simulates the light emitted from a turbulent flame to create a realistic image of the flame. Volume rendering of flames in itself is not new, see for example [1], however the use of advanced combustion models makes full use of the available numerical data for visualization purposes. While the examples shown use flamelet based modeling techniques to simulate the turbulent combustion process [2–5], the technique can just as well be used to visualize turbulent flames simulated using non-flamelet techniques. The technique has been implemented in the tool *FlameTracer* [6] and has been used successfully in the past to visualize different turbulent flames [7,8].

This paper is structured in the following manner. First, the equations solved to visualize the light emitted from the turbulent flame are presented. Next, numerical implementation issues are discussed, followed by a presentation of some select visualization results. Finally, some concluding remarks are presented.

2. Governing equations

In typical flames, only a small number of species n_Y actually emit light in the visual range, for example only CH, C_2, and soot emit noticeable levels of light in technical hydrocarbon flames. Assuming black body behavior, the intensity $I(\lambda)$ of light emitted at a wavelength λ from a given spatial coordinate $\boldsymbol{x}$ can be determined from

$$I(\lambda, \boldsymbol{x}) = \sum_{i=1}^{n_Y} \frac{w_i(\lambda)}{\iota_i} Y_i(\boldsymbol{x}) \frac{2\pi hc^2}{\lambda^5 \left(e^{\frac{hc}{\lambda kT(x)}} - 1\right)}, \quad (1)$$

with w_i and ι_i species dependent weighting factors, h the Planck constant, c the speed of light, k the Boltzmann constant, Y_i the mass fraction of species i, and T the temperature. The weighting factors $w_i(\lambda)$ determine the hue of the emitted light from a given species and can be determined from visual observations of flames summarized by Gaydon [9]. For CH and C_2 these are

$$\begin{aligned} &w_{CH}(438\,\text{nm}) = 0.2 \quad w_{CH}(474\,\text{nm}) = 0.9 \quad w_{CH}(517\,\text{nm}) = 1.0 \\ &w_{CH}(564\,\text{nm}) = 0.8 \quad w_{CH}(619\,\text{nm}) = 0.3 \\ &w_{C_2}(387\,\text{nm}) = 0.5 \quad w_{C_2}(432\,\text{nm}) = 1.0 \quad w_{C_2}(494\,\text{nm}) = 0.2. \end{aligned} \quad (2)$$

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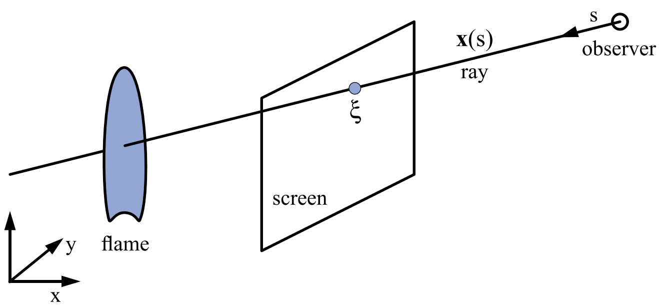

Fig. 1. Ray tracing geometry.

Since these factors have meaning only relative to the weighting factors of the same species, an additional factor ι_i is used to weight the species amongst each other,

$$\iota_i = \int_{\lambda_{min}}^{\lambda_{max}} \frac{2\pi hc^2}{\lambda^5 \left(e^{\frac{hc}{\lambda k T_{i,\mathrm{ref}}(x)}} - 1\right)} d\lambda \,, \tag{3}$$

with $T_{i,\,\mathrm{ref}}$ a species reference temperature set to

$$T_{\mathrm{CH,ref}} = 2500\,\mathrm{K} \qquad \mathrm{T}_{\mathrm{C_2,ref}} = 3000\,\mathrm{K}\,, \tag{4}$$

and λ_{min} and λ_{max} the minimum and maximum wavelength of the spectrum to be calculated. Here, we focus on the visual range of light, hence we choose $\lambda_{min} = 380\,\mathrm{nm}$ and $\lambda_{max} = 780\,\mathrm{nm}$.

To calculate an image of the flame, a rectangular screen is defined in the coordinate system of the flame, see Fig. 1 together with the coordinate of the observer. The screen is then divided into N_h by N_v equidistant pixels in the screen horizontal and vertical direction. A ray $\mathbf{x}(s)$ can then be defined from the observer location through any screen pixel coordinate $\boldsymbol{\xi}$ traversing the computational domain of the flame calculation. Integrating Eq. (1) along this ray gives the intensity of the screen pixel as a function of wavelength λ,

$$I(\lambda, \xi) = \int_0^{s_{max}} I(\lambda, \mathbf{x}(s)) ds \tag{5}$$

where s_{max} is chosen such that the ray traverses the entire computational domain of the flame calculation. However, in order to integrate Eq. (5), the temperature T and the mass fractions Y_i of all light emitting species must be determined along the ray, see Eq. (1). The straightforward way to do this is to use the calculated temperature $T^{(cv)}$ and species mass fractions $Y_i^{(cv)}$ of the combustion simulation at each mesh point/control volume cv and interpolate their values by some interpolation function f to the ray location $\mathbf{x}(s)$, i.e.,

$$T(\mathbf{x}(s)) = f(T^{(cv)})$$
$$Y_i(\mathbf{x}(s)) = f(Y_i^{(cv)})\,, \tag{6}$$

and then numerically integrate Eq. (5) along the ray. However, this approach is directly applicable only to fully resolved flame calculations, i.e., either laminar flames, or direct numerical simulations of turbulent flames, where T and Y_i of the light emitting species, e.g., CH and C_2, are directly available at every mesh point/control volume as part of the combustion simulation.

In the case of turbulent flames using for example a large eddy simulation (LES) approach, only spatially filtered mass fractions $\widetilde{Y}_i^{(cv)}$ and temperatures $\widetilde{T}^{(cv)}$ are available at each mesh point/control volume of the combustion simulation. Using the filtered quantities in Eq. (6), i.e.,

$$\widetilde{T}(\mathbf{x}(s)) = f(\widetilde{T}^{(cv)})$$
$$\widetilde{Y}_i(\mathbf{x}(s)) = f(\widetilde{Y}_i^{(cv)})\,, \tag{7}$$

thus visualizes the spatially filtered flame and not a fully resolved realization of the flame.

A further complication arises from the fact that light in non-sooting flames is emitted in the visual range by radicals that have both low concentrations and tend to be highly localized in mixture fraction space and thus typically occur only in thin sheets in physical space. To properly capture the light emitted by these radicals, the mesh of the turbulent flame calculation would have to resolve these thin radical sheets in physical space, a condition that is usually not well met even by state-of-the art turbulent combustion LES of realistic flame configurations, see Section 4.

Instead of relying on the mass fractions of light emitting species calculated at each mesh point/control volume by the combustion simulation, we propose to reconstruct sub-cell species concentrations and temperatures using a flamelet approach. Depending on whether the combustion process is non-premixed, premixed, or partially premixed, we require either the mixture fraction, its variance, and the scalar dissipation rate, and/or a distance function level set scalar and its variance or a progress variable at each mesh point/control volume of the combustion simulation. In many turbulent combustion models, these quantities are directly available as the solution variables of the model [2], or they may be reconstructed from the employed solution variables.

As an example, consider a turbulent diffusion flame calculated using a flamelet approach [2,8,10,11] employing LES. Filtered mixture fraction $\widetilde{Z}$, sub-filter mixture fraction variance $\widetilde{Z''^2}$, and scalar dissipation rate $\widetilde{\chi}$ are then readily available as part of the combustion simulation at each mesh point/control volume. These quantities exhibit significantly smaller spatial gradients than the mass fractions of the light emitting radicals and thus can readily be interpolated to the ray location, e.g.,

$$\widetilde{Z}(\mathbf{x}(s)) = f(\widetilde{Z}^{(cv)}) \tag{8}$$

$$\widetilde{Z''^2}(\mathbf{x}(s)) = f(\widetilde{Z''^2}^{(cv)}) \tag{9}$$

$$\widetilde{\chi}(\mathbf{x}(s)) = f(\widetilde{\chi}^{(cv)})\,. \tag{10}$$

Using a standard presumed shape PDF approach in conjunction with flamelet libraries, the temperature and mass fractions of the light emitting species can then be reconstructed at the ray location,

$$\widetilde{T}(\mathbf{x}(s)) = \widetilde{T}\left(f(\widetilde{Z}^{(cv)}), f(\widetilde{Z''^2}^{(cv)}), f(\widetilde{\chi}^{(cv)})\right)$$
$$\widetilde{Y}_i(\mathbf{x}(s)) = \widetilde{Y}_i\left(f(\widetilde{Z}^{(cv)}), f(\widetilde{Z''^2}^{(cv)}), f(\widetilde{\chi}^{(cv)})\right), \tag{11}$$

and used to integrate Eq. (5). This visualizes a spatially filtered flame, with the spatial filter scale being the local flow solver mesh size. The approach therefore cannot directly visualize any sub-filter wrinkling of the flame front, but visualizes only its aggregate effect on the filter scale. This limitation is not significant if the underlying LES is well resolved, i.e., the sub-filter wrinkling is small, as is the case in the visualizations presented in this paper, or the resulting picture's resolution is insufficient to resolve the sub-filter wrinkling, which is likely the case for digital photographs of full laboratory flames.

3. Numerical methods

To integrate along the ray, Eq. (5), the portion of the ray within the computational domain of the combustion simulation is subdivided into pieces of size Δs and integrated in physical space using a simple midpoint rule. This necessitates that Δs is sufficiently small to resolve the thin sheets of light emitting radicals in physical space. It would be possible to perform the integration along the ray in flamelet library space using the discrete points of the flamelet library for integration. Such an approach would ensure that even the most localized mass fraction in library space would

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