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SCALE-INVARIANT FORMS OF CONSERVATION EQUATIONS IN REACTIVE FIELDS AND A MODIFIED HYDRO-THERMO-DIFFUSIVE THEORY OF LAMINAR FLAMES

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ABSTRACT

A scale-invariant model of statistical mechanics is applied to present invariant forms of mass, energy, linear, and angular momentum conservation equations in reactive fields. The resulting conservation equations at molecular-dynamic scale are solved by the method of large activation energy asymptotics to describe the hydro-thermo-diffusive structure of laminar premixed flames. The predicted temperature and velocity profiles are in agreement with the observations. Also, with realistic physico-chemical properties and chemical-kinetic parameters for a single-step overall combustion of stoichiometric methane-air premixed flame, the laminar flame propagation velocity of 42.1 cm/s is calculated in agreement with the experimental value.

1. INTRODUCTION

The universality of turbulent phenomena from stochastic quantum fields to classical hydrodynamic fields resulted in recent introduction of a scale-invariant model of statistical mechanics and its application to the field of thermodynamics [4]. The implications of the model to the study of transport phenomena and invariant forms of conservation equations have also been addressed [5]. In the present study, the invariant forms of the conservation equations are described and the results are employed to introduce a modified hydro-thermo-diffusive theory of laminar premixed flames.

2. A SCALE-INVARIANT MODEL OF STATISTICAL MECHANICS

Following the classical methods [1-3], the invariant definitions of the density ρ_β, and the velocity of *atom* $\mathbf{u}_\beta$, *element* $\mathbf{v}_\beta$, and *system* $\mathbf{w}_\beta$ at the scale β are given as [4]

$$\rho_\beta = n_\beta m_\beta = m_\beta \int f_\beta d\mathbf{u}_\beta \quad , \quad \mathbf{u}_\beta = \mathbf{v}_{\beta-1} \quad , \quad \mathbf{v}_\beta = \rho_\beta^{-1} m_\beta \int \mathbf{u}_\beta f_\beta d\mathbf{u}_\beta \quad , \quad \mathbf{w}_\beta = \mathbf{v}_{\beta+1} \qquad (2.1)$$

The scale-invariant model of statistical mechanics for equilibrium fields of . . . eddy-, cluster-, molecular-, atomic-dynamics . . . at the scale β = e, c, m, a, and the corresponding *non-equilibrium* laminar flow fields are schematically shown in Fig.1. Each statistical field, described by a distribution function $f_\beta(\mathbf{u}_\beta) = f_\beta(\mathbf{r}_\beta, \mathbf{u}_\beta, t_\beta)\, d\mathbf{r}_\beta d\mathbf{u}_\beta$, defines a "system" that is composed of an ensemble of "elements", each element is composed of an ensemble of small particles viewed as *point-mass* "atoms". The element (system) of the smaller scale (β) becomes the atom (element) of the larger scale ($\beta+1$). The three length scales associated with the atom, the element, and the system at any scale β are ($l_\beta = \lambda_{\beta-1}, \lambda_\beta, L_\beta = \lambda_{\beta+1}$) where $\lambda_\beta = <l^2_\beta>^{1/2}$ is mean-free-path of the atoms [5].

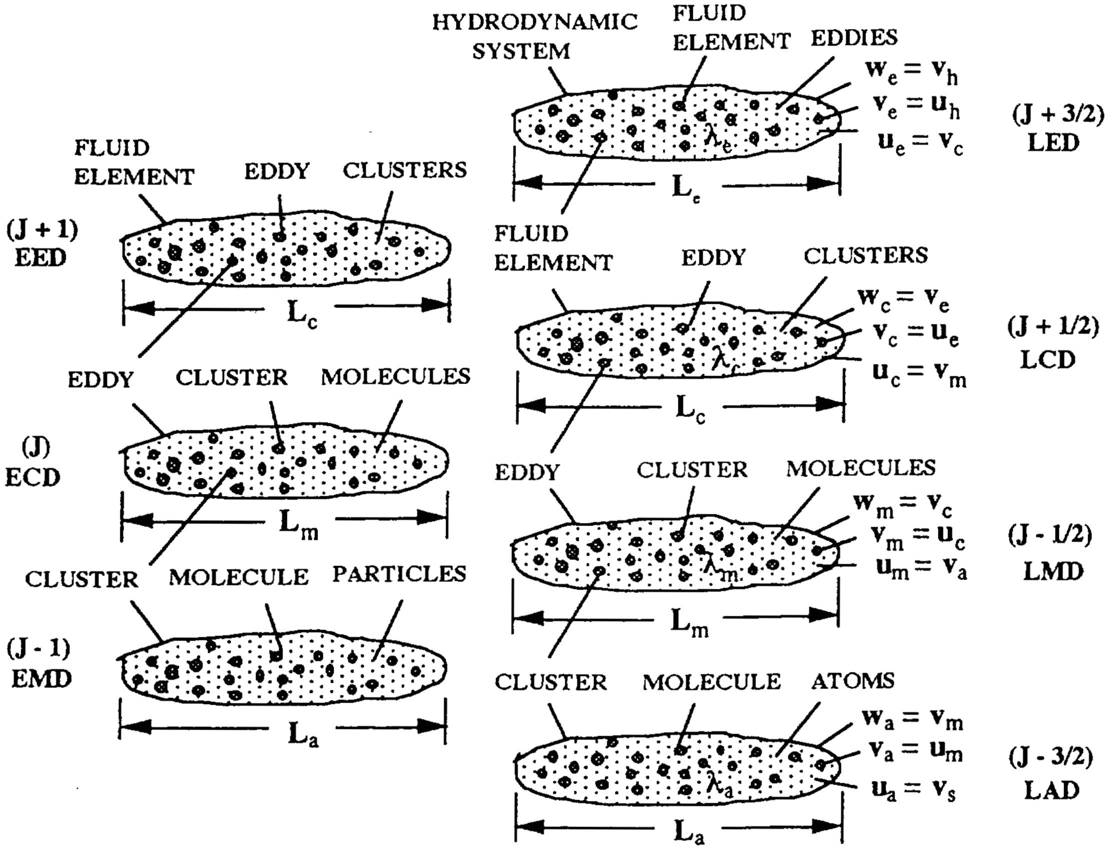

Fig.1 Hierarchy of statistical fields for equilibrium eddy-, cluster-, and molecular-dynamic scales and the associated laminar flow fields.

The invariant definitions of the peculiar and the diffusion velocities have been introduced as [4]

$$\mathbf{V'}_\beta = \mathbf{u}_\beta - \mathbf{v}_\beta \quad , \quad \mathbf{V}_\beta = \mathbf{v}_\beta - \mathbf{w}_\beta \tag{2.2}$$

such that

$$\mathbf{V}_\beta = \mathbf{V'}_{\beta+1} \tag{2.3}$$

The above definitions are applied to introduce the invariant definitions of equilibrium and non-equilibrium thermodynamic translational temperature and pressure as [4]

$$3kT_\beta = m_\beta \langle u_\beta^2 \rangle \quad , \quad P_\beta = \rho_\beta \langle u_\beta^2 \rangle /3 \tag{2.4}$$

and

$$3k\mathbb{T}_\beta = m_\beta \langle V'^2_\beta \rangle \quad , \quad \mathbb{P}_\beta = n_\beta m_\beta \langle V'^2_\beta \rangle /3 \tag{2.5}$$

leading to the corresponding *invariant ideal "gas" laws* [4]

$$P_\beta V = N_\beta k T_\beta \qquad \text{and} \qquad \mathbb{P}_\beta V = N_\beta k \mathbb{T}_\beta \tag{2.6}$$

3. SCALE-INVARIANT FORM OF THE CONSERVATION EQUATIONS FOR CHEMICALLY REACTIVE FIELDS

Following the classical methods [1-3], the scale-invariant forms of mass, thermal energy, linear and angular momentum conservation equations [5] at scale β are given as

$$\frac{\partial \rho_\beta}{\partial t} + \nabla . (\rho_\beta \mathbf{v}_\beta) = \Omega_\beta \tag{3.1}$$

$$\frac{\partial \varepsilon_\beta}{\partial t} + \nabla . (\varepsilon_\beta \mathbf{v}_\beta) = 0 \tag{3.2}$$

$$\frac{\partial \mathbf{p}_\beta}{\partial t} + \nabla . (\mathbf{p}_\beta \mathbf{v}_\beta) = 0 \tag{3.3}$$

$$\frac{\partial \pi_\beta}{\partial t} + \nabla . (\pi_\beta \mathbf{v}_\beta) = 0 \tag{3.4}$$

where $\varepsilon_\beta = \rho_\beta h_\beta$, $\mathbf{p}_\beta = \rho_\beta \mathbf{v}_\beta$, and $\pi_\beta = \rho_\beta \omega_\beta$ are the *volumetric density* of thermal energy, linear and angular momentum of the field, respectively and $\omega_\beta = \nabla \times \mathbf{v}_\beta$ is the vorticity. Also, Ω_β is the chemical reaction rate, and h_β is the absolute enthalpy [5].

The local velocity $\mathbf{v}_\beta$ in (3.1)-(3.4) is expressed as the sum of convective $\mathbf{w}_\beta = \langle \mathbf{v}_\beta \rangle$ and diffusive velocities [5]

$$\mathbf{v}_\beta = \mathbf{w}_\beta + \mathbf{V}_{\beta g} \quad , \quad \mathbf{V}_{\beta g} = -D_\beta \nabla \ln(\rho_\beta) \tag{3.5a}$$

$$\mathbf{v}_\beta = \mathbf{w}_\beta + \mathbf{V}_{\beta tg} \quad , \quad \mathbf{V}_{\beta tg} = -\alpha_\beta \nabla \ln(\varepsilon_\beta) \tag{3.5b}$$

$$\mathbf{v}_\beta = \mathbf{w}_\beta + \mathbf{V}_{\beta hg} \quad , \quad \mathbf{V}_{\beta hg} = -\nu_\beta \nabla \ln(\mathbf{p}_\beta) \tag{3.5c}$$

$$\mathbf{v}_\beta = \mathbf{w}_\beta + \mathbf{V}_{\beta rhg} \quad , \quad \mathbf{V}_{\beta rhg} = -\nu_\beta \nabla \ln(\pi_\beta) \tag{3.5d}$$

where ($\mathbf{V}_{\beta g}$, $\mathbf{V}_{\beta tg}$, $\mathbf{V}_{\beta hg}$, $\mathbf{V}_{\beta rhg}$) are respectively the diffusive, the thermo-diffusive, the linear hydro-diffusive, and the angular hydro-diffusive velocities. For unity Schmidt and Prandtl numbers $Sc_\beta = Pr_\beta = \nu_\beta / D_\beta = \nu_\beta / \alpha_\beta = 1$, one may express

$$\mathbf{V}_{\beta tg} = \mathbf{V}_{\beta g} + \mathbf{V}_{\beta t}$$
$$\mathbf{V}_{\beta hg} = \mathbf{V}_{\beta g} + \mathbf{V}_{\beta h}$$
$$\mathbf{V}_{\beta rhg} = \mathbf{V}_{\beta g} + \mathbf{V}_{\beta rh}$$

that involve the thermal $\mathbf{V}_{\beta t}$, the linear (translational) hydrodynamic $\mathbf{V}_{\beta h}$, and the angular (rotational) hydrodynamic $\mathbf{V}_{\beta rh}$ diffusion velocities defined as [5]

$$\mathbf{V}_{\beta t} = -\alpha_\beta \nabla \ln(h_\beta) \tag{3.6a}$$
$$\mathbf{V}_{\beta h} = -\nu_\beta \nabla \ln(\mathbf{v}_\beta) \tag{3.6b}$$
$$\mathbf{V}_{\beta rh} = -\nu_\beta \nabla \ln(\omega_\beta) \tag{3.6c}$$

Since for an ideal gas $h_\beta = c_{p\beta}T_\beta$, when $c_{p\beta}$ is constant and $T = T_\beta$, Eq.(3.6a) reduces to the *Fourier* law of heat conduction

$$q = \rho h_\beta \mathbf{V}_{\beta t} = -\kappa_\beta \nabla T \tag{3.7}$$

where κ_β and $\alpha_\beta = \kappa_\beta/(\rho_\beta c_{p\beta})$ are the thermal conductivity and diffusivity. Similarly, (3.6b) may be identified as the shear stress associated with diffusional flux of linear momentum and expressed by the generalized *Newton* law of viscosity [5]

$$\tau_{ij\beta} = \rho_\beta v_{j\beta} \mathbf{V}_{ij\beta h} = -\mu_\beta \nabla \mathbf{v}_\beta = -\mu_\beta \partial v_{j\beta}/\partial x_i \tag{3.8}$$

Finally, (3.6c) may be identified as the shear stress induced by diffusional flux of angular momentum (torsional stress) and expressed as

$$\tau_{ijr\beta} = \rho_\beta \omega_{j\beta} \mathbf{V}_{ij\beta rh} = -\mu_\beta \nabla \omega_\beta = -\mu_\beta \partial \omega_{j\beta}/\partial x_i \tag{3.9}$$

Substitutions from (3.5a)-(3.5d) into (3.1)-(3.4), neglecting cross-diffusion terms and assuming constant transport coefficients with $Sc_\beta = Pr_\beta = 1$, result in

$$\frac{\partial \rho_\beta}{\partial t} + \mathbf{w}_\beta \cdot \nabla \rho_\beta - D_\beta \nabla^2 \rho_\beta = \Omega_\beta \tag{3.10}$$

$$h_\beta \left[\frac{\partial \rho_\beta}{\partial t} + \mathbf{w}_\beta \cdot \nabla \rho_\beta - D_\beta \nabla^2 \rho_\beta \right] + \rho_\beta \left[\frac{\partial h_\beta}{\partial t} + \mathbf{w}_\beta \cdot \nabla h_\beta - \alpha_\beta \nabla^2 h_\beta \right] = 0 \tag{3.11}$$

$$\mathbf{v}_\beta \left[\frac{\partial \rho_\beta}{\partial t} + \mathbf{w}_\beta \cdot \nabla \rho_\beta - D_\beta \nabla^2 \rho_\beta \right] + \rho_\beta \left[\frac{\partial \mathbf{v}_\beta}{\partial t} + \mathbf{w}_\beta \cdot \nabla \mathbf{v}_\beta - \nu_\beta \nabla^2 \mathbf{v}_\beta \right] = 0 \tag{3.12}$$

$$\omega_\beta \left[\frac{\partial \rho_\beta}{\partial t} + \mathbf{w}_\beta \cdot \nabla \rho_\beta - D_\beta \nabla^2 \rho_\beta \right] + \rho_\beta \left[\frac{\partial \omega_\beta}{\partial t} + \mathbf{w}_\beta \cdot \nabla \omega_\beta + \omega_\beta \cdot \nabla \mathbf{w}_\beta - \nu_\beta \nabla^2 \omega_\beta \right] = 0 \tag{3.13}$$

The above forms of the conservation equations perhaps help to better reveal the coupling between the gravitational versus the inertial contributions to total energy and momentum densities of the field. Except for possible externally imposed sources, ε_β, $\mathbf{p}_\beta$ and π_β have no *internal sources* as reflected in (3.2)-(3.4). However, in the presence of chemical reactions the loss of gravitational mass could result in the production of inertial thermal energy, or linear and angular momenta. For example, the first and the second parts of (3.11) respectively correspond to the *gravitational* and the *thermal* contributions to the total energy density of the field. For instance, the loss of gravitational mass induced by chemical reaction in the body of a person results in the generation of thermal energy (heat) in this persons body. Similarly, the first and the second parts of (3.12) respectively correspond to the *gravitational* and the *inertial* contributions to the total linear momentum density of the field. Now, one considers a stationary person with no initial linear momentum that suddenly starts to run, thus producing substantial linear momentum without the action of any *external forces*. In this case, there is no violation of the conservation of momentum, but rather because of chemical reactions in the body of such a person, the first part of (3.12) changes thus leading to a compensating change in the second part. Finally, the first and the second parts of (3.13) respectively correspond to the *gravitational* and the *inertial* contributions to the total angular momentum density of the field. For example, (3.13) may be used to describe the change of angular velocity of a ballet dancer. Here, the loss of mass by chemical reactions in the body of a spinning dancer that pulls the arms inwards, thus doing work against centrifugal forces, leads to an increase in the dancer's angular momentum. Because of the large value of the velocity of light c in $E = mc^2$, the actual loss of gravitational mass in the above examples will be exceedingly small.

Substitutions from (3.10) into (3.11)-(3.13) result in scale-invariant forms of conservation equations [5]

$$\frac{\partial \rho_\beta}{\partial t} + \mathbf{w}_\beta \,.\, \nabla \rho_\beta - D_\beta \nabla^2 \rho_\beta = \Omega_\beta \tag{3.14}$$

$$\frac{\partial T_\beta}{\partial t} + \mathbf{w}_\beta \,.\, \nabla T_\beta - \alpha_\beta \nabla^2 T_\beta = - \; h_\beta \Omega_\beta / (\rho_\beta c_{p\beta}) \tag{3.15}$$

$$\frac{\partial \mathbf{v}_\beta}{\partial t} + \mathbf{w}_\beta \,.\, \nabla \mathbf{v}_\beta - \nu_\beta \nabla^2 \mathbf{v}_\beta = - \; \mathbf{v}_\beta \Omega_\beta / \rho_\beta \tag{3.16}$$

$$\frac{\partial \boldsymbol{\omega}_\beta}{\partial t} + \mathbf{w}_\beta \,.\, \nabla \boldsymbol{\omega}_\beta - \nu_\beta \nabla^2 \boldsymbol{\omega}_\beta = - \; \boldsymbol{\omega}_\beta \,.\, \nabla \mathbf{w}_\beta - \boldsymbol{\omega}_\beta \Omega_\beta / \rho_\beta \tag{3.17}$$

Equation (3.17) is the modified form of the *Helmholtz* vorticity equation for chemically reactive flow fields. The last two terms of (3.17) respectively correspond to vorticity generation by vortex-stretching and chemical reactions. Also, equation (3.16) is the *scale-invariant equation of motion in reactive fields* [5] that includes the reaction term $(-\mathbf{v}_\beta \Omega_\beta / \rho_\beta)$ representing generation $\Omega_\beta < 0$ (annihilation $\Omega_\beta > 0$) of linear momentum accompanied by release (absorption) of thermal energy associated with exothermic (endothermic) chemical reactions. It is known that as flames propagate, they convert *stationary* reactants to *moving* combustion products because of thermal expansion. Another important feature of the modified equation of motion (3.16) is that it involves a convective velocity $\mathbf{w}_\beta$ that is different from the local fluid velocity $\mathbf{v}_\beta$. Consequently, when the convective velocity vanishes $\mathbf{w}_\beta = 0$, equation (3.16) reduces to the diffusion equation similar to mass and heat conservation equations (3.14)-(3.15). Because the convective velocity $\mathbf{w}_\beta$ is not *locally-defined* it cannot occur in *differential form* within the conservation equations [5]. This is because one cannot differentiate a function that is not locally, i.e. differentially, defined. To determine $\mathbf{w}_\beta$, one needs to go to the next higher scale (β+1) where $\mathbf{w}_\beta = \mathbf{v}_{\beta+1}$ becomes a local velocity. However, at this new scale one encounters yet another convective velocity $\mathbf{w}_{\beta+1}$ which is not known, requiring consideration of the higher scale (β+2). This unending chain constitutes the *closure problem* of the statistical theory of turbulence discussed earlier [5].

By summation of (3.1)-(3.4) over (β) one can arrive at the conservation equations at the next higher scale of (β+1). By such procedure, one can move from molecular-dynamic to cluster-dynamic scale or from cluster-dynamic to eddy-dynamic scale within the cascade of embedded statistical fields (Fig.1). The summation of Eq.(3.1) is simple since

$$\Sigma_\beta \, \rho_\beta = \rho_{\beta+1} \tag{3.18}$$

and

$$\Sigma_\beta \, \rho_\beta \mathbf{v}_\beta = \Sigma_\beta \, [\rho_{\beta+1} Y_\beta \mathbf{v}_\beta] = \rho_{\beta+1} \, \Sigma_\beta \, [Y_\beta \mathbf{v}_\beta] = \rho_{\beta+1} \mathbf{v}_{\beta+1} \tag{3.19}$$

For Eq.(3.3), the summation of the first term is identical to that shown in (3.19)

$$\Sigma_\beta \, \mathbf{p}_\beta = \Sigma_\beta \, \rho_\beta \mathbf{v}_\beta = \Sigma_\beta \, [\rho_{\beta+1} Y_\beta \mathbf{v}_\beta] = \rho_{\beta+1} \, \Sigma_\beta \, [Y_\beta \mathbf{v}_\beta] = \rho_{\beta+1} \mathbf{v}_{\beta+1} = \mathbf{p}_{\beta+1} \tag{3.20}$$

To treat the summation of the second term of (3.3), one starts with the relation based on (2.1)-(2.2)

$$\mathbf{v}_\beta = \mathbf{w}_\beta + \mathbf{V}_\beta = \mathbf{v}_{\beta+1} + \mathbf{V}'_{\beta+1} \tag{3.21}$$

Multiplying (3.21) by ($Y_{\beta+1} \rho_\beta \mathbf{v}_\beta$) and summing over ($\beta$) and ($\beta$+1) leads to

$$\Sigma_{\beta+1} \, \Sigma_\beta \, [Y_{\beta+1} \rho_\beta \mathbf{v}_\beta \mathbf{v}_\beta] = \Sigma_{\beta+1} \Sigma_\beta \, [Y_{\beta+1} \rho_\beta \mathbf{v}_\beta \mathbf{v}_{\beta+1}] + \Sigma_{\beta+1} \, \Sigma_\beta \, [Y_{\beta+1} \rho_\beta \mathbf{v}_\beta \mathbf{V}'_{\beta+1}]$$

or

$$\begin{aligned}
\Sigma_\beta \, [\rho_\beta \mathbf{v}_\beta \mathbf{v}_\beta] &= \Sigma_{\beta+1} \Sigma_\beta \, [\rho_\beta \mathbf{v}_\beta Y_{\beta+1} \mathbf{v}_{\beta+1}] + \Sigma_{\beta+1} \, \Sigma_\beta \, [\rho_\beta \mathbf{v}_\beta Y_{\beta+1} \mathbf{V}'_{\beta+1}] = \\
&= \Sigma_\beta \, [\rho_\beta \mathbf{v}_\beta \mathbf{w}_{\beta+1}] + \Sigma_\beta \, [\rho_\beta \mathbf{v}_\beta \mathbf{V}_{\beta+1}] = \\
&= \rho_{\beta+1} \mathbf{v}_{\beta+1} \mathbf{w}_{\beta+1} + \rho_{\beta+1} \mathbf{v}_{\beta+1} \mathbf{V}_{\beta+1} = \\
&= \rho_{\beta+1} \mathbf{v}_{\beta+1} (\mathbf{w}_{\beta+1} + \mathbf{V}_{\beta+1}) = \rho_{\beta+1} \mathbf{v}_{\beta+1} \mathbf{v}_{\beta+1} = \mathbf{p}_{\beta+1} \mathbf{v}_{\beta+1}
\end{aligned} \tag{3.22}$$

where Y_β is mass fraction and use was made of the relation $\mathbf{v}_{\beta+1} = \mathbf{w}_{\beta+1} + \mathbf{V}_{\beta+1}$ from (2.2) in the last step. The summation of the energy (3.2) and vorticity (3.4) equations follow procedures similar to those used above in (3.21)-(3.22).

4. CONNECTION BETWEEN THE MODIFIED FORM OF EQUATION OF MOTION AND THE NAVIER-STOKES EQUATION

The original form of the *Navier-Stokes* equation with constant coefficients is given as [1, 2]

$$\rho \frac{\partial \mathbf{v}}{\partial t} + \rho \mathbf{v} . \nabla \mathbf{v} = - \nabla P + \mu \nabla^2 \mathbf{v} + \frac{1}{3} \mu \nabla(\nabla . \mathbf{v}) \tag{4.1}$$

when the coefficient of bulk viscosity is considered to be negligible [6]. Since thermodynamic pressure P_t is an isotropic scalar, P in (4.1) is not P_t. Rather, the pressure P is generally identified as the *mechanical pressure* that is defined in terms of the total stress tensor $T_{ij} = - P_t \delta_{ij} + \tau_{ij}$ as [6]

$$P_m = - (1/3) T_{ii} = P_t - (1/3) \tau_{ii} \tag{4.2}$$

The normal viscous stress is given by (3.8) as $(1/3)\, \tau_{ii} = (1/3)\, \rho \mathbf{v}_i \mathbf{V}_{ii} = - (1/3)\, \mu \nabla . \mathbf{v}$ and since $\nabla P_t \approx 0$ because of isotropic nature of P_t, the gradient of (4.2) becomes

$$\nabla P = \nabla P_m = \nabla \frac{1}{3} \mu (\nabla . \mathbf{v}) = \frac{1}{3} \mu \nabla (\nabla . \mathbf{v}) \tag{4.3}$$

Substituting from (4.3) in (4.1), the *Navier-Stokes* equation assumes the form

$$\frac{\partial \mathbf{v}}{\partial t} + \mathbf{v} . \nabla \mathbf{v} - \nu \nabla^2 \mathbf{v} = 0 \tag{4.4}$$

that is almost identical to the modified equation of motion (3.16) with $\Omega_\beta = 0$ except that in the latter the convective velocity $\mathbf{w}_\beta$ is different from the local velocity $\mathbf{v}_\beta$. However, because (4.4) includes a diffusion term and the velocities $\mathbf{w}_\beta$ and $\mathbf{v}_\beta$ are related by $\mathbf{v}_\beta = \mathbf{w}_\beta + \mathbf{V}_\beta$, it is clear that (4.4) should in fact be written as (3.16).

An example of exact solution of the modified equation of motion (3.16) was recently introduced [7] for the classical *Blasius* problem [2] of laminar flow over a flat plate. For this steady problem Eq.(3.16) in the boundary layer, with $w'_y = 0$ and $\Omega = 0$, reduces to

$$w'_x \frac{\partial \mathbf{v}'_x}{\partial x'} = \nu \frac{\partial^2 \mathbf{v}'_x}{\partial y'^2} \tag{4.5}$$

$$y' = 0 \qquad v'_x = 0 \tag{4.5a}$$

$$y' = \infty \qquad v'_x = w'_o \tag{4.5b}$$

where w'_o is the constant free-stream velocity outside of the boundary layer and (x', y') are the coordinates along and normal to the wall, respectively. The local velocity v'_x varies from $v'_x = 0$ at the wall $y' = 0$ to $v'_x \approx w'_o$ at the edge of the boundary layer at all axial positions. Therefore, the convective velocity $w'_x = \langle v'_x \rangle$, i.e. the mean value of the local velocity v'_x inside the boundary layer, will have the constant value of $w'_x = w'_o/2$. Substituting for this convective velocity in (4.5) one obtains [7]

$$2\eta \frac{dv_x}{d\eta} + \frac{d^2 v_x}{\partial \eta^2} = 0 \tag{4.6}$$

$$\eta = 0 \qquad v_x = 0 \tag{4.7a}$$

$$\eta = \infty \qquad v_x = 1 \tag{4.7b}$$

in terms of the similarity variable $\eta = y'/(2x'^{0.5})$, where $v_x = v'_x / w'_o$. The solution of (4.6)-(4.7) is the predicted velocity profile $v_x = \text{erf}\, \eta$ that is in excellent agreement with the experimental observations of *Nikuradze* [2].

The solution of (3.16) for the classical problem of *Hagen-Poiseuille* flow [2] in circular tubes has also been investigated [7]. It was found that the geometry of the predicted velocity profile involving *Bessel* function was quite similar to the classical parabolic profile and hence in agreement with the experimental observations. Finally, the exact solution of the modified *Helmholtz* vorticity equation (3.17) was recently reported [8] for the steady problem of non-reactive flow within a stationary liquid droplet that is located at the stagnation-point between two axisymmetric counter-flowing gaseous streams. It was found that such a spherical flow could be expressed by the stream function [8]

$$\Psi = - r^2 z (1 - r^2 - z^2) \tag{4.8}$$

representing two rings vortices, rather than a single spherical *Hill* vortex for the classical problem of a droplet in a uniform stream [6], that are located above and below the stagnation plane. Therefore, the preliminary investigations discussed above show that the modified equation of motion (3.16) does indeed lead to realistic solutions in agreement with experimental observations for these classical problems for which exact solutions of the *Navier-Stokes* equation are available.

5. MODIFIED HYDRO-THERMO-DIFFUSIVE THEORY OF LAMINAR FLAMES

Theory of laminar flames is the most fundamental problem of combustion science and subject of many classical [9-18] as well as more recent [3, 19-24] studies. For one-dimensional propagation of a planar flame one introduces the dimensionless parameters

$$\theta = (T - T_u)/(T_b - T_u) \;, \qquad y = Y_F/Y_{Fu} \;, \qquad \Lambda \equiv [\nu_F W_F B \alpha/(\rho v'^2_o)]\, e^{-\beta/x} \tag{5.1}$$

The adiabatic flame temperature T_b, the Zeldovich number β, and the coefficient of thermal expansion χ are

$$T_b = T_u + QY_{Fu}/(\nu_F W_F c_p) \ , \qquad \beta = E(T_b - T_u)/RT_b^2 \ , \quad \chi = (T_b - T_u)/T_b \qquad (5.2)$$

and one assumes that $\beta >> 1$. Also, Q, E, and R are heat release per mole of fuel, activation energy, and universal gas constant. Prandtl, Schmidt, and Lewis numbers are assumed to be unity $\nu = \alpha = D$, such that outside of reaction zone where $\Lambda = 0$, the θ, y, and **v** fields will be similar under identical boundary conditions. Equations (3.14)-(3.16) for molecular-dynamic scale with the dimensionless coordinate, time, and velocity defined as $x = x'/(\alpha/v'_o)$, $t = t'/(\alpha/v'^2_o)$, and $\mathbf{v} = \mathbf{v}'/v'_o$ become

$$\frac{\partial y}{\partial t} + w\frac{\partial y}{\partial x} = \frac{\partial^2 y}{\partial x^2} - \Lambda\, y\, e^{\beta(\theta - 1)}\, \delta(x) \qquad (5.3)$$

$$\frac{\partial \theta}{\partial t} + w\frac{\partial \theta}{\partial x} = \frac{\partial^2 \theta}{\partial x^2} + \Lambda\, y\, e^{\beta(\theta - 1)}\, \delta(x) \qquad (5.4)$$

$$\frac{\partial \mathbf{v}}{\partial t} + w\frac{\partial \mathbf{v}}{\partial x} = \frac{\partial^2 \mathbf{v}}{\partial x^2} + \mathbf{v}\, \Lambda\, y\, e^{\beta(\theta - 1)}\, \delta(x) \qquad (5.5)$$

where v'_o is the flame propagation speed.

5.1 Far-Field Convective Coordinate

For laminar flames propagating in quiescent reactive fields, there is no forced convection $w = 0$, and (5.3)-(5.5) reduce to non-homogeneous diffusion equations with nonlinear sources. Because of thermal expansions in the flame, the stationary cold reactants are converted to moving hot combustion products resulting in a velocity jump across the flame sheet as schematically shown in Fig.2a. When viewed from the perspective of the physical or far-field coordinate x', the flame appears as a mathematical surface of discontinuity without any spatio-temporal structures.

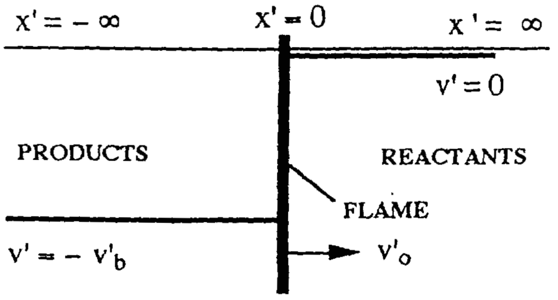

Fig.2a A propagating laminar flame viewed from far-field coordinate x'.

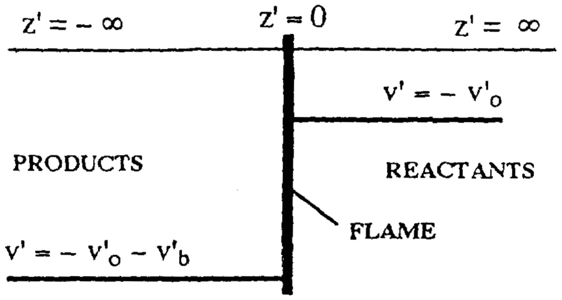

Fig.2b A stationary laminar flame viewed from far-field coordinate z'.

Outside of the thin flame zone chemical reactions will be frozen $\Lambda = 0$, and the governing equations (5.3)-(5.5) become

$$\frac{\partial f}{\partial t'} = \nu_m \frac{\partial^2 f}{\partial x'^2} \qquad f = y, \theta, v \tag{5.6}$$

To an observer in the coordinate x' only the mean velocity $w'_f = -v'_o - v'_b/2$ will be detectable and this velocity will be without any spatial structure. If one introduces a coordinate system that moves with the flame $z' = x' - w'_f t'$, one obtains from (5.6)

$$w'_f \frac{df}{dz'} = -\nu_m \frac{d^2 f}{dz'^2} \qquad f = y, \theta, v \tag{5.7}$$

and the flame becomes stationary with velocity jump $(-v'_o, -v'_o - v'_b)$ across the flame front ($z' = 0+$, $z' = 0-$) as shown in Fig.2b . However, the hydro-thermo-diffusive structure of the flame will be hidden from this observer in the far-field coordinate z'.

5.2 Outer Convective-Diffusive Coordinate

In terms of the convective-diffusive stretched coordinate $x = x'/l_T$, where l_T is the flame thermal thickness $l_T = \alpha/v'_o$, the hydro-thermo-diffusive structure of the flame becomes visible as shown in Fig.3a. However, the convective-diffusive coordinate is being applied to the colder regions outside of the thin reaction zone such that chemical reactions remain frozen $\Lambda = 0$ because $\beta >> 1$. With linear approximation, the values of velocities (v, w, V) within the flame structure at the locations $x = (-1/2, 0, 1/2)$ will be $v = (-v_b, -v_b/2, 0)$, $w = (-3v_b/4, -v_b/2, -v_b/4)$, and $V = (-v_b/4, 0, v_b/4)$ as shown in Fig.3a, when $v_b = v'_b/v'_o$. Hence, the flame hydrodynamic structure involves a variable convective velocity w, and the relation $v = w + V$ is satisfied, while the sign of V as well as that of curvature of the velocity profile change across $x = 0$.

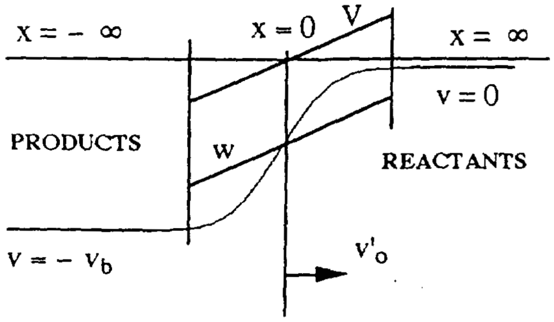

Fig.3a Hydrodynamic structure of a propagating laminar flame viewed from thermo-diffusive coordinate x.

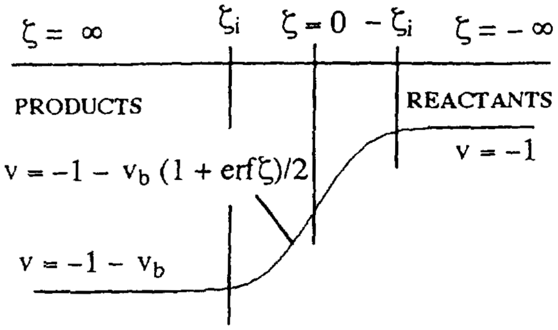

Fig.3b Hydrodynamic structure of a stationary laminar flame viewed from thermo-diffusive coordinate z.

The velocity of the burned gas v'_b will be related to the laminar flame propagation velocity v'_o by the mass conservation across the flame $\rho_o v'_o = \rho_b(v'_o + v'_b)$ that is valid to a very high degree of accuracy. It is important to emphasize however that mass is not strictly conserved across flame fronts and in fact an exceedingly small amount of gravitational mass (rest energy) of the reactants will be converted to other forms of energy (inertial energy) such as thermal energy of products of combustion and photons as discussed in sec. 3.

For the steady problem, the convective-diffusive coordinate that moves with the flame is $z = x - w\,t$ where $w = w'/v'_o$, $z = z'/l_T$, and $t = t'/(l_T/v'_o)$. One notes however that in terms of the stretched coordinate z, the velocity $w = -1 + v_b(z - 1)/2$ is no longer constant but has spatial structure as shown in Figs.3a-3b. One further notes that the average value of w at the flame center $z = 0$ is $w_f = -1 - v_b/2$ that is exactly the mean flame speed as seen by the far-field coordinate z' discussed in sec.5.1 above. Furthermore, for an observer that moves with the flame front, this velocity profile $w = \langle v \rangle = -1 + v_b(z - 1)/2$ remains invariant such that Eq.(5.7) becomes

$$[1 - v_b(z - 1)/2]\frac{df}{dz} = \frac{d^2f}{dz^2} \qquad f = y, \theta, v \tag{5.8}$$

$$z \rightarrow \infty \qquad y - 1 = \theta = v + 1 = 0 \tag{5.9}$$

$$z \rightarrow -\infty \qquad y = \theta - 1 = v + 1 + v_b = 0 \tag{5.10}$$

Introducing the new variable $\sqrt{v_b}\,\zeta = 1 - v_b(z - 1)/2$ into (5.8)-(5.10) gives

$$2\zeta\frac{df}{d\zeta} + \frac{d^2f}{d\zeta^2} = 0 \qquad f = y, \theta, v \tag{5.11}$$

$$\zeta \rightarrow -\infty \qquad y - 1 = \theta = v + 1 = 0 \tag{5.12}$$

$$\zeta \rightarrow \infty \qquad y = \theta - 1 = v + 1 + v_b = 0 \tag{5.13}$$

with the solutions

$$\theta = 1 - y = -(v + 1)/v_b = (1 + \operatorname{erf}\zeta)/2 \tag{5.14}$$

According to (5.14), the steady flame structure is given by a traveling error function schematically shown in Fig.4b. This result, while being in harmony, is fundamentally different from that discussed in an earlier study [25], and perhaps provides a clearer description of the steady flame structure. The predicted geometry of the temperature profile involving error function (5.14) is in close agreement with the experimental observations [26-28]. In addition, the predicted profiles are consistent with the measured temperature profiles of counterflow premixed flames [29] in the limit of vanishing rates of stretch. On the other hand, the temperature profile within the flame structure according to the classical theories of laminar flame is given by an exponential function as schematically shown in Fig.4b. More experimental measurements of temperature profiles in unsteady propagating laminar flames are needed in order to further test the validity of the modified versus the classical theory. The slope of the temperature profile of the outer convective-diffusive zone at the position of the reaction zone ζ_i (Fig.4a) is obtained from (5.14) as

$$\left(\frac{d\theta}{d\zeta}\right)_{\zeta=\zeta_i} = \frac{e^{-\zeta_i^2}}{\sqrt{\pi}} \tag{5.15}$$

that will be matched with the solution within the reaction zone to be described next.

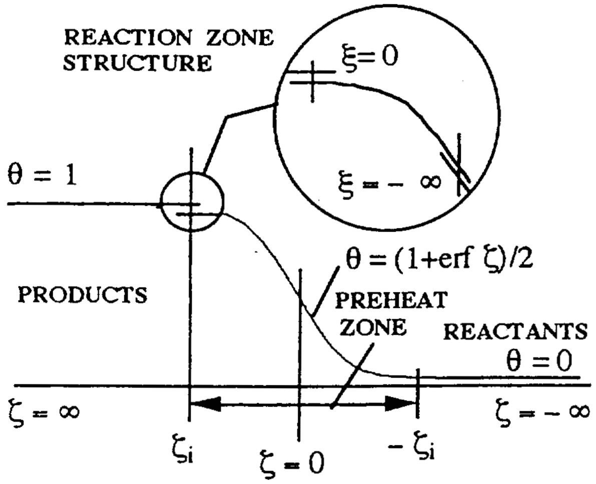

Fig.4a Flame structure according to the modified theory of laminar flame.

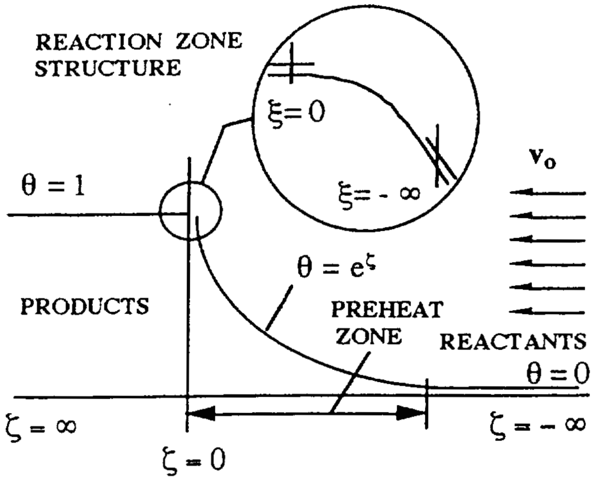

Fig.4b Flame structure according to the classical theories of laminar flame.

5.3 Inner Reactive-Diffusive Coordinate

The analysis of the thin reaction zone follows the classical methods [3, 19-24] and involves the stretched coordinate

$$\xi = \beta(\zeta_i - \zeta) \tag{5.16}$$

along with the temperature and concentration expansions

$$\theta = 1 + \Theta_1/\beta + \ldots \qquad \text{and} \qquad y = 0 + Y_1/\beta + \ldots \tag{5.17}$$

that are introduced into Eqs.(5.3)-(5.4) to obtain, to the first order in $\varepsilon = 1/\beta << 1$

$$\frac{d^2Y_1}{d\xi^2} = \frac{4\Lambda}{v_b\,\beta^2}\, Y_1\, e^{\Theta_1} \tag{5.18}$$

$$\frac{d^2\Theta_1}{d\xi^2} = -\frac{4\Lambda}{v_b\,\beta^2}\, Y_1\, e^{\Theta_1} \tag{5.19}$$

From the coupling of Eqs.(5.18)-(5.19) and the boundary conditions at $\xi \rightarrow \pm\infty$, one obtains $\Theta_1 + Y_1 = 0$ such that Eq.(5.19) becomes

$$\frac{d^2\Theta_1}{d\xi^2} = \frac{4\Lambda}{v_b\,\beta^2}\,\Theta_1\,e^{\Theta_1} \tag{5.20}$$

that may also be expressed as

$$\frac{d}{d\Theta_1}\left(\frac{d\Theta_1}{d\xi}\right)^2 = \frac{8\Lambda}{v_b\,\beta^2}\,\Theta_1\,e^{\Theta_1} \tag{5.21}$$

The first integral of the above equation, and matching of the slopes of the temperature profiles on either side of the reaction zone with the outer solutions in Eq.(5.15) results in

$$\exp(-2\zeta_i^2) = [8\pi\,\nu_F W_F B\alpha/(\rho v_b v'^2_o\,\beta^2)]\,e^{-\beta/\chi} \tag{5.22}$$

that relates the reaction zone position ζ_i and hence the ignition temperature θ_i, to the flame propagation velocity v'_o. The parameter B in (5.1) is related to the actual preexponential factor B' in the law of mass action [3] under *Arrhenius* kinetics by

$$B = B'\rho\rho_O/(W_F W_O) \tag{5.23}$$

Also, the mass balance across the flame front $\rho_u v'_o = \rho_b(v'_o + v'_b)$ leads to

$$v'_b = v'_o(\rho_u - \rho_b)/\rho_b \tag{5.24}$$

By substitution from (5.23)-(5.24) into (5.22), one obtains the analytic expression

$$v'^2_o = \frac{8\pi\,\nu_F\,\rho_b\rho_O\,\alpha\,B'}{(\rho_u - \rho_b)W_O\beta^2}\,e^{-\beta/\chi}\,e^{2\zeta_i^2} \tag{5.25}$$

for calculation of laminar flame propagation velocity.

For single-step overall combustion of stoichiometric premixed methane-air flame at the flame temperature of 2100 K the relevant physico-chemical properties are $\nu_F = 1$, $\rho_O = 1.38$ kg/m^3, $W_O = 32$, $\alpha \approx 6\times10^{-4}$ m^2/s (thermal diffusivity of air at the flame temperature of 2100 K), $E \approx 46$ kcal/mole , $B' \approx 4.33\times10^7$ m^3/kmol-s [30], $\chi \approx 0.86$, $\beta \approx 10$, and the ignition temperature of $\theta_i = 0.99$ that by (5.13) gives the reaction zone position $\zeta_i \approx 1.75$. Also, from the temperatures of reactants 300 K and combustion products 2100 K and the ideal gas law under constant pressure, one obtains the density ratio $\rho_u/\rho_b = 7$. With these realistic values of the physico-chemical properties, the value of flame propagation velocity calculated from (5.25) is about $v'_o = 42.1$ cm/s in close agreement with the experimentally observed value [27, 28, 31-32]. Although this level of agreement between the theory and experiments is considered to be encouraging, it should be viewed with caution because of the well-known uncertainties in the overall chemical-kinetic parameters (E, B'). The value of about $v'_o = 42$ cm/s has also been obtained in a number of numerical investigations using complex multi-step kinetic models [33-36].

6. CONCLUDING REMARKS

A scale invariant model of statistical mechanics was applied to present invariant forms of mass, energy, linear, and angular momentum conservation equations in chemically-reactive flow fields. The summation procedures for relating adjacent families within the hierarchy of statistical fields was described. Also, the coupling between the gravitational versus the inertial contributions to the energy-momentum density of the field was discussed. The connection between the modified equation of motion and the classical *Navier-Stokes* equation was established. The exact solution of the modified equation of motion for the classical problem of *Blasius* for laminar flow over a flat plate was presented. Also, a modified form of the *Helmholtz* vorticity equation was presented with a source of vorticity due to chemical reactions. The conservation equations at the molecular-dynamic scale were then applied to present a modified hydro-thermo-diffusive theory of laminar flames. The predicted flame structure was found to be in agreement with experimental observations as well as numerical calculations. With realistic physico-chemical properties for one-step combustion of stoichiometric methane-air premixed flames, the flame propagation velocity of 42.1 cm/s was calculated in accordance with experimental observations.

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