TOWARDS UNCERTAINTY QUANTIFICATION OF PREMIXED LAMINAR FLAMES USING BAYESIAN STATISTICS

by

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These are my acknowledgements

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Abstract

This is my abstract

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Introduction

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2.1 Governing Equations

Need transition description (will write later)

2.1.1 Problem definition

The The flow of a compressible fluid is described in terms of the velocity (u^*), pressure (p^*), density (ρ^*), and temperature(T^*) fields. These fields are solutions of the compressible Navier Stokes equations that describe the dynamics of the system and that are statements of conservation of mass, momentum and energy and a state equation relating the thermodynamic variables.

The system of equation that needs to be solved reads

$$\frac{D\rho^*}{Dt^*} = -\rho^* \, \nabla \cdot u^* \tag{2.1}$$

$$\rho^* \frac{Du^*}{Dt} = -\nabla p^* + \nabla \cdot \tau^* + \rho^* g^* \tag{2.2}$$

$$\rho^* C_p^* \frac{DT^*}{Dt^*} = \tau^* \nabla \cdot u^* - \nabla \cdot q^* + \beta^* T^* \frac{Dp^*}{Dt^*} \tag{2.3}$$

$$\frac{D\rho^*}{Dt^*} = -\beta^* T^* \frac{D\rho^*}{Dt^*} + \alpha^* \rho^* \frac{Dp^*}{Dt^*} \tag{2.4}$$

Where u^* is the velocity vector,ρ^* is the density,β^* is the thermal expansion coefficient,p^* is the pressure ,τ^* is the viscous stress term, g^* is the gravitational vector,c_p^* is the specific heat, T^* is the temperature, q^* is the heat flux vector.

for Newtonian fluid,

$$\tau^* = \mu^*(\nabla u^* + (\nabla u^*)^T)) - \frac{2}{3}\mu^* \nabla \cdot u^* I$$

By fourier law's,

$$q^* = k^* \nabla T^*$$

μ^* is the dynamic viscocity. k^* is the thermal conductivity.

The following are the quantities in equation of state, $\beta^* = -\frac{1}{\rho^*}\frac{\partial \rho^*}{\partial T^*}$ and $\alpha^* = \frac{1}{\rho^*}\frac{\partial \rho^*}{\partial p^*}$.

2.1.2 Low mach number asymtotic analysis

We nondimensionalize the Equations by using reference quantities denoted by the subscript ∞, e.g. farfield or stagnation conditions, and a typical length scale L^* of the considered flow. The thermodynamic reference quantities are assumed to be related by the equation of state for a perfect gas. We have used perfect gas law because we are dealing with gases in combustion environment. We define the nondimensional quantities by:

$\rho = \frac{\rho^*}{\rho_\infty}$, $p = \frac{p^*}{p_\infty}$, $u = \frac{u^*}{u_\infty}$, $T = \frac{T^*}{T_\infty}$, $\mu = \frac{\mu^*}{\mu_\infty}$, $k = \frac{k^*}{k_\infty}$,$x = \frac{x^*}{L^*}$, $t = \frac{t^*}{L^*/u^*_\infty}$, $\beta^* = \frac{\beta}{\beta_\infty}$,

$C_p^* = \frac{C_p}{C_{p}{}^*_\infty}$.

Using the relations above. we may write the nondimensional Navier-Stokes equations and other equations of interest as follows:

$$\frac{D\rho}{Dt} = -\rho\,\nabla\cdot u \tag{2.5}$$

$$\rho\frac{Du}{Dt} = -\frac{1}{M^2}\,\nabla p \;+\; \frac{1}{Re}\nabla\cdot\tau + \frac{1}{Fr^2}\rho g \tag{2.6}$$

$$\rho C_p\frac{DT}{Dt} = \frac{M^2}{Re\lambda}\,\tau\nabla\cdot u \;-\; \frac{1}{RePr}\;\nabla\cdot(k\nabla T) + \frac{\beta T}{\lambda}\frac{Dp}{Dt} \tag{2.7}$$

$$\frac{D\rho}{Dt} = -\beta T\frac{D\rho}{Dt} + \alpha\rho\,\frac{Dp}{Dt} \tag{2.8}$$

Where the following nondimensional quantities are

$$M = \frac{u_\infty}{a_\infty}$$

.

$$Re = \frac{u_\infty\rho_\infty L}{\mu_\infty}$$

.

$$Pr = \frac{C_{p\infty}\mu_\infty L}{k_\infty}$$

$$Fr = \sqrt{\frac{u_\infty^2}{g_\infty L}}$$

.

a_∞ is the reference speed of sound. M is the mach number,Re is the reynolds number,Pr is the prandtl number,Fr is the froude number and λ is defined as $\frac{C_{p\infty}T_\infty}{a_\infty^2}$.

By definition

$$\beta^* = -\frac{1}{\rho^*}\frac{\partial\rho^*}{\partial T^*}$$

We non dimensional this term as follows

$$\beta^* = -\frac{1}{\rho_\infty\rho}\frac{\rho_\infty}{T_\infty}\frac{\partial\rho}{\partial T}$$

$$\beta^* = \frac{1}{T_\infty}\beta$$

Where $\beta_\infty = \frac{1}{T_\infty}$.

By definition

$$a^{*2} = \frac{\partial p^*}{\partial \rho^*}$$

We non dimensional this term as follows

$$a^{*2} = \frac{p_\infty}{\rho_\infty}\frac{\partial p}{\partial \rho}$$

$$a^{*2} = \frac{p_\infty}{\rho_\infty}a^2$$

Where $a_\infty = \sqrt{\frac{p_\infty}{\rho_\infty}}$.

2.1.3 Asymptotic analysis

We do asymptotic analysis with respect to Mach number. We use the following equation in terms of Mach number

$$\xi(x,t,M) = \xi^0(x,t) + M\xi^1(x,t) + M^2\xi^2(x,t) + O(M^3)$$

Where ξ can be u, p, ρ. We use non dimensional form of navier stokes equation do the asymptotic equation. We show the example of asymptotic analysis for mass conservation.

$$\frac{D}{Dt}(\rho^0+M\rho^1+M^2\rho^2+O(M^3)) + (\rho^0+M\rho^1+M^2\rho^2+O(M^3))\ \nabla\cdot(u^0+Mu^1+M^2u^2+O(M^3)) = 0$$

Collecting equal order terms together we get,

$$\left(\frac{D\rho^0}{Dt} + \rho^0\ \nabla\cdot u^0\right) + M\left(\frac{\partial \rho^1}{\partial t} + + \rho^1\ \nabla\cdot u^0 + + \rho^0\ \nabla\cdot u^1\right) + O(M^2) = 0$$

Therefore zeroth order terms can be written.

$$\frac{D\rho^0}{Dt} + \rho^0\ \nabla\cdot u^0 = 0 \tag{2.9}$$

The asymptotic relation for momentum are obtained are as follows. The zero, first and second order momentum equation are written as follows respectively

$$M^{-2}\nabla p^{(0)} = 0 \tag{2.10}$$

$$M^{-1}\nabla p^{(1)} = 0 \tag{2.11}$$

$$\rho^0\frac{Du^0}{Dt} = -\nabla p^2 + \nabla\cdot\tau^0 + \rho^0 g \tag{2.12}$$

The asymptotic relation for momentum are obtained are as follows.

$$\rho^0 C_p^0\frac{DT^0}{Dt} = -\frac{1}{RePr}\nabla.(k^0\nabla T^0) + \frac{\beta^0 T^0}{\lambda}\frac{dp^0}{dt} \tag{2.13}$$

We have seen from momentum asymptotic analysis that $p^0 = p^0(t)$ and therefore

$$\frac{Dp^0}{Dt} = \frac{dp^0}{dt}$$

.
The nondimensional equation of state is same as that of the dimensional form. Now same asymptotic expansion of the state equation is done in order to get zeroth order state equation which is given below.

$$\frac{D\rho^0}{Dt} = -\beta^0 T^0 \frac{D\rho^0}{Dt} + \alpha^0 \rho^0 \frac{Dp^0}{Dt} \tag{2.14}$$

From mass conservation equation and since $p^0 = p^0(t)$, we get the following equation

$$-\nabla \cdot u^0 = -\beta^0 \frac{DT^0}{Dt} + \alpha^0 \frac{dp^0}{dt} \tag{2.15}$$

From energy conservation equation

$$-\rho^0 C_p^0 \nabla \cdot u^0 = \frac{1}{RePr} \nabla \cdot q^0 + \left(\frac{C_p^0 \lambda - 1}{\lambda} \right) \frac{dp^0}{dt} \tag{2.16}$$

The final equation obtained by applying various thermodynamic properties are following

$$-\nabla \cdot u = \frac{1}{p^0} \frac{dp^0}{dt} - \frac{1}{T} \frac{DT}{Dt} \tag{2.17}$$

$$\rho \frac{Du}{Dt} = -\frac{1}{M^2} \nabla p + \frac{1}{Re} \nabla \cdot \tau + \frac{1}{Fr^2} \rho g \tag{2.18}$$

$$\rho C_p \frac{DT}{Dt} = -\frac{1}{RePr} \nabla \cdot (k \nabla T) + \frac{1}{\gamma - 1} \frac{dp^0}{dt} \tag{2.19}$$

$$\tag{2.20}$$

Chapter 3

Combustion Model

3.1 Premixed ozone oxygen laminar flame model

We shall use Heimerl and coffee's contemporary method for modelling combustion flame problem. A one dimensional, premixed, laminar, steady state ozone oxygen flame was considered in their theortical model. The reason for choosing this model was due to its simplicity. The chemical reactions involved only three species

$$O_3 + M \rightleftharpoons O + O_2 + M$$
$$O + O_3 \rightleftharpoons A_2 2O_2$$
$$A + AB \rightleftharpoons A_2 + B$$

Where M represents the third body which could be either O, O_2 or O_3.
The species conservation equation is given as

$$\frac{\partial \rho_i}{\partial t} + \nabla.(\rho_i v) \quad = \nabla.(\rho D_{ij} \nabla Y_i) + w_i \tag{3.1}$$

Where, the rate of production for species i is given by the following

Where

$$w_i = Mw_i \sum_{k=1}^{6} (v_{k,i}^{''} - v_{k,i}^{'}) B_k T^{\alpha_k} e^{\frac{-E_a}{R_u T}} \prod_{j=1}^{3} \left(\frac{X_j p}{RT} \right)^{v'_{j,k}}$$

The above equation considers all 6 reactions for all the three species.
From atomic species conservation

$$\sum_{i=1}^{N} {v_i}' M_i \rightleftharpoons \sum_{i=1}^{N} {v_i}'' M_i$$

Where E_a is the activation energy, R_u is the universal gas constant, X_j is the molar concentration of the reactant j, Mw_i is the molecular weight of the reactant. $v'_{j,k}$ is the moles of reactant j in the reaction k. $v''_{j,k}$ is the number of moles of product.

The overall continuity equation, species conservation equation and energy conservation equation are solved to calculate the flame paraneters. The energy equation considers that the pressure is constant throughout the reaction zone. The viscous dissipation is negligible and there is no body force work. The Diffusion equation is given

$$\frac{\partial X_k}{\partial x} \quad = \textstyle\sum_{j=1}^{3} \frac{X_k X_j}{D_{jk}} (V_j - V_k) \tag{3.2}$$

Where D_{jk} is the fick's diffusion coefficient. V is the diffusion velocities.
The boundaries are defined by specifying the concentration of O_3, O_2 at the inlet.

3.2 The experimental data on laminar flame speed

To compare our results we have used the experimental data given by the A.G. streng and A.V. Grosse, They have done experiments with ozone flame in tube and ozone flame on the tip of the burner. We will be using the results of the later. They have shown that laminar flame speed or burning velocity varies with the initial concentration of the ozone. The table given below shows the burning velocity with respect to initial concentration of the ozone. We concentrate on two speciifc cases where initial concentration of ozone is 53 percent and 100 percent. The laminar flame speed for 53 percent is measured in the burner with inner diameter 1.3mm and rate of 7.7 cc/sec. The laminar flame speed for 100 percent ozone is taken on .66 inner diameter tip 0.66 mm and the flow rate of 8.23 cc/sec. The measured laminar flame speed is given below. Laminar flame measurements are carried out at 300K and 1 atmosphere pressure.

Table 3.1: Experimental laminar flame speed given by A.G. Streng and A.V. Grosse

Initial Concentration of O_3 ($\pm 0.2\%$)	**Laminar Flame Speed (cm/s)**
17	9.2
20	18.2
28	52.2
40	125
46	166
53	210
75	331
100	475

Chapter 4

Finite Element Formulation

4.1 Adaptive Finite Element

Chapter 5

Bayesian Statistics

5.1 Review of Theory

5.2 Application to Problem

5.3 Methods of Solution

5.4 Software

Chapter 6

Results

Chapter 7

Conclusion