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Entropy Transport Equation in Large Eddy Simulation for Exergy Analysis of Turbulent Combustion Systems

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Abstract: The transport equation of entropy is introduced in large eddy simulation to perform exergy analysis of turbulent combustion systems. The sources of exergy destruction can be evaluated by analyzing entropy generation terms, which appear in unclosed forms in this equation. The closure is based on the filtered density function (FDF) methodology. The primary advantage of FDF is that chemical reaction and its entropy generation effects appear in closed forms. This methodology involves a stochastic model, which is being developed to account for the subgrid scale transport of entropy.

1. Introduction

Combustion of fuels is still the world's main source of energy and this is projected to continue in the foreseeable future. Considering the limited fuel reserve and the environmental effects of combustion, it is thus of prime importance to enhance the thermal and combustion efficiencies of combustion systems. From the second law of thermodynamics, combustion efficiency is the "quality" at which the thermal energy is available in the hot products of combustion [1,2]. In conventional engineering, the main

concern is energy conversion without considering the exergy destruction. Analysis of exergy loss and entropy generation, which focuses on the optimal potential work done while bringing a system into equilibrium with an environment is an effective tool to investigate combustion efficiency and irreversibilities in combustion systems [2,3].

The exergy analysis has been the subject of widespread research [1–22]. The vast majority of contributions so far has been on exergy analysis of combustion systems with laminar flow regimes [3,5, 6,11,12,19,20]. Despite the prevalence of turbulence in practical combustion devices, the application of exergy analysis to turbulent reacting flows has been very limited [8,10,16,18]. These efforts mainly involve solution of Reynolds Averaged Navier-Stokes (RANS) equations, extended to include the transport of entropy [8,10,18]. Large eddy simulation (LES) is widely known to be the optimal means of capturing the detailed, unsteady physics of turbulent reacting flows [23–29]. It can thus be utilized as an effective tool to preform exergy analysis of turbulent combustion systems. The primary challenge in LES is the accurate modeling of the subgrid scale (SGS) quantities [25]. The Filtered Density Function (FDF) methodology has proven particularly effective for this purpose [23,30]. The FDF is essentially the counterpart of the Probability Density Function (PDF) method in RANS [23] and has the unique capability to account for chemical reaction and its entropy generation effects in an exact manner. The predictive capabilities of FDF is demonstrated by applying it to several flame geometries [31–33]. The most comprehensive form of FDF to date is the joint frequency-velocity-scalar FDF [34], which accounts for the joint SGS statistics of velocity, thermo-chemical compositions and turbulent frequency. [35] provides a recent review of the state of progress in LES via FDF. In the present study, the sources of exergy destruction are accounted for by analyzing the entropy generation terms in the entropy transport equation. This equation is considered in LES of turbulent reactive flows. The unclosed terms in this equation are all accounted for by the FDF, which is particularly advantageous in providing closed forms for chemical reaction and its entropy generation effects. An exact transport equation is developed here for the FDF, which is represented by a stochastic model. In Section 2, the entropy transport equation and the rate of exergy destruction are obtained from thermodynamic principles. Section 3 involves LES implementation of entropy transport equation and calculation of exergy loss in LES. In Section 4, an FDF methodology to account for the unclosed SGS terms in entropy transport equation is developed.

2.   Theoretical Foundation

The thermodynamic efficiency of a device or process can be assessed through the measure of the irreversibilities generated, which has widely been evaluated using the second law analysis. Practical energy conversion processes are always accompanied by an irreversible increase in entropy, which leads to a decrease in exergy (available energy). Thus, even though energy is conserved, exergy decreases because energy is converted into a different form, from which less work can be obtained. Reduced entropy generation results in more efficient use of available energy in combustion systems. Therefore, to improve the performance of these systems, exergy analysis is essential to explain the sources of exergy loss. The exergy balance equation reads as:

$$\frac{dE_x}{dt} = \dot{E}_{x_t} - \dot{E}_{x_D} \tag{1}$$

where E_x is the exergy and the term on the left hand side specifies the rate of change of exergy within the system. $\dot{E}_{x_t}$ is the rate of exergy transfer due to heat, work and flow interactions and $\dot{E}_{x_D}$ denotes the rate of exergy destruction due to irreversibility and can be expressed as:

$$\dot{E}_{x_D} = T_0 \, \dot{S}_g \tag{2}$$

where T_0 is the ambient (dead state) temperature and $\dot{S}_g$ is the rate of entropy generation due to irreversibilities which can be obtained from the transport of entropy, as described below.

In exothermic, chemically reacting, variable density flows, the primary transport variables are the fluid density $\rho(\mathbf{x}, t)$, the velocity vector $u_i(\mathbf{x}, t)$, $i = 1, 2, 3$ along the x_i direction, the specific enthalpy $h(\mathbf{x}, t)$, the pressure $p(\mathbf{x}, t)$, the mass fractions of N_s species, $Y_\alpha(\mathbf{x}, t)$ ($\alpha = 1, 2, \ldots, N_s$) and the entropy $s(\mathbf{x}, t)$, where $\mathbf{x} = x_i (i = 1, 2, 3)$ and t denote space and time, respectively. These variables satisfy the conservation equations of mass, momentum, energy and species mass fractions [36] as well as the transport of entropy, which follows the thermodynamic relation [37]

$$T \rho \frac{Ds}{Dt} = \rho \frac{De}{Dt} + p \rho \frac{Dv}{Dt} - \sum_{\alpha=1}^{N_s} \mu_\alpha \rho \frac{DY_\alpha}{Dt} \tag{3}$$

where T, e and v denote the temperature, internal energy and the specific volume, respectively. $D/Dt = \partial/\partial t + u_i \, \partial/\partial x_i$ denotes the material derivative. μ_α denotes the chemical potential (per unit mass of species α),

$$\mu_\alpha = h_\alpha - T \, s_\alpha^o \tag{4}$$

in which,

$$s_\alpha^o = \frac{1}{M_\alpha} \left(\frac{\partial S}{\partial n_\alpha} \right)_{T, p, n_\beta \ (\beta \neq \alpha)} \tag{5}$$

is the partial entropy, n_α and M_α are the number of moles and molecular mass of species α, respectively. S denotes the (extensive) entropy,

$$S = m \, s = m \sum_{\alpha=1}^{N_s} Y_\alpha \, s_\alpha^o, \tag{6}$$

where m is the total mass. For an ideal gas, the partial entropy can be expressed in terms of entropy of pure substance as:

$$s_\alpha^o = s_\alpha - R_\alpha \, ln X_\alpha \tag{7}$$

In this equation, s_α denotes the entropy of pure species α, X_α denotes the mole fraction of species α and R_α is the gas constant for species α ($R_\alpha = R_u/M_\alpha$ and R_u is the universal gas constant). In Equation (4), h_α is the enthalpy of species α,

$$h_\alpha = h_\alpha^0 + \int_{T_r}^{T} c_{p_\alpha}(T')dT' \tag{8}$$

in which h_α^0 denotes the enthalpy of species α at reference temperature T_r and c_{p_α} represents specific heat at constant pressure for species α. By substituting for De/Dt and DY_α/Dt from conservation equations of energy and chemical species mass fraction [24], we obtain a transport equation for entropy,

$$\frac{\partial \rho\, s}{\partial t} + \frac{\partial \rho\, u_i s}{\partial x_i} = \frac{1}{T}\left[\tau_{ij}\frac{\partial u_i}{\partial x_j} - \frac{\partial \dot{q}_i}{\partial x_i} + \sum_{\alpha=1}^{N_s}\mu_\alpha\frac{\partial J_i^\alpha}{\partial x_i} - \sum_{\alpha=1}^{N_s}\rho\mu_\alpha S_{\omega_\alpha}\right] \tag{9}$$

In this equation, τ_{ij} and J_i^α denote the viscous stress tensor and the scalar fluxes, respectively. Assuming a Newtonian fluid and Fick's law of diffusion, these are represented as

$$\tau_{ij} = \mu\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} - \frac{2}{3}\frac{\partial u_k}{\partial x_k}\,\delta_{ij}\right) \tag{10}$$

$$J_i^\alpha = -\gamma_\alpha\frac{\partial Y_\alpha}{\partial x_i} \tag{11}$$

where μ is the molecular viscosity and γ_α denotes the mass molecular diffusivity of species α. In Equation (9), S_{ω_α} is a source term due to chemical reaction, defined as

$$S_{\omega_\alpha} = \frac{1}{\rho}M_\alpha\dot{\omega}_\alpha \tag{12}$$

where $\dot{\omega}_\alpha$ is the molar rate of production/destruction of species α due to chemical reaction. Also in Equation (9), $\dot{q}_i$ is the energy flux term, expressed as

$$\begin{aligned}
\dot{q}_i &= -\lambda\frac{\partial T}{\partial x_i} + \sum_{\alpha=1}^{N_s}h_\alpha J_i^\alpha \\
&= -\lambda\frac{\partial T}{\partial x_i} - \sum_{\alpha=1}^{N_s}\gamma_\alpha\,h_\alpha\frac{\partial Y_\alpha}{\partial x_i}
\end{aligned} \tag{13}$$

where the rate of heat transfer by radiation is neglected. In this equation λ denotes the thermal conductivity. The entropy transport equation, Equation (9), can be written in a form consistent with that in [37],

$$\begin{aligned}
\frac{\partial \rho\, s}{\partial t} + \frac{\partial \rho\, u_i s}{\partial x_i} = \frac{1}{T}&\left[\tau_{ij}\frac{\partial u_i}{\partial x_j} - \frac{1}{T}(\dot{q}_i - \sum_{\alpha=1}^{N_s}h_\alpha J_i^\alpha)\frac{\partial T}{\partial x_i} - \sum_{\alpha=1}^{N_s}\rho\mu_\alpha S_{\omega_\alpha} - \underbrace{\sum_{\alpha=1}^{N_s}J_i^\alpha\left(\frac{\partial \mu_\alpha}{\partial x_i} + s_\alpha^o\frac{\partial T}{\partial x_i}\right)}_{IV}\right] \\
&-\underbrace{\frac{\partial}{\partial x_i}\left[\frac{1}{T}(\dot{q}_i - \sum_{\alpha=1}^{N_s}h_\alpha J_i^\alpha) + \sum_{\alpha=1}^{N_s}s_\alpha^o J_i^\alpha\right]}_{V}
\end{aligned} \tag{14}$$

Utilizing Equation (8), the term IV on the right hand side (RHS) of this equation can be expressed as:

$$-\sum_{\alpha=1}^{N_s} \frac{J_i^\alpha}{T} \left(\frac{\partial \mu_\alpha}{\partial x_i} + s_\alpha^o \frac{\partial T}{\partial x_i} \right) = -\sum_{\alpha=1}^{N_s} \frac{J_i^\alpha}{T} \left(c_{p_\alpha} \frac{\partial T}{\partial x_i} - T \frac{\partial s_\alpha^o}{\partial x_i} \right) \tag{15}$$

For an ideal gas, taking derivative of Equation (7) results in,

$$\frac{\partial s_\alpha^o}{\partial x_i} = \frac{1}{T} c_{p_\alpha} \frac{\partial T}{\partial x_i} - \frac{R_\alpha}{Y_\alpha} \frac{\partial Y_\alpha}{\partial x_i} + \frac{R_\alpha}{n} \frac{\partial n}{\partial x_i} - \overbrace{\frac{R_\alpha}{p} \frac{\partial p}{\partial x_i}}^{\approx 0} \tag{16}$$

where the last term can be neglected in low Mach number combustion processes [10,23,38]. By employing Equation (16), the term IV in Equation (14) can thus be written as:

$$-\sum_{\alpha=1}^{N_s} \frac{J_i^\alpha}{T} \left(\frac{\partial \mu_\alpha}{\partial x_i} + s_\alpha^o \frac{\partial T}{\partial x_i} \right) = -\sum_{\alpha=1}^{N_s} R_\alpha J_i^\alpha \left(\frac{1}{Y_\alpha} \frac{\partial Y_\alpha}{\partial x_i} - \frac{1}{n} \frac{\partial n}{\partial x_i} \right) \tag{17}$$

In Equation (14), the term V can be further simplified by using Equations (11, 13) as:

$$-\frac{\partial}{\partial x_i} \left[\frac{1}{T} (\dot{q}_i - \sum_{\alpha=1}^{N_s} h_\alpha J_i^\alpha) + \sum_{\alpha=1}^{N_s} s_\alpha^o J_i^\alpha \right] = \frac{\partial}{\partial x_i} \left[\frac{\lambda}{T} \frac{\partial T}{\partial x_i} + \sum_{\alpha=1}^{N_s} \gamma_\alpha s_\alpha^o \frac{\partial Y_\alpha}{\partial x_i} \right] \tag{18}$$

This equation can further be simplified by employing Equation (16) and assuming equal mass diffusivity for all species ($\gamma_\alpha = \gamma$, $\alpha = 1, \ldots, N_s$) and unity Lewis number ($Le = \lambda/(\gamma \, c_p) = 1$, where $c_p = \sum_{\alpha=1}^{N_s} c_{p_\alpha} Y_\alpha$). Therefore, the term V in Equation (14) reduces to diffusion of entropy:

$$-\frac{\partial}{\partial x_i} \left[\frac{1}{T} (\dot{q}_i - \sum_{\alpha=1}^{N_s} h_\alpha J_i^\alpha) + \sum_{\alpha=1}^{N_s} s_\alpha^o J_i^\alpha \right] = \frac{\partial}{\partial x_i} \left(\gamma \frac{\partial s}{\partial x_i} \right) \tag{19}$$

By substituting Equations (17, 19) into Equation (14), another useful form of entropy transport equation can be obtained,

$$\frac{\partial \rho s}{\partial t} + \frac{\partial \rho \, u_i s}{\partial x_i} = \frac{\partial}{\partial x_i} \left(\gamma \frac{\partial s}{\partial x_i} \right) + \frac{1}{T} \tau_{ij} \frac{\partial u_i}{\partial x_j} - \frac{\rho}{T} \sum_{\alpha=1}^{N_s} \mu_\alpha S_{\omega_\alpha} + \frac{\lambda}{T^2} \frac{\partial T}{\partial x_i} \frac{\partial T}{\partial x_i}$$
$$+ \sum_{\alpha=1}^{N_s} \gamma R_\alpha \frac{1}{Y_\alpha} \frac{\partial Y_\alpha}{\partial x_i} \frac{\partial Y_\alpha}{\partial x_i} - \sum_{\alpha=1}^{N_s} \gamma R_\alpha \frac{1}{n} \frac{\partial Y_\alpha}{\partial x_i} \frac{\partial n}{\partial x_i} \tag{20}$$

In this equation, the last five terms on the RHS constitute the volumetric rate of generation of entropy $\dot{S}'''_g$. Therefore,

$$\dot{S}'''_g = \frac{1}{T} \tau_{ij} \frac{\partial u_i}{\partial x_j} - \frac{\rho}{T} \sum_{\alpha=1}^{N_s} \mu_\alpha S_{\omega_\alpha} + \frac{\lambda}{T^2} \frac{\partial T}{\partial x_i} \frac{\partial T}{\partial x_i} + \sum_{\alpha=1}^{N_s} \gamma R_\alpha \frac{1}{Y_\alpha} \frac{\partial Y_\alpha}{\partial x_i} \frac{\partial Y_\alpha}{\partial x_i} - \sum_{\alpha=1}^{N_s} \gamma R_\alpha \frac{1}{n} \frac{\partial Y_\alpha}{\partial x_i} \frac{\partial n}{\partial x_i} \tag{21}$$

As this equation demonstrates, the irreversible processes involved in entropy generation are: viscous dissipation, chemical reaction, heat conduction, mass transfer due to change in mass fraction of

individual species and mass transfer due to change in total number of moles. Similar transport equations are considered in [10,18] to perform exergy analysis of turbulent diffusion flames via RANS. Due to capacity of LES to predict instantaneous flow characteristics and resolve turbulent flow structures, in this work the entropy transport is implemented in LES to facilitate more accurate prediction of exergy losses in turbulent reactive flows.

3. Entropy Transport in Large Eddy Simulation

We consider LES implementation of entropy transport equation along with conservation equations of mass, momentum, energy and species mass fractions. LES involves the spatial filtering operation [23,39,40]

$$\langle Q(\mathbf{x},t) \rangle = \int_{-\infty}^{+\infty} Q(\mathbf{x}',t)\mathcal{G}(\mathbf{x}',\mathbf{x})d\mathbf{x}' \tag{22}$$

where $\mathcal{G}$ denotes the filter function of width $\Delta_{\mathcal{G}}$, and $\langle Q(\mathbf{x},t) \rangle$ represents the filtered value of the transport variable $Q(\mathbf{x},t)$. In reacting flows, it is convenient to consider the Favre filtered quantity, $\langle Q(\mathbf{x},t) \rangle_L = \langle \rho\, Q \rangle / \langle \rho \rangle$. We consider spatially invariant and localized filter functions, $\mathcal{G}(\mathbf{x}',\mathbf{x}) \equiv \mathcal{G}(\mathbf{x}'-\mathbf{x})$ with the properties [41] $\mathcal{G}(\mathbf{x}) = \mathcal{G}(-\mathbf{x})$, and $\int_{-\infty}^{\infty} \mathcal{G}(\mathbf{x})d\mathbf{x} = 1$. We consider "positive" filter functions [42] for which all the moments $\int_{-\infty}^{\infty} x^m \mathcal{G}(x)dx$ exist for $m \geq 0$. The filtered variables satisfy the filtered form of conservation equations of mass, momentum, energy and species mass fractions [43] as well as entropy transport equation. This equation is obtained by filtering Equation (20) according to Equation (22) as

$$\frac{\partial \langle \rho \rangle \langle s \rangle_L}{\partial t} + \frac{\partial \langle \rho \rangle \langle u_i \rangle_L \langle s \rangle_L}{\partial x_i} = \frac{\partial}{\partial x_i}\left(\gamma \frac{\partial \langle s \rangle_L}{\partial x_i} \right) - \frac{\partial \langle \rho \rangle \tau(u_i,s)}{\partial x_i} + \left\langle \dot{S}'''_g \right\rangle \tag{23}$$

where

$$\tau(a,b) = \langle a\, b \rangle_L - \langle a \rangle_L \langle b \rangle_L \tag{24}$$

denotes the second-order SGS correlations. The last two terms on the RHS of Equation (23), representing the SGS entropy flux and the filtered volumetric rate of entropy generation, are unclosed. The filtered entropy generation term can be expressed as the filtered form of individual irreversible processes, according to Equation (21):

$$\begin{aligned}
\left\langle \dot{S}'''_g \right\rangle = {} & \left\langle \frac{1}{T}\tau_{ij}\frac{\partial u_i}{\partial x_j} \right\rangle - \left\langle \frac{\rho}{T}\sum_{\alpha=1}^{N_s}\mu_\alpha S_{\omega_\alpha} \right\rangle + \left\langle \frac{\lambda}{T^2}\frac{\partial T}{\partial x_i}\frac{\partial T}{\partial x_i} \right\rangle + \left\langle \sum_{\alpha=1}^{N_s}\gamma R_\alpha \frac{1}{Y_\alpha}\frac{\partial Y_\alpha}{\partial x_i}\frac{\partial Y_\alpha}{\partial x_i} \right\rangle \\
& - \left\langle \sum_{\alpha=1}^{N_s}\gamma R_\alpha \frac{1}{n}\frac{\partial Y_\alpha}{\partial x_i}\frac{\partial n}{\partial x_i} \right\rangle
\end{aligned} \tag{25}$$

These terms are all accounted for by the methodology described in the next section. By calculating the filtered entropy generation term, the filtered rate of exergy destruction can consequently be obtained according to Equation (2).

4. The Filtered Density Function Methodology

In this section, the filtered density function (FDF) methodology is developed to account for the unclosed terms in the entropy transport equation. This methodology contains the complete statistical information about the joint SGS variation of velocity, scalar, frequency and entropy fields [30,34]. This form of FDF, denoted by $\mathcal{F}(\boldsymbol{v}, \boldsymbol{\psi}, \theta, r, \mathbf{x}; t)$, is defined by

$$\mathcal{F}(\boldsymbol{v}, \boldsymbol{\psi}, \theta, r, \mathbf{x}; t) = \int_{-\infty}^{+\infty} \rho(\mathbf{x}', t)\, \xi\left[\boldsymbol{v}, \boldsymbol{\psi}, \theta, r\, ; \boldsymbol{u}(\mathbf{x}', t), \boldsymbol{\phi}(\mathbf{x}', t), \omega(\mathbf{x}', t), s(\mathbf{x}', t)\right] \mathcal{G}(\mathbf{x}' - \mathbf{x}) d\mathbf{x}'$$

(26)

where

$$\xi\left[\boldsymbol{v}, \boldsymbol{\psi}, \theta, r\, ; \boldsymbol{u}(\mathbf{x}, t), \boldsymbol{\phi}(\mathbf{x}, t), \omega(\mathbf{x}, t), s(\mathbf{x}, t)\right] =$$
$$\delta\left(r - s(\mathbf{x}, t)\right) \delta\left(\theta - \omega(\mathbf{x}, t)\right) \times \prod_{i=1}^{3} \delta\left(v_i - u_i(\mathbf{x}, t)\right) \prod_{\alpha=1}^{N_s+1} \delta\left(\psi_\alpha - \phi_\alpha(\mathbf{x}, t)\right)$$

(27)

is the "fine-grained" density [23,44,45] and δ denotes the Dirac delta function. The sample space variables $\boldsymbol{v}$, $\boldsymbol{\psi}$, θ and r correspond to the velocity $\boldsymbol{u}(\mathbf{x}, t)$, the scalar array $\boldsymbol{\phi}(\mathbf{x}, t) = [Y_1, \ldots, Y_{N_s}, h]$, the SGS frequency $\omega(\mathbf{x}, t)$ and the entropy $s(\mathbf{x}, t)$, respectively. Following the procedure detailed in [34,43,46], the FDF satisfies an *exact* transport equation,

$$\frac{\partial \mathcal{F}}{\partial t} + \frac{\partial (v_i \mathcal{F})}{\partial x_i} = -\sum_{\alpha=1}^{N_s} \frac{\partial}{\partial \psi_\alpha} [S_{\omega_\alpha}(\boldsymbol{\psi})\mathcal{F}] + \frac{\partial}{\partial r}\left[\frac{1}{T}\sum_{\alpha=1}^{N_s} \mu_\alpha(\boldsymbol{\psi}) S_{\omega_\alpha}(\boldsymbol{\psi})\mathcal{F}\right]$$
$$+ \frac{\partial}{\partial v_i}\left[\left\langle \frac{1}{\rho}\frac{\partial p}{\partial x_i} \,\Big|\, \boldsymbol{v}, \boldsymbol{\psi}, \theta, r \right\rangle \mathcal{F}\right] - \frac{\partial}{\partial v_i}\left[\left\langle \frac{1}{\rho}\frac{\partial \tau_{ij}}{\partial x_j} \,\Big|\, \boldsymbol{v}, \boldsymbol{\psi}, \theta, r \right\rangle \mathcal{F}\right]$$
$$+ \sum_{\alpha=1}^{N_s} \frac{\partial}{\partial \psi_\alpha}\left[\left\langle \frac{1}{\rho}\frac{\partial J_i^\alpha}{\partial x_i} \,\Big|\, \boldsymbol{v}, \boldsymbol{\psi}, \theta, r \right\rangle \mathcal{F}\right] - \frac{\partial}{\partial \theta}\left[\left\langle \frac{D\omega}{Dt} \,\Big|\, \boldsymbol{v}, \boldsymbol{\psi}, \theta, r \right\rangle \mathcal{F}\right]$$
$$- \frac{\partial}{\partial r}\left[\left\langle \frac{1}{\rho}\frac{\partial}{\partial x_i}\left(\gamma \frac{\partial s}{\partial x_i}\right) \,\Big|\, \boldsymbol{v}, \boldsymbol{\psi}, \theta, r \right\rangle \mathcal{F}\right]$$
$$- \frac{\partial}{\partial r}\left[\left\langle \frac{1}{\rho T}\tau_{ij}\frac{\partial u_i}{\partial x_j} \,\Big|\, \boldsymbol{v}, \boldsymbol{\psi}, \theta, r \right\rangle \mathcal{F}\right] - \frac{\partial}{\partial r}\left[\left\langle \frac{\lambda}{\rho T^2}\frac{\partial T}{\partial x_i}\frac{\partial T}{\partial x_i} \,\Big|\, \boldsymbol{v}, \boldsymbol{\psi}, \theta, r \right\rangle \mathcal{F}\right]$$
$$- \frac{\partial}{\partial r}\left[\left\langle \frac{1}{\rho}\sum_{\alpha=1}^{N_s} \gamma R_\alpha \frac{1}{Y_\alpha}\frac{\partial Y_\alpha}{\partial x_i}\frac{\partial Y_\alpha}{\partial x_i} \,\Big|\, \boldsymbol{v}, \boldsymbol{\psi}, \theta, r \right\rangle \mathcal{F}\right] + \frac{\partial}{\partial r}\left[\left\langle \frac{1}{\rho}\sum_{\alpha=1}^{N_s} \gamma R_\alpha \frac{1}{n}\frac{\partial Y_\alpha}{\partial x_i}\frac{\partial n}{\partial x_i} \,\Big|\, \boldsymbol{v}, \boldsymbol{\psi}, \theta, r \right\rangle \mathcal{F}\right]$$

(28)

where $\left\langle\, \big|\, \right\rangle$ denotes the "conditional" filtered values. As this equation shows, the effects of SGS convection (the second term on the left hand side), combustion (the first term on the RHS) and the entropy generation due to combustion (the second term on the RHS) are all in closed forms. However,

all of the terms involving conditional filtered values require closures. The filtered value of any function $\hat{Q}$ of the velocity, scalar, frequency and/or entropy is calculated by

$$\langle \rho(\mathbf{x},t) \rangle \langle Q(\mathbf{x},t) \rangle_L = \int_{-\infty}^{+\infty} \hat{Q}(\boldsymbol{v},\boldsymbol{\psi},\theta,r)\mathcal{F}(\boldsymbol{v},\boldsymbol{\psi},\theta,r,\mathbf{x};t)\,d\boldsymbol{v}\,d\boldsymbol{\psi}\,d\theta\,dr \tag{29}$$

The unclosed terms in Equation (28) are modeled by a stochastic model which is in the form of coupled stochastic differential equations (SDE). In [34,43,46] the SDEs corresponding to position, velocity, scalar and SGS frequency are constructed. To account for the unclosed terms in the entropy transport equation in this work, the system of SDEs is supplemented with a SDE for entropy, which is currently under development. This SDE follows the thermodynamic laws and has the general form of a diffusion process [47],

$$ds^+(t) = D(\mathbf{X}^+, \mathbf{U}^+, \boldsymbol{\phi}^+, s^+, \omega^+; t)\,dt + B_j(\mathbf{X}^+, \mathbf{U}^+, \boldsymbol{\phi}^+, s^+, \omega^+; t)\,dW_j(t) \tag{30}$$

where $\mathbf{X}^+$, $\boldsymbol{U}^+$, $\boldsymbol{\phi}^+$, ω^+ and s^+ are probabilistic representations of position, velocity vector, scalar array, frequency and entropy, respectively. The D and B terms denote the drift and diffusion coefficients, respectively. The W term represents the Wiener-Lévy processes [48,49]. The system of SDEs models the FDF transport equation (Equation (28)) at the level of one-point one-time statistics and is solved by a Lagrangian Monte Carlo (MC) procedure [43]. Similar to previous FDF simulations [34,43,46,50,51], a hybrid Eulerian/Langrangian numerical solution procedure is being developed in which a Lagrangian setting is used to solve the SDEs. In the Eulerian part, the physical domain is discretized and the filtered continuity, momentum and scalar transport equations are solved via finite difference (FD) or finite volume (FV) methods. The FDF is represented by an ensemble of MC particles. Each of these particles carry information pertaining to the physical field (*i.e.* all of the FDF variables) and also the position vector. These variables are updated via temporal integration of the modeled SDEs.

5. Conclusions

The transport of entropy is introduced in large eddy simulation (LES) to perform more accurate exergy analysis of turbulent combustion systems. The filtered entropy transport equation includes several unclosed terms which represent the effects of entropy generation (exergy destruction). These terms are due to subgrid scale (SGS) viscous dissipation, heat conduction, mass transfer and chemical reaction. A novel methodology based on filtered density function (FDF) is developed for the closure of filtered entropy transport equation. In this methodology, the effects of chemical reaction and its entropy generation contribution appear in closed forms. An exact transport equation is derived for the FDF which is further modeled by a set of stochastic differential equations.

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