

TOWARDS UNCERTAINTY QUANTIFICATION OF PREMIXED LAMINAR FLAMES USING BAYESIAN STATISTICS

by

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Contents

Acknowledgements	iii
List of Figures	vii
List of Tables	ix
Abstract	xi
1 Introduction	1
1.1 Literature Review	1
2 Mathematical Model	3
2.1 Governing Equations	3
2.1.1 Problem definition	3
2.1.2 Low mach number asymptotic analysis	4
2.1.3 Asymptotic analysis	5
3 Combustion Model	7
3.1 Premixed ozone oxygen laminar flame model	7
3.2 The experimental data on laminar flame speed	8
4 Finite Element Formulation	9
4.1 Weak formulation	9
4.2 Need for stability	10
4.2.1 Streamline Upwind Petrov Galerkin Method	10
4.2.2 Pressure-Stabilizing/Petrov-Galerkin (PSPG)	11
4.2.3 Stabilized Navier Stokes Equation	11
4.3 Adaptive Finite Element	11
5 Bayesian Statistics	13
5.1 Review of Theory	13
5.2 Application to Problem	13
5.3 Methods of Solution	13
5.4 Software	13
6 Results	15
7 Conclusion	17

List of Figures

List of Tables

3.1	Experimental laminar flame speed given by A.G. Streng and A.V. Grosse	8
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Abstract

This is my abstract

Chapter 1

Introduction

It is important to understand deeply the dynamics of reacting flows as it is inherent in number of areas of science and engineering like combustion, surface chemistry etc . To understand these systems in detail, large simulations are necessary. It also requires simultaneous numerical resolution of chemical reactions, diffusive transport and fluid mechanics. The combination of three factor make simulations some of the most demanding in the area of combustion. In the deflagration (combustion wave that propagates through a gas or across the surface of an explosive at subsonic speeds, driven by the transfer of heat) regime where the burning speed (also known as laminar flame speed) and associated velocity scales are much smaller than the speed of sound in the fluid, the problem is acute.

For low speed combustion flows, Low Mach number asymptotics of the flow equations exploit the inherent separation of scales in such systems by analytically eliminating acoustic wave propagation entirely from the dynamics, while preserving the important compressibility effects arising from reactions and transport.

1.1 Literature Review

It is shown by Muller [1] that a multiple-time scale, single-space scale asymptotic analysis of the compressible Navier-Stokes equations reveals that the zeroth-order global thermodynamic pressure, the divergence of velocity and the material change of density are affected by heat-release rate and heat conduction at low-Mach-numbers.

His result show that the acoustic time change of the heat-release rate as the dominant source of sound in low-Mach-number flow. The asymptotic expansion of all flow variables show that the viscous and buoyancy forces enter the computation of the second-order incompressible pressure in low-Mach-number flow in a similar way as they enter the pressure computation in incompressible flow, except that the velocity-divergence constraint is non zero. He averaged flow equation over an acoustic wave period, the averaged velocity tensor described the net acoustic effect on the averaged flow field. Once acoustics were removed from the equations altogether it lead to the low-Mach-number equations.

As many flows of interest can be considered as incompressible. The incompressibility assumption makes the problem simpler than if a full compressible flow is considered. Codine [?] proposed that for ideal fluids, with isentropic condition, solutions of the incompressible Navier Stokes equations can be found as the limit of solutions of the compressible ones as the Mach number tends to zero under certain assumptions on the initial data.

In her paper she showed that small Mach number limit gives rise to a separation of the pressure into a constant-in-space thermodynamic pressure and a mechanical pressure that has to be used in the momentum equation. This leads to a removal of the acoustic modes and the flow behaves as incompressible, in the sense that the mechanical pressure is determined by the mass conservation equation and not by the state equation. However, large variations of density due to temperature variations are allowed. She showed that when the Mach number is small the hyperbolic wave equation for the pressure becomes an elliptic equation for the first order pressure $p(2)$, thus showing the implicit (incompressible or mechanical) character of this pressure component

A.G Streng and A.V. Grosse [?] studied the ozone oxygen flame experimentally. The stability of ozone and the rates of decomposition or explosion were investigated by Armour research foundation. Ozone was burned to oxygen from a simple burner tip in the range from 17 percent to 100 percent initial concentration of ozone in the mixture. The flame temperatures were calculated from enthalpy data and dissociation constants of oxygen using kelley's tables. The concentration of ozone was kept constant with error of 0.2 percent. Two methods were used to determine burning velocity i.e open tube method and the burning tip method. We will be using experimental burning velocity of the burning tip method. The burner tip experiments were carried out in standard apparatus, using pyrex glass aluminium tips with an inner diameter of 3 to 0.65mm. The flames were readily observed by the standard schlieren method at all concentrations above 30 mole percent. The measurements were all carried out in the laminar flow region and the reynolds number of the flow was below 2000. The initial conditions are 300K temperature and 1.0 atmosphere pressure. The results of burning velocities of ozone flames were compared with theoretical burning velocities of Dr. Von Karman and his associates. They were found to be in close agreements.

Chapter 2

Mathematical Model

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

$$\frac{D\rho^*}{Dt^*} = -\rho^* \nabla \cdot u^* \quad (2.1)$$

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

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

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

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 viscosity. 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 asymptotic 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:

$$\frac{D\rho}{Dt} = -\rho \nabla \cdot u \quad (2.5)$$

$$\rho \frac{Du}{Dt} = -\frac{1}{M^2} \nabla p + \frac{1}{Re} \nabla \cdot \tau + \frac{1}{Fr^2} \rho g \quad (2.6)$$

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

$$\frac{D\rho}{Dt} = -\beta T \frac{D\rho}{Dt} + \alpha \rho \frac{Dp}{Dt} \quad (2.8)$$

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

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

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

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.

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

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

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

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

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

The asymptotic relation for momentum are obtained are as follows.

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

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.

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

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

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

From energy conservation equation

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

The final equation obtained by applying various thermodynamic properties are following

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

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

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

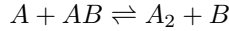
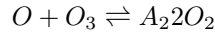
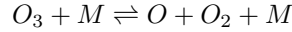
$$(2.20)$$

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 theoretical model. The reason for choosing this model was due to its simplicity. The chemical reactions involved only three species



Where M represents the third body which could be either O , O_2 or O_3 .

The species conservation equation is given as

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

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 parameters. 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

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

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 Weak formulation

The final equation obtained by applying various thermodynamic properties are following

$$-\nabla \cdot u = \frac{1}{p^0} \frac{dp^0}{dt} - \frac{1}{T} \frac{DT}{Dt} \quad (4.1)$$

$$\rho \frac{Du}{Dt} = -\frac{1}{M^2} \nabla p + \frac{1}{Re} \nabla \cdot (\mu(\nabla u + (\nabla u)^T)) - \frac{2}{3} \mu \nabla \cdot u I + \frac{1}{Fr^2} \rho g \quad (4.2)$$

$$\rho C_p \frac{DT}{Dt} = -\frac{1}{RePr} \nabla \cdot (k \nabla T) + \frac{1}{\gamma - 1} \frac{dp^0}{dt} \quad (4.3)$$

$$(4.4)$$

The 2D finite element weak form is given as

$$\begin{aligned} \int_0^L \int_0^L \rho \frac{\partial u^h}{\partial t} \psi + \int_0^L \int_0^L (\rho u^h \cdot \nabla u^h) \psi &= \int_0^L \int_0^L -\frac{1}{M^2} (\nabla p^h) \phi + \int_0^L \int_0^L \frac{1}{Re} (\nabla \cdot \tau^h) \psi + \\ &\quad \int_0^L \int_0^L \frac{1}{Fr^2} (\rho g) \psi \\ \int_0^L \int_0^L \rho C_p \frac{\partial T^h}{\partial t} \varphi + \int_0^L \int_0^L \rho C_p (u^h \cdot \nabla T^h) \varphi &= \int_0^L \int_0^L -\frac{1}{RePr} (\nabla \cdot k \nabla T^h) \varphi + \int_0^L \int_0^L \frac{1}{\gamma - 1} \frac{dp^h}{dt} \phi \end{aligned}$$

Integrating by parts and applying boundary conditions

$$\begin{aligned} \int_0^L \int_0^L \rho \dot{u}^h \psi_i \psi_j + \int_0^L \int_0^L \rho u^h \cdot \nabla u^h \psi_i &= \int_0^L \int_0^L -\frac{1}{M^2} \nabla p^h \phi_i - \int_0^L \int_0^L \frac{1}{Re} \tau^h \nabla \psi + [\tau \psi]_0^L + \\ &\quad \int_0^L \int_0^L \frac{1}{Fr^2} \rho g \psi \\ \int_0^L \int_0^L \rho C_p \dot{T}^h \varphi_i \varphi_j + \int_0^L \int_0^L \rho C_p u^h \cdot \nabla T^h \varphi_i &= \int_0^L \int_0^L +\frac{1}{RePr} (k \nabla T^h) \nabla \varphi - \frac{1}{RePr} [k \nabla T^h \varphi]_0^L \\ &\quad + \int_0^L \int_0^L \frac{1}{\gamma - 1} \frac{dp^h}{dt} \phi \end{aligned}$$

4.2 Need for stability

Using numerical methods in a straightforward way for the approximation of arbitrary differential equations may cause severe problems. There are Oscillations, locking, singular matrices and other problems in the result in certain concrete problem. Thus, stabilization is needed. To obtain satisfactory approximations stabilization may be needed. The matrix of the advective term is non-symmetric (non-self adjointness of the convective operator) and the best approximation property is lost. As a result Bubnov-Galerkin methods applied to these problems are far from optimal and show spurious oscillations in the solutions, worsening with growing convection-domination.

To characterize the relative importance of convective and diffusive effects in a given flow problem, it is useful to introduce the mesh Peclet number.

$$Pe = \frac{ah}{2\nu}$$

which expresses the ratio of convective to diffusive transport. The Galerkin solution is corrupted by non-physical oscillations when the Peclet number is larger than one. The Galerkin method loses its best approximation property when the non-symmetric convection operator dominates the diffusion operator in the transport equation, and consequently spurious node-to-node oscillations appear.

All stabilization schemes applied are Petrov-Galerkin approaches. They all add perturbations to the original Bubnov-Galerkin weak form. These perturbations are formulated in terms of modifications of the Bubnov-Galerkin test functions. They are multiplied with the residuals of the differential equations and thereby ensure consistency. Additionally, a stabilization parameter ξ weights the influence of the added stabilization terms.

4.2.1 Streamline Upwind Petrov Galerkin Method

To ensure that the solution of the differential equation is also a solution of the weak form, it is necessary to stabilize the convective term in a consistent manner. To accomplish this an extra term over the element interiors is added to the Galerkin weak form. This term has to be a function of the residual of the differential equation or else the equation will not be consistent. It introduces a certain amount of artificial diffusion in streamline direction only. The latter aspect ensures that no diffusion perpendicular to the flow direction is introduced, which was the reason for excessive over diffusion in other methods.

Stabilization through a product of a perturbation and the residual is a fundamental aspect of successful stabilization schemes and is realized in all stabilization method applied here. The following term is added to the galerkin weak form of the differential equation.

$$\sum_e \int_{\Omega^e} P(w) \xi R(u) d\Omega$$

Where $P(w)$ is a certain operator applied to the test function, ξ is the stabilization parameter (also called intrinsic time), and $R(u)$ is the residual of the differential equation. The stabilization techniques are characterized by the definition of $P(w)$

The SUPG stabilization technique is defined by taking

$$P(w) = a \cdot \nabla w$$

where a is the convection velocity. w is the test function. This corresponds to the perturbation of the test function. The space of the test functions does not coincide with the space of the interpolation functions, hence it is called as PetrovGalerkin formulation.

For simple convection diffusion equation $\tau = \frac{\vec{\nu}}{\|\vec{a}\|^2}$. For 1D $\vec{\nu} = \frac{\beta ah}{2}$ and $\beta = \coth(Pe) - \frac{1}{Pe}$

4.2.2 Pressure-Stabilizing/Petrov-Galerkin (PSPG)

In mixed convection-dominated problems, such as the incompressible Navier-Stokes equations with high Reynolds-numbers, SUPG and PSPG (called herein SUPG/PSPG) stabilization have to be applied to obtain satisfactory results. It should also be mentioned that the PSPG stabilization parameter does not necessarily have to be identical with the SUPG stabilization parameter

The terms associated with parameter ξ_{pspg} (pressure-stabilizing/Petrov-Galerkin) allow the use of mixed elements with equal-order interpolations for the velocity and pressure. All stabilization terms are weighted residuals, therefore ensuring the consistency of the formulation. The following term is added to the galerkin weak form of the differential equation.

$$\sum_e \int_{\Omega^e} \nabla \phi \xi_{pspg} R(u) d\Omega$$

4.2.3 Stabilized Navier Stokes Equation

From the stabilization discussions we can now write the stabilized form of Navier stokes equation. The Residual of momentum and energy equation are given as follows

$$\begin{aligned} R1(u) &= \rho \frac{Du^h}{Dt} + \frac{1}{M^2} \nabla p^h - \frac{1}{Re} \nabla \cdot (\mu^* (\nabla u^h + (\nabla u^h)^T)) - \frac{2}{3} \mu^h \nabla \cdot u^h I - \frac{1}{Fr^2} \rho g \\ R2(T) &= \rho C_p \frac{DT^h}{Dt} + \frac{1}{RePr} \nabla \cdot (k \nabla T^h) - \frac{1}{\gamma - 1} \frac{dp^h}{dt} \end{aligned}$$

Now adding the pressure stabilization and convection stabilization to momentum and energy equations we get the following expressions

$$\begin{aligned} \int_0^L \int_0^L \rho \dot{u}^h \psi_i \psi_j + \int_0^L \int_0^L \rho u^h \cdot \nabla u^h \psi_i + \int_0^L \int_0^L \frac{1}{M^2} \nabla p^h \phi_i + \int_0^L \int_0^L \frac{1}{Re} \tau^h \nabla \psi + \\ - \int_0^L \int_0^L \frac{1}{Fr^2} \rho g \psi + \sum_e \int_{\Omega^e} P(\psi) \xi R1(u) d\Omega + \sum_e \int_{\Omega^e} \nabla \phi \xi_{pspg} R1(u) d\Omega = [\tau \psi]_0^L \\ \int_0^L \int_0^L \rho C_p \dot{T}^h \varphi_i \varphi_j + \int_0^L \int_0^L \rho C_p u^h \cdot \nabla T^h \varphi_i - \int_0^L \int_0^L \frac{1}{RePr} (k \nabla T^h) \nabla \varphi - \\ \int_0^L \int_0^L \frac{1}{\gamma - 1} \frac{dp^h}{dt} \phi + \sum_e \int_{\Omega^e} S(\varphi) \xi R2(T) d\Omega + \sum_e \int_{\Omega^e} \nabla \varphi \xi_{pspg} R2(T) d\Omega = -\frac{1}{RePr} [k \nabla T^h \varphi]_0^L \end{aligned}$$

4.3 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

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