

Chapter 1

Introduction

Turbulent flows in the presence of one more solid surface, referred to as wall bounded flows, are prevalent in various practical situations. Wall bounded flows are important due to their extended use in engineering applications, such as the external flow around cars, ships, and buildings, the internal flows in engine pistons, pipes and channels. Many of these flows can also include the presence of a reacting region such as the combustor of jet engine or the flame spread along walls during accidental fires. The presence of reaction zones increases the complexity of the flow as well as the difficulty to understand and predict the flows using models. Further understanding of wall bounded turbulent flows where strong velocity and temperature gradients play a major role is clearly needed. The focus of this proposal is to present the numerical framework necessary to study the flow and heat transfer characteristics of wall bounded turbulent flows.

1.1 Numerical approach to turbulence computation

Often conducting wind tunnel experiments to study turbulent flows can be expensive and numerical simulations may provide an attractive low cost option. The solution of turbulent flows is possible through computational simulations that vary by their level of resolution and accuracy. The most reliable computational strategy is Direct Numerical Simulation (DNS) in which all length-scales are fully resolved; due to its unparalleled accuracy and high computational cost it is only feasible for low Reynolds number flows. At the other end of the spectrum, Reynolds Averaged Navier Stokes Equation (RANS) resolve only the mean motion and rely on modeling

the entire Reynolds stress tensor, it has been most widely used in the engineering community for simulating practical high Reynolds number or complex flows. However, RANS will typically fail to capture large scale instabilities that are fundamental to turbulent flow transport. Large Eddy Simulations (LES) represent a compromise between DNS and RANS since it does not intend to numerically resolve all turbulent length scales, but only a fraction of the larger energy-containing scales within the inertial sub range. Modeling is then applied to represent the smaller unresolved (SGS) scales, which contain only a small fraction of the turbulent kinetic energy.

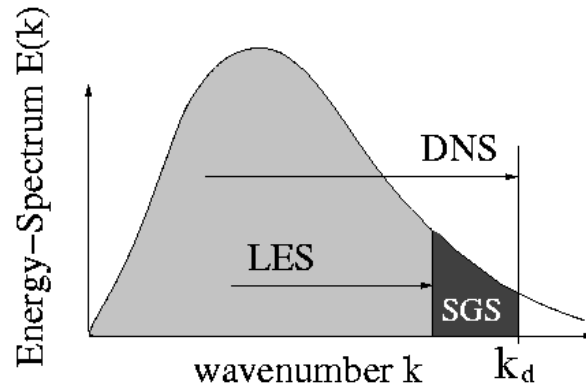


Figure 1. Energy Spectra for all scales of turbulent flow.

The solution of turbulent flow problems is theoretically possible through the direct numerical simulation (DNS) of the Navier-Stokes equations (with appropriate boundary conditions). This method constitutes the conceptually simplest approach to the problem of turbulence. Practically, however, the cost of DNS confines this approach to simple applications in terms of Reynolds number and geometry complexities. In fact, in DNS all scales of motion must be resolved, from the integral to the Kolmogorov scales. The computational domain must be on the order of the largest scale. This results in a number of grid points in each direction that is proportional to the ratio between the largest and the smallest scale, L/η . Defining a Reynolds

number based on the integral scale L, Re_L , the number of grid points (in each direction) will be proportional to $Re_L^{\frac{3}{4}}$, so a total number of points proportional to $Re_L^{\frac{9}{4}}$ is required by DNS. Moreover, the time step of the calculation Δt is typically limited by a CFL condition, that is $\Delta t < \frac{\Delta x}{U}$ where U is the local velocity determined by the integral time and length scale, we have that the total number of steps in time is $T/\Delta t$ again proportional to L/η . Thus the total cost of a DNS calculation will be on the order of Re_L^3 . This mean that for high Re numbers, DNS corresponds to a prohibitive computational cost: assuming that computer power will increase by a factor of 5 every five years, Spalart [1] estimates that DNS will not be applicable for the study of the flow over an airliner or a car until 2080. In this context, Large-eddy simulations (LES) presents a feasible alternative to DNS calculations since modeling is limited to the smallest scales of the flow. The large eddies containing the bulk of the energy, typically anisotropic and dependent on boundary conditions, are simulated directly. The fact that the small, dissipative eddies are modeled helps reduce the cost of LES considerably compared to DNS.

1.2 Boundary layer flows

Wall bounded flows are constrained by the presence of a solid wall which will enforce the no-slip condition (the velocity of the fluid at the surface must be equal to the velocity of the surface). They present a challenge since velocity and temperature gradients must be resolved and computed accurately to provide useful quantities such as wall shear stress, skin friction and heat fluxes. They may be categorized into homogenous or non-homogeneous according to certain characteristic presented along the direction of the mainstream. This feature is related to the behavior of the flow parameters after some distance or period due to a restriction imposed to the

flow. Typical examples are given by flow in pipes and channels after the development section, where boundary layers merge leading to a fully developed flow. From this point, the flow becomes homogeneous in the stream and spanwise and periodic conditions can be established. On the contrary, a spatially evolving boundary layer is a case of non-homogeneous flow due to the unrestricted growth downstream. The non-homogeneity showed along the flow direction makes them much more challenging to compute numerically than homogeneous flows because of the need to prescribe turbulent inflow information at the inlet of the domain at each time step.

The presence of turbulence in wall-bounded flows presents an additional challenge since they are characterized by much less universal properties than free shear flows and are thus more challenging to compute. A two layer model is normally assumed where the near wall region where viscosity (and diffusion) dominates is referred to viscous sublayer and the region outside of this called the outer (log) layer. Within the viscous sublayer, the characteristic velocity and length scales are set by the friction velocity and the viscosity providing wall viscous-units (See Chapter 4). As the Reynolds number increases and the thickness of the viscous sublayer decreases, the number of grid points required to resolve the near-wall structures increases. Thus, when LES is applied to wall-bounded flows at moderate to high Reynolds number it is still very demanding because of the inner layer resolution. In fact, as found in Chapman [2], considering a flat plate boundary layer, the outer part has energy-carrying structures on the order of the boundary layer thickness, δ . Assuming that the grid spacing is fixed in the streamwise and spanwise direction and on the order of 0.1δ , Chapman estimates a total number of grid points proportional to $Re_L^{0.4}$. In the inner part of the boundary layer, on the other hand, the number of points must be based on the inner layer scales; in fact, the dimension of quasi-streamwise vortices are constant in wall units (i.e., normalized by kinematic viscosity, wall stress and fluid

density). In this way, the total cost of the calculation in the inner layer is estimated to be proportional to $Re_L^{1.8}$ which makes this technique only suitable for moderate Reynolds number applications.

Alternatives to wall-resolved methods are wall-layer models for Large-eddy simulations in which three classes of models exist: Equilibrium stress models, zonal models, and hybrid LES/RANS methods. Equilibrium laws typically make use of wall-function relationships that provide the mean velocity (or temperature) in the near-wall region as a function of distance from the wall. The idea is to bypass the inner layer by using approximate boundary conditions. These boundary conditions assume the existence of an equilibrium layer in which the stress is constant resulting in the existence of a logarithmic layer that is typically used to relate the velocity in the outer layer to the wall stress. However, this technique is likely to fail for engineering flows having strong pressure gradients, separated flows or flows where the mean velocity is three dimensional (since these conditions eliminate the equilibrium stress layer approximation). These observations fueled the development of hybrid models in which simpler transport equations are solved in the inner layer and coupled to the outer flow LES. This idea was proposed by Balaras et al [3], Two-layer model (TLM), with a weak coupling between the inner and outer layers. A fine one-dimensional grid is embedded between the first grid point and the wall, and a simplified set of equations (generally, the Reynolds-averaged turbulent boundary-layer equations) is solved in the embedded mesh. The outer-layer LES provide the boundary condition for the inner layer, whereas the inner-layer calculation provides the wall stress required by the LES [3]. Hybrid simulations in which the RANS equations are used in the inner layer, while the filtered Navier–Stokes equations (LES) are solved in the outer layer are also of practical interest. Several

strategies can be used to switch between one model and the other, such as changing the length scale in the model from a RANS mixing length to one related to the grid size, or using a blending function to merge the SGS and RANS eddy viscosities. In terms of computational cost Equilibrium models are the least expensive. According to Piomelli et al [4], the cost of this simulation scales like the outer layer, $Re_L^{0.6}$. Zonal models require between 10% and 20% more CPU time for the solution of the boundary layer equations (in the inner layer), and an additional memory overhead. The cost of Hybrid RANS/LES methods is higher due to the restriction of resolving the wall normal direction ($y^+ \sim 1$) and the number of grid points in the wall-normal direction is proportional to $\log(Re_L)$ making the cost scale like $Re_L^{0.6} \log(Re_L)$.

1.2.1 Streamwise homogeneous flows: fully developed turbulent channel

Correct modeling of wall-bounded turbulent flows require special attention to the use of accurate boundary conditions. Furthermore, inflow turbulent conditions present additional challenges and are difficult to prescribe. In this context, fully developed turbulent channel flow can be considered from the end of the developing section, as seen in figure 1.2, and do not present the shortcomings associated with the time-dependent turbulent inflow conditions and represent a valuable precise tool for analyzing the near wall turbulent structures. This can be achieved numerically by prescribing periodic boundary conditions in the homogenous directions where the computational domain is assumed to be infinite. One of the first DNS of plane channels is attributed to Kim et al [4] where in their predictions, the Reynolds number is based on the wall friction velocity and the channel half-height, Re_τ was 180. Years later, this investigation was followed by a number of new plane channel predictions at much higher Reynolds numbers: Moser et al [5], Leonardi [6] and Jimenez's group [7]-[8] to name a few.

More recently, Hoyas and Jimenez [9] performed direct numerical simulations on a turbulent plane channel at $Re_t = 2000$ concluding that streamwise velocity fluctuations do not scale appropriately in wall units neither near nor away from the wall.

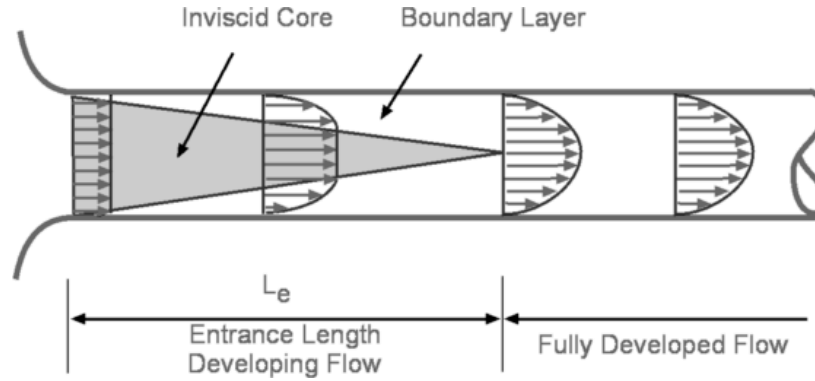


Figure 2. Fully Developed Planar Channel Flow Schematic.

1.2.2 Streamwise nonhomogeneous flows: spatially-developing flows

The case where the flow is allowed to develop naturally downstream, without any imposed restrictions, can be described as non-homogeneous in the streamwise direction. The classical canonical case of this is the spatially-developing boundary layer where if turbulent it presents a steep challenge for numerical predictions due to the specification of inflow fluctuations as a crucial boundary condition. It is observed from the literature that numerical simulations, both DNS and LES, about fully developed turbulent channel are numerous. On the contrary, numerical predictions of spatially evolving turbulent boundary layers are rather scarce because of the numerical challenge to prescribe time-dependent fluctuations at the domain inlet. Therefore, simulating a streamwise evolving flow implies the selection and application of a procedure able to generate realistic turbulent inflow data with a relatively high computational cost.

Several techniques for turbulent inflow generation have been employed with different degrees of success and a comprehensive review of these methods can be found in Lund et al [10] and Moin and Mahesh [11], and more recently in Keating et al [12]. The first DNS of a spatially developing boundary layer was carried out by Spalart [13]. He used a coordinate transformation to treat the streamwise inhomogeneity of evolving boundary layers as a homogeneous flow, and, consequently, agreeable to periodic conditions. The pioneering Spalart's approach is very ingenious but is limited to flows whose mean streamwise velocity variation is small as compared to the vertical variation, such as zero-pressure gradient (ZPG) flows. Consequently, in numerical simulations of more complex flows, both inflow and outflow boundary conditions must be established introducing an additional model for the treatment of flow leaving the domain. Originally, inflow conditions were generated by specifying a mean velocity profile and superimposing some random fluctuations, so called synthetic turbulence. Le and Moin [14] produced inflow conditions for DNS of a backward-facing step basically from a three dimensional, divergence free field of random fluctuations with prescribed moments and spectra. Random fluctuations were created by the proposed method of Lee et al [15]. Thus, this turbulent field was convected through the inflow plane by using the Taylor's hypothesis. However, the inlet turbulent structures required a long distance for accommodation and reaching a realistic state because the inflow information was void of the phase information of the real turbulent eddies. It was reported by Le and Moin [14] that 50 displacement thicknesses from the inlet channel were required to get a realistic turbulent flow, which seriously penalized the streamwise length of the computational box and, thus, increased the cost of the simulation. An improvement of the previous approach was proposed and tested by Na and Moin [16], and Akselvoll and Moin [17] by convecting an instantaneous turbulent field computed from an auxiliary temporal

simulation. This modification was observed to shorten significantly the evolution distances but at a high computational cost of having an extra numerical simulation.

More recently, Batten et al [18] introduced a new method to generate synthetic turbulence that takes into account the anisotropy of the flow. The method by Batten et al is based on the superposition of sinusoidal modes with random frequencies and wave-numbers, with given moments and spectra. Their approach includes an ingenious way to modify the wave numbers to yield eddies that are more elongated in the direction of larger Reynolds stresses, thus introducing more realistic anisotropic eddies into the flow. Spille-Kohoff [18] recently proposed a method that seeks to establish the correct Reynolds stress profiles earlier in the domain. They used a synthetic turbulent field at the inflow and a number of control planes downstream. At these planes, a controller amplifies the wall-normal velocity fluctuations to try to match the required Reynolds shear stress. These last two methods are further analyzed in the turbulence validation section of chapter 4. Finally, the simulations of even more complex evolving flows, of great need in engineering applications, require the use of appropriate methodologies for inflow conditions which is part of the focus of the present study.

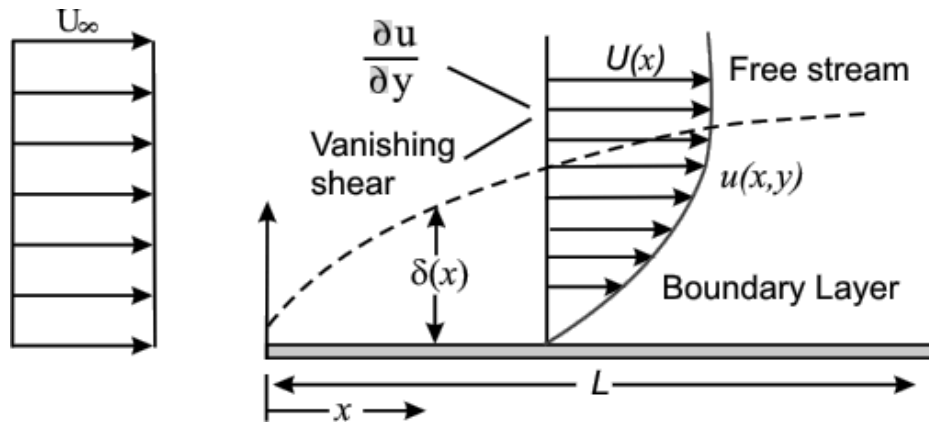


Figure 3. Canonical boundary layer flow schematic.

1.3 Transport of scalars in wall-bounded flows

The transport of scalars is important in various engineering applications ranging from combustors, boilers to thermal boundary layers as found in turbine blade film cooling. In many cases, there is a two way coupling between the scalars and the flow: the transported field can influence the velocity field – which is known as active scalar transport. This is the case, for example, of the temperature field that acts on velocity through density changes. Conversely, situations where the feedback of the scalar field is negligible and the velocity determines the properties of the scalar, but not vice versa, are termed passive. This ideal case is well approximated by the use of dye in laboratory experiments or by the transport of smoke and low concentration pollutants. Although active and passive scalars are governed by the same advection-diffusion equation, their nature is radically different. Passive scalars belong to the category of linear problems, despite being highly nontrivial. Celani et al [19] reports that as a consequence of the statistical independence of the temperature fields and the advected velocity, the transported fields depend linearly on the temperature. This property allows a theoretical treatment of the problem, and has the major consequence that the passive scalar scaling laws are universal with respect to the injection mechanism. On the contrary, for active fields, the presence of the feedback couples the velocity with the transported scalar and makes the problem fully nonlinear. In this case, the theoretical tools developed for studying the passive problem may fall short of explaining the behavior of active scalars, and the current understanding of active turbulent transport lags far behind the knowledge accumulated on the passive counterpart.

One of the first numerical simulations with respect to the transport of passive scalar fields was performed by Kim and Moin [20] at a Reynolds number of 180 (based on wall friction velocity and channel-half width) and at various molecular Prandtl numbers. They considered two

different types of boundary conditions. In the first case, the heat is generated internally and removed from isothermal walls at the same temperature. In the second case, isothermal walls at different temperatures create a temperature gradient and drive the heat transfer. More recent work of DNS of turbulent heat transfer in channels have been performed and a comprehensive progress of the topic can be found in Kasagi and Iida [21], Kasagi et al [22] and Keating [12].

In the following sections, a literature review of investigations on active scalars is presented for streamwise homogeneous and non-homogeneous wall bounded flows.

1.3.1 Fully developed turbulent channel with heat transfer

The case of streamwise homogeneous flows with strong heat transfer and variable property has been studied extensively by various researchers. Two regimes of interest often found in the literature with this configuration are: subsonic, low Mach number flow and compressible high Mach number flow; where the role of pressure becomes vital in understanding the difference between the two methods. Fully compressible numerical formulations are constrained by the need to resolve fast acoustic wave motions; hence the density is dependent on both temperature and pressure increasing the complexity of the system. In the low Mach number limit where density becomes independent of pressure, the role of pressure is to act on velocity through continuity so that conservation of mass is satisfied. For low speed flows, the pressure gradient needed to drive the velocities through momentum conservation is of such magnitude that the density is not affected significantly and the flow can be considered nearly incompressible. Hence, density and pressure are very weakly related. Thus for slow flows, the low Mach number formulation, where the acoustic properties are filtered out becomes a computationally cost efficient method to use.

One of the first variable property channel flow numerical study was carried out by Wang and Pletcher [24]. They performed an LES study of low Mach number isothermal channel flows with one hot wall and one cold wall, with temperature ratios as high as 3. The heat transferred by the hot wall was removed from the channel through the cold wall so there was no bulk temperature rise. Results showed the minimum velocity fluctuations at the center because there was no mean velocity gradient at that location. However, the temperature fluctuations remained large near the center of the channel. Since there is energy transfer from the heated to the cooled wall, the whole domain contains temperature gradients including the center of the channel. The compressible formulation of the dynamic SGS model was utilized in a staggered grid finite volume method that was fully implicit.

Nicoud and Poinso [25] applied DNS to a very similar configuration and pointed out that some of the observed effects might be explained through the different local values of Reynolds number obtained near the hot and cold walls. A higher Reynolds number was observed near the cold wall and a lower one was found near the hot wall. The variations in Reynolds number were thought to be responsible for a variation in the size of the turbulent structures. The structures near the hot wall were much larger than those near the cold wall. These different Reynolds numbers were obviously due to different density and viscosity values which were functions of temperature. This configuration will be explained in more detail in the LES validation chapter of this proposal.

1.3.2 Natural convection heat transfer

Modeling transport in thermal boundary layers is the main objective of this proposal. The target configuration corresponds to a non-homogeneous natural convecting shear layer obtained through the interaction of a hot surface in quiescent surrounding fluid. This configuration has been extensively studied analytically, experimentally and more recently computationally. A similarity solution was carried out by Ostrach [26] for various Prandtl numbers which were in good agreement with previous experiments and is now a classical problem for flows in the laminar regime.

Turbulent natural convection boundary layer next to a heated vertical surface was analyzed by George & Capp [27] using classical scaling arguments. In this theoretical investigation, the boundary layer is treated in two parts. An inner region in which the mean convection terms are negligible and is identified as a constant heat flux layer and an outer region which makes up most of the boundary layer (log-region) where conduction terms are negligible. In this work, universal velocity and temperature profiles for asymptotic values of Rayleigh number (approaching infinity) are suggested for both constant heat flux and constant temperature boundary conditions. The proposed theory was modified later by Wosnik & George [28] and it was claimed that the new scaling functions were valid both in the limit of infinite Rayleigh number and for any position downstream well into the turbulent regime.

Turbulent transport in a natural convection along a vertical plate has been studied experimentally and it was shown that the large eddy motions play an important role on the turbulent transport. Tsuji & Nagano [29] performed an experimental study of natural convecting heat transfer boundary layer in detail compared to previous researches. Characteristics of the

near wall region were studied and applicability of the conventional analogy between heat and momentum transfer and the concept of the viscous sublayer for natural convection were investigated. The structure of turbulent natural convection boundary layer was studied further by Tsuji & Nagano [30] and it was shown that this phenomenon has a unique turbulent structure which is rarely seen in other turbulent boundary layers.

Natural convecting boundary layer has also been studied numerically. Many investigations have been carried out and useful results have been proposed. Considering RANS computations, a v^2-f and a $k-\epsilon$ model were compared with the experimental data for two different geometries by Tiezen et al [31] while at CTR Stanford University. The two considered geometries were a vertical plate and a differentially heated cavity. Three treatments of buoyancy/turbulence coupling were compared and it was shown that the v^2-f model together with employment of a buoyant production term which was defined based on generalized diffusion hypothesis yielded the best results.

Peng & Davidson [32] studied the LES of turbulent flow in a confined cavity and compared the results with the experiment of Tian & Karayiannis [33] and Tian & Karayiannis [34]. It was shown that mean flow quantities were in good agreement with the experimental results. However, there were some discrepancies in the prediction of turbulence statistics especially in the shear layer region between the wall boundary layer flow and the cavity core region. It is suggested that special attention should be paid to the flow physics and numerical treatment in this region. A comparative study of LES of turbulent buoyant flow in a cavity with different SGS models and grid resolutions was also performed by Peng & Davidson [35]. It was shown that although the proposed SGS model was able to predict mean flow quantities, it was

unable to recreate the turbulence quantities particularly in the core region. It was also shown that the energetic flow structures which are enhanced by buoyancy in the boundary layer along the heated and cooled walls of the cavity, exist in the outer layer neighboring the nearly stagnant core region of the cavity. Using DNS, Natural convection between two vertical differentially heated walls was studied by Nieuwstadt & Versteegh [36]. The major topic of investigation in this study was the self-similarity behavior of the results following the scaling hypothesis proposed by George & Capp [27]. It was shown that the proposed scaling approach leads to self-similarity for the mean temperature profile but it fails for the mean velocity profile. In another study, Versteegh & Nieuwstadt [37] investigated the turbulent budgets of natural convection in an infinite, differentially heated, vertical channel. It was found that close to the wall, the shear production of turbulence was negative. It was also mentioned that modeling of pressure strain and transport as separate terms is not a good idea while the combination of these terms behaves in a more continuous way especially near wall.

1.4 Boundary Layer Combustion – Flame spread

The main, long-term objective of this work is the detailed study of diffusion flame-spread along vertical walls. The literature and experimental results for this configuration is wide providing an ample database for flame spread validation cases. Studies starting with de Ris [38] and followed by Altenkirch et al. [39], Zhou et al. [40], Wichman et al. [41-42], and Bhattacharjee et al. [43-44] have focused on opposed flow flame spread (air flow opposed to the spread direction). Other studies have focused on vertical flame spread (wind-aided or concurrent flow spread). Concurrent flow flame spread rates are faster than opposed flow flame spread rates and are inherently unsteady, accelerating as pyrolysis heights increase. Markstein and de Ris [45]

investigated upward fire spread over textiles. They found an accelerating flame spread rate and characterized it by a power-law relationship between pyrolysis spread rate V_p and pyrolysis height H_p : $V_p = \beta H_p^n$. Orloff et al. [46] examined the upward fire spread rate for vertical polymethyl methacrylate (PMMA). With 4.5 cm thick, 41 cm wide, and 157 cm high vertical PMMA slabs, they observed flame spread remained relatively constant for pyrolysis heights from 10 to 15 cm and subsequently became proportional to H_p : $V_p = 0.0041H_p^{0.964}$.

Fire behavior of PMMA was studied comprehensively by Tewarson and Ogden [47]. They also found flame spread rates accelerate for upward spread. The total heat fluxes to the solid flame region ranged from 20 to 30 kW/m² for 0.61 m PMMA samples, which agreed with the analysis by Quintiere et al. [48]. Wu et al. [49] conducted a 5 m high PMMA vertical wall panel experiment. The heat release rate and pyrolysis heights increased exponentially as a function of time. Total heat fluxes to the fuel surface varied from 30 to 40 kW/m².

1.4 Outline of current work

The main objective of this dissertation is to present the development of an in-house low-mach number boundary layer solver with LES capabilities. The main feature of this new software is its ability to handle variable density flows while using advanced turbulence models. It is intended to be a prediction tool that can provide high-fidelity, high resolution numerical studies of laboratory experimental configurations. This proposal organized as follows: The numerical methods and LES variable density developments are discussed and presented in Chapter 2. Chapter 3 presents validation studies of forced convection boundary layers and classical results from laminar and

turbulent flows with and without heat transfer. Chapter 4 presents another validation study conducted in the natural convection regime, results from the classical Ostrach solution is presented as well as the classical result from Tsuji & Nagao and the fidelity of the code is established. Lastly, Chapter 5 presents the direction and outline of future work, including further development and validation plans to address turbulent boundary layer combustion problems.

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