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Large eddy simulation-based analysis of entropy generation in a turbulent nonpremixed flame

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ABSTRACT

LES (large eddy simulation) is employed for prediction and analysis of entropy generation in turbulent combustion. The entropy transport equation is considered in LES. This equation contains several unclosed entropy generation terms corresponding to irreversible processes: heat conduction, mass diffusion, chemical reaction and viscous dissipation. The SGS (subgrid scale) closure of these effects is provided by a methodology termed the En-FDF (entropy filtered density function), which contains complete statistical information about SGS variation of scalars and entropy. In the En-FDF, the effects of chemical reaction and its associated entropy generation appear in closed forms. The methodology is applied for LES of a nonpremixed jet flame. Predictions show good agreements with the experimental data. Analysis of entropy generation shows that heat conduction and chemical reaction are the main sources of irreversibility in this flame. The sensitivity of individual entropy generation effects to turbulence intensity is studied.

1. Introduction

Improved energy efficiency is a key objective in development of modern energy systems. To achieve optimum efficiency in energy conversion, it is essential to minimize the irreversible losses in the system. In practice, transport processes are always accompanied by irreversibilities, causing destruction of exergy (availability) of the working-fluid and thus, reduction of energy efficiency, according to the second law of thermodynamics. The rate of exergy destruction can be characterized in terms of entropy generation according to the Gouy-Stodola theorem, $I_D = T_0 S_g$ [1], where I_D, T_0 and S_g denote the rate of exergy destruction (also known as lost power), ambient (dead state) temperature and entropy generation rate, respectively. Therefore, optimizing the energy efficiency relies on minimizing the overall exergy destruction by reducing the entropy generated within the system. During the past several decades the second-law analysis has been the subject of broad investigations; see, *e.g.*, Refs. [1–3]. A system-level analysis, often termed exergy analysis, is used to obtain the net rate of exergy destruction. Alternatively, analysis of local generation of entropy reveals the specific agents contributing to irreversible losses. Such analysis applied to laminar flows has been the subject of many studies; some of the recent contributions are as follows. Briones et al. [4] studied the entropy generation processes in a partially-premixed flame. Bidi et al. [5] performed flame stabilization and burner optimization in a porous media using entropy generation minimization method. Makhanlall et al. [6] considered entropy generation associated with viscous dissipation, heat transfer and thermal radiation in a solar collector filled with a radiative participating gas. Anand [7] studied entropy generation due to heat transfer in a two-dimensional pressure driven micro-channel flow. In turbulent flows, analysis of entropy generation based on DNS (direct numerical simulation) has been conducted in a few studies. Okong'o & Bellan [8] performed DNS studies of entropy generation effects in supercritical, multicomponent shear flows. Farran & Chakraborty [9] used DNS to analyze the entropy generation in a turbulent premixed flame. Borghesia & Bellan [10] used a DNS database of a high pressure, reacting temporal mixing layer to study the influence of initial pressure and exhaust gas recirculation on each individual entropy generation term. In contrast to DNS, RANS (Reynolds Averaged Navier–Stokes) has been a more common approach to investigate entropy generation in turbulent reacting flows. As examples of recent contributions in RANS, Emadi & Emami [11] studied entropy generation in a turbulent hydrogen enriched methane/air bluff-body flame. Makhanlall

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et al. [12] studies the second-law efficiency of thermal radiation in turbulent diffusion natural gas flames. Saqr & Wahid [13] used RANS predictions to investigate the effect of inlet swirl intensity on local entropy generation. Jiang et al. [14] studied entropy generation distribution in H_2/air premixed flame in micro-combustors with baffles. Chakraborty [15] performed modeling and simulation of entropy generation terms in a turbulent premixed flame and assessed the results using DNS data. Despite the benefits of LES (large eddy simulation) in turbulence simulations, its application for entropy generation analysis has been insubstantial. This is mainly due to the challenges to SGS (subgrid scale) modeling of the unclosed entropy generation terms. An effective strategy to account for SGS effects in turbulent reacting flows is the FDF (filtered density function) methodology. This methodology has been the subject of extensive previous contributions. These include the development of scalar FDF (S-FDF) by Colucci et al. [16] and Jaberi et al. [17]; the velocity FDF by Gicquel et al. [18]; the velocity-scalar (VS-FDF) FDF by Sheikhi et al. [19] and [20]; and the frequency-velocity-scalar FDF by Sheikhi et al. [21]. Some of the applications of this methodology in turbulent combustion include the S-FDF simulation of turbulent jet [22] and [23], bluff-body [24] and swirl [25] flames; and the VS-FDF simulation of turbulent jet flames [26] and [27]; see, *e.g.*, Refs. [28] and [29] for comprehensive reviews of the FDF. In recent works by Sheikhi et al. [30] and Safari & Sheikhi [31], a FDF-based methodology, termed the En-FDF (entropy FDF) has been introduced which allows LES prediction of entropy transport and entropy generation in turbulent reacting flows. In this study, the marginal form of this methodology [31] is considered which contains the complete statistical information on entropy and scalar fields and thus, accounts for individual entropy generation effects. The En-FDF is applied to predict a nonpremixed methane jet flame (Sandia Flame D) [32]. The objectives are to assess the accuracy of the En-FDF and to demonstrate its effectiveness for prediction and analysis of entropy generation in turbulent reacting flows.

2. Mathematical modeling

We consider the compressible form of the continuity, Navier–Stokes, energy (enthalpy), mass fraction and entropy transport equations in low Mach number flows. Along with the ideal gas equation of state, these equations describe transport of fluid density $\rho(\mathbf{x},t)$, the velocity vector $u_i(\mathbf{x},t)$, the pressure $p(\mathbf{x},t)$, the specific enthalpy $h(\mathbf{x},t)$, mass fraction of N_s number of chemical species $Y_\alpha(\mathbf{x},t)$ ($\alpha = 1,\ldots,N_s$) and the specific entropy $s(\mathbf{x},t)$. Large eddy simulation involves the use of filtering operation.

$$\langle Q(\mathbf{x},t)\rangle = \int_{-\infty}^{+\infty} Q(\mathbf{x}',t)G(\mathbf{x}',\mathbf{x})d\mathbf{x}' \tag{1}$$

where $\langle Q\rangle$ is the filtered variable and G is the filter function with characteristic width Δ. We consider a filter function which is spatially invariant, localized and symmetric with $\int_{-\infty}^{+\infty} G(\mathbf{x})d\mathbf{x} = 1$. We assume existence of all moments $\int_{-\infty}^{+\infty} \mathbf{x}^m G(\mathbf{x})d\mathbf{x}$, $(m \geq 0)$. In compressible flows we use the Favre filter variable $\langle Q\rangle_L = \langle \rho Q\rangle/\langle\rho\rangle$. Applying the filtering operation to the transport equations we obtain

$$\frac{\partial\langle\rho\rangle}{\partial t} + \frac{\partial\langle\rho\rangle\langle u_i\rangle_L}{\partial x_i} = 0 \tag{2}$$

$$\frac{\partial\langle\rho\rangle\langle u_i\rangle_L}{\partial t} + \frac{\partial\langle\rho\rangle\langle u_i\rangle_L\langle u_j\rangle_L}{\partial x_j} = -\frac{\partial\langle p\rangle}{\partial x_i} + \frac{\partial\langle\tau_{ij}\rangle_L}{\partial x_j} - \frac{\partial\langle\rho\rangle\tau(u_i,u_j)}{\partial x_j} \tag{3}$$

$$\frac{\partial\langle\rho\rangle\langle\phi_\alpha\rangle_L}{\partial t} + \frac{\partial\langle\rho\rangle\langle u_i\rangle_L\langle\phi_\alpha\rangle_L}{\partial x_i} = \frac{\partial}{\partial x_i}\left(\gamma\frac{\partial\langle\phi_\alpha\rangle_L}{\partial x_i}\right) - \frac{\partial\langle\rho\rangle\tau(u_i,\phi_\alpha)}{\partial x_i} + \langle\rho S_\alpha\rangle \tag{4}$$

$$\begin{aligned}\frac{\partial\langle\rho\rangle\langle s\rangle_L}{\partial t} + \frac{\partial\langle\rho\rangle\langle u_i\rangle_L\langle s\rangle_L}{\partial x_i} = {} & \frac{\partial}{\partial x_i}\left(\gamma\frac{\partial\langle s\rangle_L}{\partial x_i}\right) - \frac{\partial\langle\rho\rangle\tau(u_i,s)}{\partial x_i} + \left\langle\frac{1}{T}\tau_{ij}\frac{\partial u_i}{\partial x_j}\right\rangle \\ & + \left\langle\gamma\frac{c_p}{T^2}\frac{\partial T}{\partial x_i}\frac{\partial T}{\partial x_i}\right\rangle + \sum_{\alpha=1}^{N_s}\left\langle\frac{\gamma R_\alpha}{X_\alpha}\frac{\partial\phi_\alpha}{\partial x_i}\frac{\partial X_\alpha}{\partial x_i}\right\rangle \\ & - \left\langle\frac{\rho}{T}\sum_{\alpha=1}^{N_s}\mu_\alpha S_\alpha\right\rangle\end{aligned} \tag{5}$$

where R_α, X_α, μ_α and S_α are gas constant, mole fraction, specific chemical potential and chemical reaction source term for species α, respectively. Variables T and c_p denote the temperature and the specific heat capacity at constant pressure for the mixture; γ denotes the thermal and mass molecular diffusivity coefficients for all the scalars. We assume unity Lewis number and we set the molecular Schmidt (and Prandtl) number as $Sc = Pr = 0.75$. We use the scalar array $\boldsymbol{\phi} = [\phi_1,\ldots,\phi_{N_s+1}]$ to represent mass fraction and enthalpy in a common form with $\phi_\alpha \equiv Y_\alpha$ for $\alpha = 1,\ldots,N_s$ and $\phi_{N_s+1} \equiv h$. In these equations, we employ Fourier's law of heat conduction and Fick's law of diffusion and we assume a Newtonian fluid with the molecular stress tensor $\tau_{ij} = \mu(\partial u_i/\partial x_j + \partial u_j/\partial x_i - (2/3)(\partial u_k/\partial x_k)\delta_{ij})$ where μ denotes the molecular viscosity which is proportional to $T^{0.7}$. Equation (5) is the filtered entropy transport equation. This equation is derived in previous work [33] for low Mach number flows with unity Lewis number and equal mass diffusivity for all chemical species.

The last four terms in Eq. (5) correspond to irreversible generation of entropy by viscous dissipation S_{gV}, heat conduction S_{gH}, mass diffusion S_{gM} and chemical reaction S_{gC}, respectively. These terms constitute the total rate of entropy generation, denoted by S_g. According to the second law of thermodynamics, the modeled filtered entropy generation terms must be positive semidefinite. The closure problem in Eqs. (2)–(5) is associated with SGS stress $\tau(u_i,u_j)$, scalar flux $\tau(u_i,\phi_\alpha)$ and entropy flux $\tau(u_i,s)$, where $\tau(a,b) = \langle ab\rangle_L - \langle a\rangle_L\langle b\rangle_L$; in addition, the filtered chemical reaction source term (the last term on the RHS of Eq. (4)) and the entropy generation terms (the last four term on the RHS of Eq. (5)) appear in unclosed forms. For modeling of SGS stress tensor we employ the Modified Kinetic Energy Viscosity (MKEV) closure [17]. To represent the scalar and entropy flux terms we use the SGS diffusivity $\gamma_t = \nu_t/Sc_t$, where the SGS viscosity ν_t is described by MKEV and the turbulent Schmidt (and Prandtl) number is $Sc_t = 0.75$ [17].

The closure of chemical reaction source term and the entropy generation effects is provided by the En-FDF methodology, denoted by $\mathscr{F}_{en}(\widehat{\boldsymbol{\phi}},\widehat{s},\mathbf{x};t)$. The En-FDF contains complete statistical information about scalar and entropy fields and is formally defined as

$$\mathscr{F}_{en}\left(\widehat{\boldsymbol{\phi}},\widehat{s},\mathbf{x};t\right) = \int_{-\infty}^{+\infty} \rho(\mathbf{x}',t)\zeta\left[\widehat{\boldsymbol{\phi}},\widehat{s};\boldsymbol{\phi}(\mathbf{x}',t),s(\mathbf{x}',t)\right]G(\mathbf{x}'-\mathbf{x})d\mathbf{x}' \tag{6}$$

where

$$\zeta\left[\widehat{\boldsymbol{\phi}},\widehat{s};\boldsymbol{\phi}(\mathbf{x},t),s(\mathbf{x},t)\right] = \delta(\widehat{s}-s(\mathbf{x},t))\prod_{\alpha=1}^{N_s+1}\delta\left(\widehat{\phi}_\alpha-\phi_\alpha(\mathbf{x},t)\right) \tag{7}$$

is the fine-grained density [34] and δ denotes the Dirac delta function. The sample space variables $\widehat{\boldsymbol{\phi}}$ and $\widehat{s}$ correspond to scalar