Containment Analysis Incorporating Boundary Layer Heat and Mass Transfer Techniques

by

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Abstract

A new condensation heat transfer methodology has been implemented into a coarse-mesh finite-volume computer code. This methodology combines heat transfer logic based on bulk properties with the flow representation required to capture boundary layer phenomena. Application of the methodology increases the ability of the finite-volume code to predict thermal stratification, which in certain situations depends on resolving boundary layer flow adjacent to a vertical condensing surface. To achieve this, the meshing strategy employs relatively small computational cells near the surface. This approach was originally identified by Gavrilas, who proposed a noding strategy consisting of a single narrow near-wall cell and an associated heat transfer model. These concepts are extended in the present work, in which the boundary layer hypothesis is proposed and tested. The boundary layer hypothesis consists of: 1) utilizing two near-wall computational cells having prescribed thicknesses; and 2) employing an appropriate condensation model. In order to demonstrate the utility of the boundary layer hypothesis, the source code of the GOTHIC 4.1c containment analysis program was modified to include the chosen condensation model and to extend the computational algorithm to allow the condensation model to be implemented correctly. A test computational problem demonstrating stratification is presented and a proposed experiment to test code capabilities is described.

A thorough literature search was performed to assess the applicability and usefulness of the available condensation models for use in the boundary layer hypothesis. The diffusion layer model (DLM), originally proposed by Peterson, was chosen as the most appropriate model for three reasons. First, the DLM is more general and accurate than the empirical model of Uchida, which is widely used in containment analysis. Second, a modified version of the DLM has been verified against experimental data from facilities which are representative of advanced containment designs. Third, the DLM is physically grounded in mass transfer theory, consistent with the assumption of a downward flowing boundary layer, and compatible with the formulation of the boundary layer hypothesis and most finite-volume containment codes. The physical basis allows the DLM to be useful for both BWR and PWR prototypic accident scenarios, where the noncondensible gas concentration is low and high, respectively. A thorough analysis of the DLM was performed to compare the model qualitatively and quantitatively to other condensation models and to experimental data covering a range of expected containment conditions. An analysis to determine model sensitivity to changes in key properties was also performed. The results of these analyses show that the DLM is more capable than the other models studied to correctly account for the influence of air, helium, and hydrogen on the condensation process.

Thesis Advisor: Dr. Neil E. Todreas
KEPCO Professor of Nuclear Engineering
and Professor of Mechanical Engineering
Dedication

To my parents, Beverly and Kenneth, and my sister Jeanette,

for their patience and support in this endeavor
Acknowledgements

I would like to express my sincere appreciation for the help and guidance that my thesis advisors, Professor Neil Todreas and Professor Michael Driscoll, have given me over the course of this endeavor. Working with them has been a worthwhile and enjoyable experience, both personally and professionally. Thanks to Professor Mirela Gavrilas, University of Maryland, for her friendship, guidance, and encouragement in tackling some of the subject matter in this thesis. Tom George, NAI, deserves a great deal of credit for facilitating the modifications to the GOTHIC source code. Without his timely advice and assistance the code modifications would not have been possible. Professor Peter Griffith, MIT, helped me to refine the specifications for the boundary layer hypothesis. Dr. Mark Anderson and Professor Corradini at the University of Wisconsin-Madison were instrumental in my quest to evaluate the diffusion layer condensation model. They provided information on their experimental data, computer code listings, and preprints of their articles on the subject. Dr. Anderson also helped significantly by participating in several lengthy exchanges to resolve technical questions concerning the derivation of some key elements of the model. Thanks especially to Jennifer deVries Gwinn, MIT, for her assistance in keeping my paychecks coming over the course of the project. Finally, thanks to Dr. David Freed, Tanya Williams, and Paul Fallon for their steadfast friendship and constant encouragement. I could not have done it without them.

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NOMENCLATURE

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<thead>
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<th>Symbol</th>
<th>Description</th>
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<tr>
<td>( B_m )</td>
<td>mole transfer diffusion driving force</td>
</tr>
<tr>
<td>( \varepsilon_m )</td>
<td>mass transfer diffusion driving force</td>
</tr>
<tr>
<td>( c_p )</td>
<td>heat capacity at constant pressure</td>
</tr>
<tr>
<td>( c )</td>
<td>gas concentration (molar density)</td>
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<tr>
<td>( C^* )</td>
<td>blowing factor (suction factor)</td>
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<tr>
<td>( C_f )</td>
<td>skin friction coefficient</td>
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<td>( d )</td>
<td>tube diameter</td>
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<td>( D_{12} )</td>
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<td>time</td>
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\( T \) \([\text{K}]\)  \( u,v,w \) \([\text{m} / \text{s}]\)  velocity vector components  
\( u_* \) \([\text{m} / \text{s}]\)  friction velocity  
\( v' \) \([\text{m} / \text{s}]\)  molar-average mixture velocity (scalar)  
\( v' \) \([\text{m} / \text{s}]\)  molar-average mixture velocity (vector)  
\( v_n \) \([\text{m} / \text{s}]\)  absolute velocity of species \( n \) (scalar)  
\( v_n \) \([\text{m} / \text{s}]\)  absolute velocity of species \( n \) (vector)  
\( V \) \([\text{m} / \text{s}]\)  velocity vector  
\( U,V,W \) \([\text{m} / \text{s}]\)  average velocity components  
\( W \) \([\text{m} / \text{s}]\)  mass fraction  
\( x,y,z \) \(-------\)  coordinate directions  
\( X \) \(-------\)  mole fraction

**Greek symbols**

\( \alpha \) \([\text{m}^2 / \text{s}]\)  thermal diffusivity  
\( \Gamma \) \([\text{(kg} / \text{m}^2-\text{s}) / \text{m}]\)  mass flux per unit circumference  
\( \delta \) \([\text{m}]\)  thickness  
\( \delta_{ij} \) \(-------\)  Kronecker delta  
\( \varepsilon \) \([\text{kg} / \text{m} \cdot \text{s}^3]\)  dissipation rate of turbulent kinetic energy  
\( \mu \) \([\text{kg} / \text{m} \cdot \text{s}]\)  dynamic viscosity  
\( \nu \) \([\text{m}^2 / \text{s}]\)  kinematic viscosity (momentum diffusivity)  
\( \rho \) \([\text{kg} / \text{m}^3]\)  density  
\( \sigma_k \) \(-------\)  turbulent Prandtl number for \( K \)  
\( \sigma_\varepsilon \) \(-------\)  turbulent Prandtl number for \( \varepsilon \)  
\( \tau \) \([\text{N} / \text{m}^2]\)  shear stress  
\( \nu \) \([\text{m}^3 / \text{kg}]\)  specific volume  
\( \Theta \) \(-------\)  blowing or suction factor

**Dimensionless Groups**

\( \text{Gr}_x \) \( = \left( \frac{\Delta \rho}{\rho} \right) x^3 / v^2 \)  Grashof number  
\( \text{Ja} \) \( = c_p \left( T_b - T_i \right) / h_f \)  Jacob number  
\( \text{Le} \) \( = \left( \alpha / D_{12} \right) = (Sc / Pr) \)  Lewis number  
\( \text{Nu}_x \) \( = h x / k \)  Nusselt number  
\( \text{Pr} \) \( = \left( \mu c_p / k \right) \)  Prandtl number  
\( \text{Re}_x \) \( = \left( \rho u x / \mu \right) \)  Reynolds number  
\( \text{Sc} \) \( = \left( \mu / \rho D_{12} \right) \)  Schmidt number  
\( \text{Sh}_x \) \( = \left( g_m x / c D_{12} \right) \)  Sherwood number  
\( \text{St} \) \( = h / \rho c u_b \)  Stanton number  
\( \text{St}_m \) \( = \left( g_m / \rho u \right) \)  Stanton number for mass transfer
**Subscripts**

1. without shear stress
2. with shear stress
\( a,\text{air} \) air property
\( \text{avg} \) average
\( b,\text{bulk} \) bulk steam/gas mixture property
\( c \) condensation
\( \text{cond} \) condensation
\( \text{conv} \) convection
\( e \) free stream quantity
\( fg \) liquid to vapor phase change
\( g \) noncondensable gas property
\( (\text{at gas partial pressure}) \)
\( i \) evaluated at the condensate interface
\( i,j,k \) indices for tensor notation
\( l \) liquid (condensate) property
\( \text{la} \) laminar
\( m \) steam/gas mixture property
\( \text{rad} \) radiation
\( s \) steam property
\( (\text{at steam partial pressure}) \)
\( \text{sf} \) smooth condensate film
\( t \) turbulent
\( \text{tbf} \) turbulent boundary layer
\( T \) total
\( v \) vapor (steam)
\( w \) evaluated at the wall
\( \text{wf} \) wavy condensate film

**Superscripts**

- average value
- \( FC \) forced convection
- \( NC \) natural convection
- \( \text{sat} \) water/steam saturation property
- \( \text{ss} \) steady state
- \( \text{trans} \) transient
1. INTRODUCTION AND BACKGROUND

1.1 Introduction and Reasons for this Work
The main focus of this thesis is to advance the analysis techniques which are used to evaluate and predict the performance of passive nuclear reactor containment systems. The current analysis techniques rely heavily on computerized tools to simulate phenomena such as circulation and condensation inside the containment vessel. The analyst has benefited from advances in computer speed in recent years, making detailed, computationally intensive, simulations possible. This increased level of detail allows the modeler to resolve small changes in buoyancy or mass concentration within the containment structure. This resolution is necessary for predicting the performance of passive containment systems since most passive systems rely on buoyancy differences or other small gradients to provide the driving force for operation. However, greater detail is not the only advance needed to predict passive system performance. The models which are implemented in the computational tools must be used in a manner which is consistent with their derivation. Choosing the correct phenomenological models and properly implementing them, using the appropriate level of resolution, is the key focus of this project.

The project was performed in three stages. The first stage was a thorough review of the current state of knowledge for the phenomena encountered when predicting containment performance. As such, the first stage centers primarily around evaluation of several computer codes and different condensation models. The second stage consisted of a sensitivity study on the most appropriate condensation models identified in stage one and a careful evaluation of how to implement them properly into the tools that MIT has available to predict containment performance. The third stage consisted of numerically studying natural convection, turbulent, condensation boundary layers and finally implementing a new condensation boundary layer model into the finite-volume computer code GOTHIC, which is used for overall containment assessments.

The remainder of this chapter gives some background for the work which is presented in the following chapters. Section 1.2 gives a description of the key physical phenomena which must be modeled in order to predict the performance of an advanced containment system with passive heat removal. Section 1.3 reviews several containment analysis codes which are currently available and lists their strengths and weaknesses. Section 1.4 gives an overview of the condensation models available and outlines the literature review given in Appendix A. Section 1.5 gives a short review of the condensation mass transfer theory which is central to the condensation model which is focused on in the remainder of the thesis. Finally section 1.6 gives an overview of the work presented in the remaining chapters.

1.2 Physical Phenomena in Containment Analysis
This section identifies the key phenomena that are encountered in a passive containment facility. In order to simulate the integral performance of a passive containment system, the analysis tool, usually a computer code, must predict the interaction between several different phenomena under changing conditions. The three phenomena which are most important in a passive containment system are: condensation of steam (often in the presence of a noncondensible gas); natural and
mixed convection; and stratification of liquid and vapor regions. These three phenomena are discussed in more detail below.

1.2.1 Condensation

Condensation is the primary means of removing heat and limiting the pressure increase following a loss of coolant accident (LOCA) inside any nuclear reactor containment vessel. Historically, suppression pools, fan coolers, and water sprays have been used to rapidly condense water vapor and reduce the overall containment pressure and temperature. A suppression pool, while a feature in many traditional containment designs, is also an example of a passive system that performs a primary function in limiting pressure rise. The suppression pool does not require power to function and is a fast acting and highly effective method of condensing a large amount of steam in a short period of time. However, a traditional suppression pool loses effectiveness after the initial blowdown period, when the pressure difference between the drywell and the wetwell becomes small. New designs must be employed to keep passive systems like a suppression pool functioning in order to control the long-term containment pressure in the absence of active heat removal systems.

During and after the blowdown period, condensation on heat sinks inside the containment vessel plays a key role in helping to limit the pressure in a passive containment system. In the short-term \( t < 500 \text{ seconds} \) fast acting heat sinks are very effective as cool surfaces for condensation. However, these fast acting heat sinks, which are mostly steel components, become saturated quickly, and only the large steel and concrete containment structures and in-containment water pools remain as inherent surfaces for condensation in the long term. Since decay heat continues to be released into the containment following the initial blowdown, long-term heat removal is necessary to reduce the containment pressure. This heat removal is usually accomplished by a combination of methods. The passive heat capacity of the containment structures are important contributors, and in addition several containment concepts have long-term passive heat removal systems that are designed to condense water vapor.

Modeling condensation on surfaces and in passive systems is not always a straightforward task. Two complications arise immediately. The first is the presence of a noncondensable gas, the second is the geometric layout of the containment and the heat sink surfaces. A noncondensable gas acts to severely hinder the condensation process. Whereas condensation of pure steam is generally limited by the resistance to heat transfer of the condensate film, condensation in the presence of a noncondensable gas is diffusion limited. While the steam/gas mixture moves toward the cool surface, only the steam changes phase to liquid, leaving the noncondensable gas to collect at the interface. This gas buildup forms a diffusion boundary layer. In order for the steam to condense, it must first diffuse through this noncondensable boundary layer, causing a decrease in the condensation rate. Because the noncondensable gas builds up at the interface, a very small concentration of noncondensable gas in the bulk atmosphere can cause a severe decrease in condensation rate.
Figure 1-1 illustrates the situation for a flat vertical wall. At the outer limits of the boundary layer, the partial pressures of steam and air are in equilibrium with the local atmospheric conditions. As one moves through the boundary layer toward the condensate film, the steam partial pressure decreases while the air partial pressure increases. At steady state, the partial pressure of air at the interface reaches an equilibrium condition where the amount of air being carried to the interface by the incoming steam-air mixture exactly equals the amount of air diffusing away. The condensation rate is limited by the amount of steam that can diffuse or convect through the air layer. Steam diffusion is driven by the steam partial pressure gradient between the bulk conditions and the interface, whereas steam convection is a result of fluid motion within the boundary layer. A suitable condensation model which represents these phenomena must be employed to accurately predict the condensation rate on large surfaces inside the containment. Choosing such a model is the basis for the condensation literature review which is presented in Appendix A.

Further complications for modeling condensation arise from the complex geometries involved. The containment vessel houses pumps, ladders, walkways, pools, and many other structures that act as heat sinks following a LOCA. Condensation inside tubes in a passive condenser is also different from condensation on a surface in contact with a large atmosphere. As gas flows through the tube, steam can not diffuse in from a near-infinite bulk mixture region as is the case for condensation on walls. Thus, the entire mixture inside the tube (not just the boundary layer) becomes depleted of steam. Ideally, the computer code used to analyze the containment response would be able to represent the condensation on each structure taking into account the different geometric influences on airflow and condensation rate. When trying to predict the long-term pressure response of a containment system, this approach is far too cumbersome for efficient analysis, and fortunately can be avoided based on rational arguments. Section 2.2 discusses this problem in detail.
1.2.2 Natural convection and steam stratification

In traditional containment designs, active systems such as water sprays and fan coolers force the atmosphere inside the containment to remain relatively well mixed following a LOCA. A well mixed atmosphere simplifies a containment performance analysis by allowing the analyst to treat the atmosphere as a single homogenized region. With a homogenized atmosphere, all heat sinks and containment surfaces can be assumed to be in contact with a vapor mixture that is at a uniform temperature and steam concentration. When the assumption of a well mixed atmosphere is valid, the containment pressure response can usually be evaluated using analytical methods or simple computer programs based on a lumped parameter modeling approach. When this assumption is not valid, a more complex modeling approach is necessary.

In many passive containment systems, the steam atmosphere cannot, a priori, be assumed well mixed. Immediately following a LOCA, the atmosphere will be relatively homogenous as a result of the violent mixing which occurs during the blowdown. However, after the blowdown has ceased and steam begins to condense on structures and passive systems begin to operate, the atmosphere may begin to stratify. In the case of the boiling water reactor SBWR design, the upper drywell and lower drywell are connected through a relatively small opening. In addition, the lower drywell is a “dead end” volume. The result is that during the blowdown the gas in the upper drywell is forced into the suppression pool, while the gas in the lower drywell is merely compressed by incoming steam. Thus at the end of the blowdown phase, the drywell atmosphere is not uniformly mixed in all areas. A similar situation exists in the pressurized water reactor AP-600 design. The below-operating-deck rooms in the containment are somewhat isolated from the above-deck region, and some do not participate in the violent mixing that occurs. The high concentrations of noncondensable gas in these regions cause the gas to diffuse back into the steam-rich regions. Thus the gas/steam mixture is not uniform once this later mixing begins to occur.

Many of the structures that act as passive heat sinks are located in small rooms within the containment building. After a LOCA the steam concentration in these rooms may be different from the concentration in the bulk atmosphere due to a higher condensation rate. Most importantly, however, is the approach used in representing the difference in steam concentration that exists within the bulk atmosphere of the drywell region. Steam is generally more buoyant than air, thus in the absence of strong mixing forces one would expect a steam-rich region to develop near the top of the containment vessel, with an air-rich region in the lower containment. Clearly, accurate modeling of condensation on the heat sinks in these regions will be depend on the local steam concentration, and treating the atmosphere as one homogenized region could introduce significant errors into the analysis. Also, for designs which use passive condensers, such as the SBWR, it is important to know the steam-air concentrations at the condenser inlets in order to calculate the correct rate of heat removal by the condenser units.

All of these factors point to the need for modeling natural convection within the containment atmosphere. Natural convection is a process in which buoyancy provides the forces which cause fluid motion. Correctly modeling this fluid motion is essential if one wishes to predict stratification within the containment and the correct heat transfer rates on containment surfaces. Condensation on walls will cause a cooling effect that induces the down-flow of the steam-air
mixture at the wall. This causes shear induced mixing forces in the surrounding fluid. Conversely, a hot steam plume will rise, entraining other fluid with it, causing a second type of mixing motion. Modeling these natural convection processes requires a relatively fine computational mesh within the open containment space and a computer code which can calculate two- or three-dimensional flow within a region. When the natural convection forces can be modeled by the computer code, phenomena such as stratification and location-specific heat transfer are amenable to prediction.

### 1.2.3 Thermal stratification in water pools

Stratification of steam within the containment atmosphere was discussed above in the section on natural convection. However, thermal stratification within a water pool is also a key phenomenon within a passive containment design. The two most important pools considered here are the suppression pool and the passive cooling condenser pool. A suppression pool generally has several vents which allow steam from the drywell to enter the suppression pool at different elevations. Figure 1-2 shows a typical suppression pool configuration.

For a large break LOCA, the pressure difference between the drywell and suppression pool will be sufficient that steam will be forced through all three vertical vent openings into the pool. This will cause the pool to become relatively well mixed. For a small break LOCA, the pressure rise in the drywell may only be sufficient to force steam through the top vertical vent opening. In this situation, it is expected that the suppression pool will stratify. Stratification in a suppression pool caused by a low steam flow rate was the subject of experimental investigation in Japan [Kataoka, 1992]. Kataoka showed that stratification occurs just below the steam release point and is quite well defined. The water above the stratification layer is uniformly warm, whereas the water below the stratification layer is uniformly cool. The stratification layer moves downward via conduction only. This phenomenon essentially reduces the amount of water which acts in the steam suppression process, thereby reducing the total heat capacity available for safety functions.
A more important consequence of this type of stratification can occur in the suppression pool of a SBWR type reactor, where the passive containment cooling system (PCCS) vents noncondensable gases from the passive condensers. This arrangement is also shown in Figure 1-2. In the case where the PCCS condensers are not able to condense all of the steam, there will be some steam which gets vented to the suppression pool along with the noncondensable gases. This steam will then condense in the suppression pool and cause heating of the top layer of water which is above the PCCS vent tube outlet. Since this steam/noncondensable mixture has a very low velocity, no significant mixing will result and a stratification layer is expected to form. The problem associated with this is the wetwell gas space pressure. The wetwell gas pressure is a strong function of the temperature of the water surface, since the saturation pressure of water vapor and the temperature (and thus pressure) of the noncondensable gas are closely related to the water surface temperature. A significant rise in the water surface temperature will cause a corresponding rise in the wetwell gas space pressure, and thus a rise in the pressure of the drywell. This phenomenon opposes the desired effect of long-term pressure reduction as a result of PCCS operation and should be captured in a containment performance analysis.

A second type of water pool that may become stratified during a LOCA is the PCCS pool in an advanced containment design. The passive condensers are submerged in a pool of water which acts as the secondary side heat sink. In most designs steam from the containment condenses on the tube inner surface and the heat released from condensation causes the water in the pool to boil. Since the steam/air mixture enters the condensers from the top, the highest rate of condensation occurs at the tops of the tubes. Thus the highest rate of heat transfer to the liquid is also near the top of the pool. The water at the top of the pool is at a lower hydrostatic pressure, and thus boils more rapidly than the water further down in the pool. These effects may combine to produce pool stratification, especially in the absence of vigorous boiling, which may be the case late in the transient. The effects of varying pool temperature on the PCCS system may be a significant factor in determining the overall performance of the containment system.

The ability of a computer code to predict pool stratification is directly related to how it models convection and fluid motion. A code which is able to predict natural convection in the gaseous atmosphere, should be able to predict stratification in water pools, if the code is a general two-phase code. Because liquid water has a significant density, a haphazard noding scheme can induce spurious mixing currents and force mixing in cases where stratification should be observed. Attention should be paid to the specific computer code instructions on how to avoid such numerical problems. Although pool modeling has been identified as a key parameter in containment analysis, this topic is not be covered in the remainder of the thesis. Instead, the focus is on the problem of condensation and circulation within the vapor region, which is considered to be more urgent.

1.2.4 Location of phenomena

The three basic phenomena discussed in this section have been determined to be of primary importance when evaluating the performance of a passive containment system. Figure 1-3 shows a simplified layout of a suppression pool-type advanced reactor containment system with the locations of the key phenomena indicated. The most important phenomenon is condensation in the presence of a noncondensable gas which occurs in the condenser tubes and on passive heat
sinks such as walls, floors, and steel components. Section 1.4 presents an overview of the different condensation models that are available for use in analyses of this type.

Figure 1-3: Location of key phenomena inside the volumes of a passive suppression pool-type containment system

1.3 Summary of Condensation Literature Review
A large part of the background work for this thesis consisted of a thorough literature review of condensation models for both internal and external surfaces. Since a containment atmosphere nearly always has noncondensable gases present, the literature review focused on condensation with this condition. There have been many models developed recently for both condensation on large surfaces and inside tubes. The structure of the models ranges from purely theoretical to purely empirical, with several somewhere in between. Not all of the models are easily implemented into some of the less sophisticated, early computer codes. However, advances in computer analysis techniques in the last decade have made implementation of complex models much easier. Appendix A gives a review of the most relevant condensation work published in the last fifteen years, and the reader is referred to it for an in-depth look at each of the models. This section summarizes the results of the literature review and highlights which models will be the focus for the remainder of the thesis. Most of the discussion past this point will be concerned with condensation on large external surfaces as opposed to condensation inside tubes.

1.3.1 Early empirical models
The most widely known empirical models for condensation inside a containment building are those of Uchida and Tagami [Uchida, 1965; Tagami, 1965]. These models have been used for many years as the standard tool for predicting inside containment condensation rates. Uchida and
Tagami performed condensation experiments using a small cylinder in a vessel which was initially filled with one atmosphere of a noncondensable gas. The gases studied were air, nitrogen, and argon. During the Uchida tests, the cylinder surface temperature was held constant while the vessel was filled with steam until a steady state pressure was reached. A curve fit to the Uchida steady state data results in the expression below which is often referred to as the Uchida model:

\[
\bar{h} = 379 \left( \frac{m_s}{m_r} \right)^{-0.707} (W / m^2 K)
\]  

(1.1)

Tagami gathered transient data and produced a set of equations which can be used to describe the rate of heat transfer as a function of time. The Tagami method for predicting heat transfer is very crude and should be used only when performing a cursory, lumped parameter study. The Tagami data, however, have been used for comparison by many researchers who have since developed more advanced models. The Tagami model is given as equations (A.4 - A.5) in Appendix A.

The Uchida (and Tagami) model does not take into account any local parameters, but is instead based solely on the average bulk steam and air mass fractions. This type of model is well suited to lumped parameter computer analysis, and has historically been viewed as conservative. The paper by Gido & Koestel noted that the small scale experiments produced laminar condensation data which consistently under-predicted condensation data from large surfaces, which are in the turbulent regime [Gido, 1983]. However, recently Peterson showed that the Uchida model only works well for situations that match those in which the data were taken - i.e. a noncondensable gas partial pressure of about one atmosphere [Peterson, 1996]. The theoretical study showed that the Uchida model can over-predict the rate of condensation heat transfer if the partial pressure of noncondensable gas in the containment is significantly below one atmosphere. This situation often arises in the drywell of a suppression pool-type containment, where most of the noncondensable gases are purged to the wetwell during the blowdown. This situation can also occur in sub-atmospheric containment buildings and in individual compartments of a containment that may be purged of their noncondensables for some reason. These two shortcomings have basically meant that the Uchida model has outlived its usefulness in modern containment analysis, except as a simple first approximation tool.

### 1.3.2 Simple enhancement models

One of the simplest types of theoretical condensation models is based on a heat transfer coefficient for dry air convection multiplied by an enhancement factor for condensation. This type of approach is often used in analyses of air conditioning or dehumidifier systems. An expression for the mass transfer coefficient can be written [Research and Education Association, 1984]:

\[
h_D = \frac{h_{conv}}{\rho c_p} \left( \frac{Sc}{Pr} \right)^{2/3} = \frac{h_{conv}}{\rho c_p} \frac{Le^{2/3}}{Le^{2/3}}
\]

(1.2)

\footnote{Gido and Koestel proposed their own condensation model which is a combination of natural and forced convection heat transfer expressions (see Appendix A for details).}
where the total heat transfer is given by:

\[ q^* = h_{\text{conv}} \Delta T + h_D \Delta h_{\text{fg}} \]  

(1.3)

Another such model is given by [Threlkeld, 1970]:

\[ h_{\text{humid air}} = h_{\text{dry air}} \left[ \frac{c_{p(\text{air})} + \varphi c_{p(\text{water})} + h_{\text{fg}} \frac{dp}{dT}}{c_{p(\text{air})}} \right] \]  

(1.4)

where \( \varphi \) is the mass of water vapor per unit mass of air. These models are both based on the heat and mass transfer analogy, but are limited in their range of applicability to instances where the water vapor partial pressure is small. These models are suitable for the applications cited above which generally have air temperatures less than 40°C, a total pressure of about one atmosphere, and a condensing surface below 20°C. When one attempts to apply these models to other conditions, they can incur large errors. Since the atmosphere in a post-LOCA containment building generally has a vapor partial pressure equal to or exceeding those of the noncondensable gases, this type of model is not adequate.

### 1.3.3 Modern external surface models

More recent theoretical models for external surface condensation have emerged which are capable of describing the processes of condensation and convection based on local parameters. This type of model is necessary in the analyses of an advanced containment design because the atmosphere may not be well mixed. These new models treat heat transfer through the condensate film and through the gas boundary layer as two distinct processes occurring in series. Heat transfer through the boundary layer is further treated as three parallel processes: convection (or sensible heat transfer); condensation (or latent heat transfer that accompanies mass transfer); and radiation. Equations (1.5) and (1.6) describe this process:

\[ \frac{1}{h_{\text{r}}} = \frac{1}{h_{\text{film}}} + \frac{1}{h_{\text{gas}}} \]  

(1.5)

\[ h_{\text{gas}} = h_{\text{conv}} + h_{\text{cond}} + h_{\text{rad}} \]  

(1.6)

Researchers have debated back and forth whether modeling of the condensate film is necessary for condensation in the presence of a noncondensable gas because the resistance to heat transfer from the boundary layer is much greater than that from the film. However, it has been argued that for high vapor velocities, or low noncondensable gas concentrations, the heat transfer coefficient in the boundary layer can approach that of the condensate film [Kim, 1990]. It is also necessary to include the condensate film if one wishes to have a general condensation model which can be used in a computer code to describe condensation under any circumstances, which is a desirable trait in this author’s opinion.

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2 The radiation term in equation (1.3) is usually dropped because the atmospheric temperature in most containment analyses is well below 200°C, which results in the radiation component being negligibly small.
Two researchers who have made recent advances in this field are Corradini and Peterson (see Appendix A for details of their work). Corradini assumed that condensation boundary layers on large surfaces are turbulent, and using the heat/mass transfer analogy and empirical relations for turbulent quantities devised a method to predict condensation under such conditions [Corradini, 1984]. The Corradini model was later extended to include waviness effects from the condensate film [Kim, 1990]. The Corradini approach requires knowledge of steam concentrations both inside and outside the boundary layer, and iteration on the condensate film temperature to match the heat transfer rate through the film with that through the boundary layer. Later Peterson derived an expression called the condensation conductivity, which allows the mass transfer process, which is driven by concentration gradients, to be expressed in terms of saturation temperatures[Peterson, 1993]. Then by invoking the heat and mass transfer analogy, a simple expression for treating heat transfer through the gas boundary layer was developed. Peterson’s model also requires iteration on the condensate film temperature, but is applicable to internal and external condensation since the model is general and based on choosing an appropriate Nusselt number for the particular situation being studied.

Both of these models are fundamentally derived from theory, instead of being purely empirical, which makes them more robust and applicable to a wider range of conditions than models such as Uchida. The model which is used throughout the remainder of this thesis is the Peterson model, which has a few extensions by Anderson to treat high mass transfer rates [Anderson, 1998] (also see Appendix A). The modified Peterson model is termed the diffusion layer model or DLM, and obeys the following equations:

\[ h_{\text{conv}} = \frac{k_m}{x} \frac{Nu}{x} \quad (1.7) \]

\[ h_{\text{cond}} = \frac{k_{\text{cond}}}{x} \frac{Sh}{s} \Theta \quad (1.8) \]

\[ k_{\text{cond}} = \frac{h_{\text{fg}} c M^2}{RT_b T_i \phi} \quad (1.9) \]

\[ \Theta = \frac{1 - X_{x,i}}{1 - X_{x,\text{avg}}} \quad (1.10) \]

\[ \phi = \frac{X_{g,\text{avg}}}{X_{s,\text{avg}}} = \frac{\ln\left[\frac{X_{s,b}}{X_{s,i}}\right]}{\ln\left[\frac{X_{g,b}}{X_{g,i}}\right]} \quad (1.11) \]

\[ X_{j,\text{avg}} = \frac{X_{j,b} - X_{j,i}}{\ln\left(\frac{X_{j,b}}{X_{j,i}}\right)} \quad j = s \text{ or } g \quad (1.12) \]

The DLM is in a form which can easily be implemented into a computer code for performing containment analysis. This model is also able to predict local values of the heat transfer coefficient, which makes it applicable for studies where conditions may change drastically over the length of a single surface. This type of flexibility is desirable for a model to be used in analyzing advanced containment systems. This model is studied extensively in Chapter 2 of this thesis. Several other condensation models were identified as being relevant during the literature review. Appendix A presents these additional models in detail, and discusses their strengths and weaknesses. There is also a section of Appendix A dedicated to condensation inside tubes, which is not a topic that will be discussed frequently in this thesis, although it is relevant to many types of passive containment cooling systems.

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3 A derivation for the condensation conductivity is given in Appendix B.
1.4 Review of Containment Codes

Several computer codes are currently available for the analysis of nuclear reactor containment systems. This section provides a brief overview of four major codes and presents an evaluation based on the ability of each code to simulate key phenomena in the containment system. The key physical phenomena which occur in passive containment systems were identified in section 1.2. Prediction of these phenomena often requires that a code have several distinct capabilities. These capabilities are briefly described next.

1.4.1 Necessary capabilities of a containment analysis code

The key physical phenomena that a computer code must ideally be able to simulate in the analysis of a passive containment system are:

- Condensation in the presence of noncondensable gases;
- Natural (buoyancy induced) convection and mixing;
- Stratification in liquid or gas volumes.

The first, condensation in the presence of a noncondensable gas, requires that the code be able to calculate the variables which are needed for the particular heat and mass transfer models. This usually requires the calculation of several parameters near a wall or other boundary as well as the ability to track a noncondensable gas mixture separately from the steam phase. Figure 1-4 shows the variables which a code must calculate in order to use the Uchida correlation, the Gido & Koestel correlations, or the Peterson diffusion layer model (DLM). Most codes calculate variables which are necessary for the Uchida and Gido & Koestel models. However, many codes do not calculate the liquid film interface temperature or the steam partial pressure at the interface. These quantities are necessary for the DLM.

A second and closely related process that a code must be able to simulate is natural convection. This requires that the code be able to predict buoyancy-induced driving forces for fluid motion. For the proper prediction of these forces, a code should have three-dimensional capability. The buoyancy-induced forces of free or mixed convection are localized phenomena and can not necessarily be treated symmetrically. Imposing a one-dimensional or two-dimensional solution scheme on a containment problem is forcing the problem to be treated symmetrically. Symmetry can sometimes be used to simplify a containment analysis, but in many cases it is known a priori that the problem will be asymmetric (i.e. for an off-center steam release.) Similarly, a multi-dimensional velocity and momentum solution allows for stratification to develop in different regions of the containment atmosphere. Predicting stratification is essential to being able to predict real situations. Also, the possibility of stratification indicates that heat transfer and condensation should be calculated on a local basis, not on an average basis over large surfaces.

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4 An example of a two-dimensional solution scheme would be a cylindrical coordinate representation of a cylindrical containment volume with radial divisions but no divisions in the azimuthal direction. Such a treatment models the problem as a set of concentric annuli, where the flow in each annulus is assumed homogenous. Such a situation may be envisioned for flow in pipes, but is not a realistic model for a large containment volume because of non-symmetric break release locations, heat sink distributions, and the large distances between supposedly homogenous regions.
This local heat transfer calculation requires the use of local heat transfer models and computer code logic which are set up to perform this function. Many older computer schemes do not contain this flexibility (e.g., GOTHIC version 3.4e and earlier).

The previous paragraph necessitates a discussion of the basic distinction between a “lumped parameter” (LP) computational scheme and a “distributed parameter” (DP) computational scheme. In a LP analysis, the containment is usually represented by relatively large computational volumes. These volumes are assumed to be homogenous and all fluid properties (e.g., temperature & steam partial pressure) are calculated on a volume-average basis. No fluid velocities are calculated within a LP computational cell. Velocities induced by the net change of mass between volumes is modeled as flowing through a one-dimensional junction (pipe) only and is a result of pressure difference between the volumes. By definition, local heat and mass transfer correlations cannot be used in LP studies, only average heat transfer relations can be used. It is also an assumption that any liquid present in the volume is in a pool at the bottom. Thus a condensate liquid film on a vertical wall cannot be modeled within a LP volume.

On the other hand, DP modeling refers to a situation where a single large volume is discretized into smaller subvolumes. Each subvolume is referred to as a cell. Fluid properties are still calculated on a volume average basis, but within each subvolume. Fluid velocities do exist within subvolumes and velocity directional components are calculated as the average of the velocities on opposing faces (boundaries) between cells. Each cell has six faces, thus there are velocity components in all three dimensions. The basic distinction between a computational model with a large number of LP volumes connected together and one with a single DP volume subdivided into smaller cells, is the ability to predict three-dimensional velocity and momentum transfer in the DP representation. In modern computer programs, it is generally less work to define a DP model with many subvolumes than to define a LP model with many volumes.
Historically, however, containment analysis has been performed on a LP basis. These analyses were warranted since most containment designs used active systems such as sprays or fan coolers to remove heat following a LOCA. These active systems kept the containment atmosphere well mixed, thus the basic assumption of a homogenous volume was justified. However, stratification cannot be adequately predicted using a historical LP approach. Neither can pressure or density increases due to increased depth in a pool of water. For passive containment systems, where buoyancy and other small forces provide the driving mechanism for heat transfer and containment cooling, a DP representation is required.

There are several other factors that should be considered when evaluating a computer code. The processes of condensation and convection should be treated in parallel as explained in the discussion of the DLM condensation model discussed in chapter 2. This is not a concern for the Uchida and Gido & Koestel correlations which were formulated to predict total heat transfer with saturated steam conditions. However, in a superheated steam environment there will be convection and condensation taking place at the same time. The specific convection correlations used in the codes are also of interest along with the knowledge of whether the heat and mass transfer analogy is employed. During the condensation literature review (Appendix A), it was discovered that suction plays a key role in determining the actual heat transfer rate during condensation in the presence of a noncondensable gas. Some codes do not have a built in suction correction to help compensate for the under-prediction of the heat and mass transfer analogy.

Thermal non-equilibrium between phases is a situation that exists in reality but may not be calculated in a computer code. Phase non-equilibrium allows the vapor and liquid phases of the same fluid to exist within the same volume while not being in the saturated equilibrium state. For instance this condition exists when subcooled water and superheated vapor exist in the same volume (or subvolume), or when saturated steam and superheated liquid are present. Finally some computer codes solve conservation equations for three phases: a contiguous liquid phase; a vapor/gas phase; and a liquid droplet phase. Many codes, however, do not solve equations for the droplet phase. The advantage of a droplet phase is that it allows the code to simulate drop entrainment and de-entrainment in vapor streams. Heat transfer between the droplet and vapor phases is calculated separately from heat transfer between the contiguous liquid phase and vapor, which can result in significantly higher rates of heat and mass transfer. This capability can be very useful when attempting to model realistic blowdown energy releases and other boundary conditions. Table 1.1 at the end of this section summarizes the important characteristics of the four computer codes reviewed in this study.

1.4.2 GOTHIC
The GOTHIC information presented here is taken nearly verbatim from [George, 1994] with only slight modifications. GOTHIC is a general purpose thermal hydraulics computer program developed by Numerical Applications Inc. for design, licensing, safety and operating analyses of nuclear containments and other confinement buildings. The code has origins in the COBRA-NC and FATHOMS codes and is now under EPRI sponsorship for further development and assessment. The code package includes graphical pre- and post-processors which make GOTHIC especially useful for creating complex input models with a minimum of errors.
GOTHIC solves mass, momentum, and energy balances for three separate phases; vapor, liquid, and drops. The vapor phase can be a mixture of steam and noncondensable gases with a separate mass balance being solved for each component of the vapor mixture. An ice phase is also included for ice condenser containment analysis. The phase balance equations are coupled by mechanistic models for interfacial mass, energy and momentum transfer that cover the entire flow regime from bubbly flow to film/drop flow as well as single phase flows. The interface models allow for the possibility of thermal non-equilibrium between phases and unequal phase velocities. The code can be used for three-dimensional analysis of the thermal hydraulic behavior of containment atmosphere and structures. Containment compartments can be modeled using a one-, two-, or three-dimensional rectangular grid. The option of a lumped parameter model can be used for containment volumes where the resolution of a distributed parameter model is not needed. Lumped parameter volumes are connected by junctions that employ a one-dimensional model for flow between compartments. A combination of lumped parameter and two- or three-dimensional distributed parameter analysis is also possible.

GOTHIC includes full treatment of the momentum transport terms in multidimensional models with the optional one parameter Prandtl mixing length turbulence model for turbulent shear and mass and energy diffusion. GOTHIC version 5.0 and above also incorporate the two-parameter K-ε turbulence model. Thermal conductors model heat transfer surfaces in the containment. All conduction within thermal conductors is one-dimensional and perpendicular to the surface area exposed to the containment volumes. Wall heat transfer correlations are incorporated for a wide variety of heat transfer situations, including the Uchida, Tagami, and Gido & Koestel correlations. GOTHIC 4.1c (and newer versions) contains heat transfer relations that are based on boundary layer theory which depends on the calculation of the condensate interface temperature whereas older versions have less sophisticated models. Special models for engineering safety equipment including pumps, sprays, fans, valves, heat exchanges, coolers and vacuum breakers are included. Trip logic is used to control the action of the safety equipment in response to changes in the containment atmosphere.

The code assessment program included a wide range of analytic tests, small and large-scale experimental tests which included hydrogen dispersion, suppression pool performance, single and multi-compartment water and steam blowdowns, and superheated steam blowdown.

1.4.3 RELAP5/MOD3.2

The RELAP5 information presented here is taken nearly verbatim from [RELAP5/MOD3, 1995]. RELAP5 is a light water reactor transient analysis code developed at the Idaho National Engineering Laboratory (INEL) for the U.S. Nuclear Regulatory Commission. RELAP5 was historically developed as a systems code, intended to simulate operational and accident transients within the primary and/or secondary systems of a nuclear power reactor plant. However, RELAP5 is a highly generic code that can also simulate a wide variety of hydraulic and thermal transients in both nuclear and non-nuclear systems involving mixtures of steam, water, noncondensable gases, and solute.

The RELAP5/MOD3.2 code is based on a non-homogeneous and non-equilibrium model for the two-phase system that is solved by a fast, partially implicit numerical scheme. The code includes
many generic component models from which general systems can be simulated. The component models include pumps, valves, pipes, heat releasing or absorbing structures, reactor point kinetics, electric heaters, jet pumps, turbines, separators, accumulators, and control systems components. In addition models are included for effects such as form loss, flow at an abrupt area change, branching, choked flow, boron tracking, and noncondensable gas transport. The code is a lumped parameter based representation with computational volumes being connected by one-dimensional junctions. The one-dimensional nature of the field equations for the two-fluid model precludes direct simulation of effects that depend upon transverse gradients of any physical parameter, such as velocity or energy.

Because RELAP5 is primarily a system code, most of the code logic has been developed for modeling flows which are inside pipes or vessels. Hence, the prediction of multi-dimensional velocities and momentum transfer is not possible. The RELAP5 code documentation is voluminous and confusing, which leads to a very slow ascent on the learning curve. RELAP5 has been used in recent years to study containment phenomena, but is not an ideal code for modeling containments because of the biases present for modeling confined one-dimensional flows. The lack of a pre-processor makes input and output files difficult to deal with and prone to errors.

1.4.4 GASFLOW 1.0

The GASFLOW information is taken primarily from [Wilson, 1992]. GASFLOW is being developed at Los Alamos National Laboratory under sponsorship of the US Nuclear Regulatory Commission as a best-estimate tool for predicting transport, mixing, and combustion of hydrogen and other gases in nuclear reactor containments and other facilities. The code can model geometrically complex facilities with multiple compartments and internal structures. It can simulate the effects of condensation, heat transfer to walls and internal structures, chemical kinetics, and fluid turbulence.

GASFLOW is a finite-volume, single-phase, code based on proven computational fluid dynamics methodology that solves the compressible Navier-Stokes equations for three-dimensional volumes in Cartesian or cylindrical coordinates. Wall shear stress models are provided for bulk laminar and turbulent flow. GASFLOW has transport equations for multiple gas species and one for internal energy. Three turbulence models are provided, including the well known k-ε model, to determine turbulent velocity and length scales needed to compute the turbulent viscosity. Terms for turbulent diffusion of different species are included in the mass and internal energy equations.

Heat conduction within walls and structures is one-dimensional. Heat and mass transport to walls and structures is based on a modified Reynolds analogy which accounts for increased heat transfer and condensation when the mass fraction of steam becomes a relatively large fraction of the mass of the gas mixtures.

The GASFLOW code is primarily intended to solve chemical combustion and gas flow problems within containment buildings. The code does not have the capabilities to model liquid water or water drops. Condensation can take place, but acts as an energy transfer process and a mass sink.
This seriously limits the applicability of the GASFLOW 1.0 code for containment calculations which include modeling a suppression pool or condenser pool. The code is still in development and version 2.1 was scheduled to be released in late 1997. The new version includes some options for modeling re-vaporization from sumps and other water pools [Royl, 1997].

1.4.5 TRAC-BF1/MOD1

The TRAC-BF1 information presented here is taken nearly verbatim from [Borkowski, 1992]. The transient reactor analysis series of codes for boiling water reactors (TRAC-B) has been developed by the Idaho National Engineering Laboratory to provide the US Nuclear Regulatory Commission with a best-estimate capability for the analysis of postulated accidents and transients in boiling water reactor systems and related experimental facilities. The computer code provides the capability to analyze large and small-break loss-of-coolant accidents, anticipated transients without scram, and other operations and accident transient sequences.

The code features include a full non-homogenous, non-equilibrium, two-fluid, thermal hydraulic model of two-phase flow in all portions of the BWR system, including a three-dimensional treatment of the BWR vessel, a detailed modeling of the BWR fuel bundle complete with a radiative heat transfer model, and detailed models of BWR hardware such as jet pumps and separator-drivers. Other features include a non-homogenous, thermal equilibrium critical flow model and flow-regime-dependent constitutive relations for interchanges of mass, energy, and momentum between the fluid phases and fluids and structures. Heat conduction within the thermal structures is one-dimensional. TRAC-BF1/MOD1 includes new models for balance of plant components such as turbines, feedwater heaters, steam condensers, a comprehensive control system model, boron transport, and reactivity feedback models.

The TRAC code is primarily one-dimensional, much like the RELAP5 code, and was developed to model reactor systems - not detailed containment systems. However, TRAC-BF1 does have a three-dimensional model for the BWR vessel. Recently, containment studies have been performed using the three-dimensional vessel model to represent the containment [Vierow, 1993]. This is not how the code was intended to be used, but provides the best way to apply the TRAC code to advanced containment analysis.

1.4.6 Computer codes summary

Four computer codes were described: GOTHIC, RELAP5, GASFLOW, and TRAC-BF1. Only GOTHIC and GASFLOW were originally intended to model containment structures and only these two possess general three-dimensional capabilities. All four codes have been used by different research groups to perform containment analyses. However, only GOTHIC is capable of performing all of the functions outlined which are necessary to predict the major physical phenomena identified in section 1.2, although the newer versions of GASFLOW may soon meet the criteria as well. RELAP5 and TRAC-BF1 have the ability to model primary or secondary reactor systems, thus predicting the interaction between containment modeling and the reactor system. This advantage does not aid the analysis when the long term passive cooling of the containment is studied. The reactor system at this time far into the accident sequence is easily described by known boundary conditions.
The MIT containment research group has chosen to work with GOTHIC 4.1c whenever possible. This computer code was updated to include the DLM, which is discussed in section 1.3 and chapter 2.

Table 1-1: Summary of computer code capabilities

<table>
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Turbulence Models

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Convection Correlations

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<td>$Sh = 0.13(GrSc)^{0.44}$</td>
<td>$Sh = \frac{f}{2} Re Sc^{1/3}$</td>
<td>$Sh = 0.023 Re^{0.03} Sc^{0.44}$</td>
<td>$Sh = 0.023 Re^{0.03} Sc^{0.03}$</td>
<td>$h = \frac{\tau_w c_p}{u_c}, \tau_w = \rho u_*^2$</td>
</tr>
</tbody>
</table>

5 TRAC-BF1 has a three-dimensional BWR vessel model that can be used for modeling a containment structure.
6 GOTHIC 3.4e assumes the interface temperature is at the bulk saturation temperature.
7 The treatment of noncondensable gases in TRAC-BF1 is extremely primitive.
8 $u_*$ is the wall shear speed which is calculated according to the law-of the-wall for turbulent flow [Wilson, 1992].

The mass transfer coefficient is calculated based on the heat/mass transfer analogy.
1.5 Mass Transfer Theory

Many of the condensation models discussed in this thesis rely heavily on mass transfer theory and the analogies between momentum, heat, and mass transfer. This section provides a brief description of mass transfer, including the difference between low and high mass transfer rate theory, and the analogies between the transport of heat, mass, and momentum. The information in this section is taken directly from [Mills, 1995] with a bit also from [Hines, 1985].

1.5.1 Elementary mass transfer

The phenomena associated with mass transfer is diffusion, which is described by Fick's law:

\[ \mathbf{J}_s = -c D_{12} \nabla X_s \quad \text{or} \quad \mathbf{j}_s = -\rho D_{12} \nabla m, \]  

where \( \mathbf{J}_s \) is the diffusive molar flux of steam, \( \mathbf{j}_s \) is the diffusive mass flux of steam, \( c \) is the mixture molar concentration, \( \rho \) is the mixture density, and \( D_{12} \) is the binary diffusion coefficient (sometimes called the mass diffusivity). The driving force for diffusion is the gradient of the local species concentration \((1.13a)\), or analogously, the gradient in local species mass fraction \((1.13b)\). Mass transfer can be described equivalently in terms of molar units or mass units, depending on which is easier for the situation at hand. Mechanical engineers generally use mass units, while chemical engineers tend to use molar units. The standard in this thesis will be to calculate mass transfer in terms of molar units.

Unlike temperature, which is continuous at an interface, concentration is often discontinuous at an interface. To deal with this situation, two imaginary surfaces are set up on either side of the actual interface. Figure 1-5 shows the situation for water vapor condensing onto a liquid film.

![Figure 1-5: Condensation from a steam-air mixture onto a liquid film](image)

\( \text{Figure 1-5: Condensation from a steam-air mixture onto a liquid film} \)

\(^9\) The specific notation used is consistent with the diffusion of steam through a noncondensable gas.
At the imaginary surface inside the liquid there is no air, only water, thus the mole fraction of water is unity (we ignore the small amount of air dissolved in the water). For the surface at $z = 0$, the water vapor is assumed to be in equilibrium with the air, thus the water mole fraction is set by the saturation pressure of water at the local temperature, i.e. $X_{s,i} = \frac{P_{sat}(T)}{P_{total}}$. Low mass transfer rate theory assumes that the medium through which the species is diffusing is stationary, i.e. that there is no movement of the air/gas mixture in the direction of the diffusive flux. Water vapor that crosses the interface at $z = 0$ is a result of diffusion only. The total molar flux, $N_s$, is therefore equal to the diffusive flux. For a simple one-dimensional case this can be written as:

$$N_s = J_s = cD_{12} \frac{X_{s,i} - X_{s,b}}{\delta} \tag{1.14}$$

where $\delta$ is the equivalent stagnant film distance over which the difference in mole fraction is taken. Equation (1.14) is often rewritten in terms of the mass transfer conductance, $g_m$, as:

$$N_s = g_m \left( X_{s,i} - X_{s,b} \right) \tag{1.15}$$

The mass transfer conductance is defined as:

$$g_m = \frac{cD_{12}}{\delta} \tag{1.16}$$

and the thickness $\delta$ is commonly called the boundary layer. Equations (1.14 - 1.16) are valid for low mass transfer rates, where there is a linear relationship between the driving force and the mass transfer rate. “Low mass transfer rate” is somewhat of an arbitrary definition, but it is safe to assume that the relationships are valid for small changes in mole fraction, such as $\Delta X_s < 0.1$.

1.5.2 High mass transfer rate theory

High mass transfer rate theory accounts for the convection of mass across the surface at $z = 0$ due to a net velocity in the direction normal to the surface. The total molar flux of water vapor across the interface will then be the sum of a convective component and a diffusive component. Because we no longer have a stagnant medium, we must define the specific velocities and fluxes of interest. The molar-average velocity of the mixture is defined as:

$$\mathbf{v}^* = \frac{\sum c_n \mathbf{v}_n}{\sum c_n} = \frac{\sum c_n \mathbf{v}_n}{c} = \sum X_n \mathbf{v}_n \tag{1.17}$$

where $\mathbf{v}_n$ is the absolute velocity of species $n$, that is the velocity relative to a fixed coordinate axis. The velocity of a particular species relative to the molar-average velocity is called the diffusion velocity of the species. The diffusion velocity of species $n$ is then equal to:

$$\mathbf{v}_n^* = \mathbf{v}_n - \mathbf{v}^* \tag{1.18}$$
The absolute molar flux of species $n$ (relative to a stationary coordinate axis) is then defined as:

$$N_n = c_n v_n$$  \hspace{1cm} (1.19)

The molar diffusion flux of species $n$ relative to the molar-average velocity $v^*$ is:

$$J_n = c_n v^* = c_n (v_n - v^*)$$  \hspace{1cm} (1.20)

The absolute molar flux of the mixture is:

$$N = \sum N_n = c v^*$$  \hspace{1cm} (1.21)

By substituting equation (1.18) into equation (1.19) then simplifying using equation (1.20), the absolute molar flux of species $n$ can be expressed as the sum of the convective flux and the diffusive flux:

$$N_n = c_n v^* + J_n = X_n N + J_n$$  \hspace{1cm} (1.22)

Fick’s law for the diffusion flux is still defined as before in equation (1.13a):

$$J_n = -c D_{12} \nabla X_n$$  \hspace{1cm} (1.23)

however, from the definitions of velocities and fluxes above, equation (1.23) is known precisely to be the molar diffusion flux of species $n$ relative to the molar-average velocity of the mixture. For the specific binary system of steam and a noncondensable gas, substituting equation (1.23) for Fick’s law into equation (1.22) yields:

$$N_s = c_s v^* - c D_{12} \nabla X_s = X_s (N_s + N_g) - c D_{12} \nabla X_s$$  \hspace{1cm} (1.24)

One final equation which is of use is the conservation equation for species. One form is listed in Appendix C as equation (C.15). For the present purposes, a conservation equation in molar quantities is appropriate (where $\dot{R}_n^s$ is a source term, equal to 0 in this case):

$$\frac{\partial c_n}{\partial t} + \nabla \cdot N_n = \dot{R}_n^s$$  \hspace{1cm} (1.25)

Now the above equations will be used to perform a one-dimensional analysis on the condensation boundary layer shown in Figure 1-5. At steady state there will be no time rate of change of concentration of either species. Also, for an ideal gas mixture with relatively small temperature and pressure changes across the boundary layer, the total concentration will be nearly independent of position. Using these two assumptions, equation 1.25 for each species reduces to:
\[ \frac{d}{dz}(N_g) = 0 \quad \frac{d}{dz}(N_s) = 0 \] (1.26, 1.27)

This result is also intuitive, since at steady state we do not expect the velocity (in the direction normal to the interface) of either the gas or the steam to be changing, but to be constant. Thus the flux of each of these species should be constant as well. If we assume that the noncondensable gas is not soluble in water, there will be no net flux of the gas across the interface:

\[ N_g \bigg|_{z=0} = 0 \] (1.28)

and from equation (1.27) it follows that the steady state gas flux is zero everywhere:

\[ N_g = 0 \] (1.29)

Using equation (1.24) the steam flux can be written as the sum of a convective and diffusive component:

\[ N_s = X_s (N_s + N_g) - cD_{12} \frac{dX_s}{dz} \] (1.30)

Substituting equation (1.29) for \(N_g\) into equation (1.30) and solving for \(N_s\):

\[ N_s = -\frac{cD_{12} \frac{dX_s}{dz}}{1 - X_s \frac{dz}{dz}} \] (1.31)

Now substitution of equation (1.31) into equation (1.26) gives the differential equation:

\[ \frac{d}{dz} \left( N_s \right) = \frac{d}{dz} \left( -\frac{cD_{12} \frac{dX_s}{dz}}{1 - X_s \frac{dz}{dz}} \right) = 0 \] (1.32)

We have already made the assumption that the concentration is independent of position, and since the temperature and pressure changes are assumed small, the binary diffusion coefficient is independent of position as well\(^{10}\). We are then left with the following simplified equation for the steam mole fraction which is subject to the listed boundary conditions:

\[ \frac{d}{dz} \left( \frac{1}{1 - X_s \frac{dz}{dz}} \right) = 0 \] (1.33)

\(^{10}\) Binary diffusion coefficients for gases are proportional to temperature, inversely proportional to pressure, and virtually independent of the exact concentration ratio of the two gases.
\begin{align*}
  z = 0: & \quad X_s = X_{s,i} \\
  z = \delta: & \quad X_s = X_{s,b}
\end{align*}

(1.34a)

(1.34b)

Integrating equation (1.33) with respect to \( z \):

\[
\frac{1}{1 - X_s} \frac{dX_s}{dz} = C_1
\]

(1.35)

Integrating equation (1.35) with respect to \( z \) once again yields:

\[-\ln(1 - X_s) = zC_1 + C_2\]

(1.36)

Applying the boundary conditions in equation (1.34) to evaluate the integration constants yields:

\[C_2 = -\ln(1 - X_{s,i})\]

(1.37)

\[C_1 = \frac{1}{\delta} \ln \left( \frac{1 - X_{s,i}}{1 - X_{s,b}} \right)\]

(1.38)

Plugging equations (1.37) and (1.38) back into (1.36) and rearranging results in the relationship for the steam mole fraction distribution:

\[
\frac{1 - X_s}{1 - X_{s,i}} = \left( \frac{1 - X_{s,b}}{1 - X_{s,i}} \right)^{1/\delta}
\]

(1.39)

To calculate the molar flux of steam, we re-write equation (1.31) as follows:

\[
N_s = N_s \bigg|_{z=0} = -\frac{cD_{12}}{1 - X_{s,i}} \frac{dX_s}{dz} \bigg|_{z=0}
\]

(1.40)

The derivative of the steam mole fraction can be evaluated by plugging equation (1.38) into (1.35) to get:

\[
\frac{dX_s}{dz} = \frac{1 - X_s}{\delta} \ln \left( \frac{1 - X_{s,i}}{1 - X_{s,b}} \right)
\]

(1.41)

\[
\left. \frac{dX_s}{dz} \right|_{z=0} = \frac{1 - X_{s,i}}{\delta} \ln \left( \frac{1 - X_{s,i}}{1 - X_{s,b}} \right)
\]

(1.42)

Substituting equation (1.42) back into (1.40) and simplifying gives:
The steam flux can also be expressed in terms of the gas mole fractions by using the identity ($X_g = 1 - X_s$) as:

$$N_s = N_{s,i} = \frac{cD_{12}}{\delta} \ln \left( \frac{1 - X_{s,i}}{1 - X_{s,b}} \right) = \frac{cD_{12}}{\delta} \ln \left( \frac{1 - X_{s,b}}{1 - X_{s,i}} \right)$$  \hspace{1cm} (1.43)

The logarithmic mean value of the gas mole fraction will be used, which is defined as:

$$\left( X_g \right)_{lm} = \frac{X_{g,b} - X_{g,i}}{\ln \left( X_{g,b} / X_{g,i} \right)}$$  \hspace{1cm} (1.45)

Substituting the logarithmic mean value (1.45) into (1.44) results in an expression for steam flux of the form:

$$N_s = \frac{cD_{12}}{\delta \left( X_g \right)_{lm}} \left( X_{s,i} - X_{s,b} \right)$$  \hspace{1cm} (1.46)

Comparing equation (1.46) for a high mass flux to equation (1.14) for a low mass flux, we see that the only difference is the inclusion of the log mean value in the evaluation of the high rate equation. This term has a limiting value of one for a small diffusion potential (i.e. small $\Delta X_s$) which results in reproducing the low mass transfer expression. As the potential increases, the log mean term decreases, causing a departure from the linear relationship for low mass transfer rates. This nonlinear behavior for a large diffusion potential is the key difference between low and high mass transfer rate theory.

The concept of the mass transfer conductance is also useful for high mass transfer rate analyses. Reviewing equations (1.14) and (1.16) we can write the mass transfer conductance as:

$$g_m = \frac{J_{s,i}}{(X_{s,i} - X_{s,b})}$$  \hspace{1cm} (1.47)

The mass transfer conductance, more correctly called the mole transfer conductance in this case, is defined in terms of the diffusive molar flux. From equation (1.22) the absolute flux of steam at the interface is defined to be:

$$N_{s,i} = X_{s,i} N_i + J_{s,i}$$  \hspace{1cm} (1.48)
Recall that the absolute flux of gas, \( N_g \), is zero everywhere. Thus equation (1.48) can be written as:

\[ N = N_x = X_{x,i}N + J_{x,i} \]  

(1.49)

Substituting equation (1.47) into (1.49) we can write the total flux in terms of the mole transfer conductance:

\[ N = N_x = g_m \left( \frac{X_{s,b} - X_{s,i}}{X_{s,i} - 1} \right) \]  

(1.50)

Equation (1.50) is often rearranged in the following manner:

\[ N = g_m B_{ms} \]

\[ B_{ms} = \left( \frac{X_{s,b} - X_{s,i}}{X_{s,i} - 1} \right) \]  

(1.51)

where \( B_{ms} \) is called the mole transfer driving force. For most mass transfer analyses, the mole transfer conductance is normalized by the value it takes in the limit of zero mass transfer, \( g_m^* \):

\[ g_m^* = \lim_{m' \to 0} g_m \]  

(1.52)

which allows equation (1.51) to be written as:

\[ N = (g_m^* \Theta)B_{ms} \]  

(1.53)

The term \( \Theta \) is called the blowing factor\(^{11} \), and it relates the actual mole transfer conductance to the mole transfer conductance in the limit of zero mass transfer. If we equate equations (1.53) and (1.43) we can write:

\[ N = (g_m^* \Theta)B_{ms} = \frac{c D_{12}}{\delta} \ln \left( \frac{1 - X_{s,b}}{1 - X_{s,i}} \right) \]  

(1.54)

which can be rewritten again as:

\[ N = (g_m^* \Theta)B_{ms} = \frac{c D_{12}}{\delta} \ln \left( 1 + \frac{X_{s,b} - X_{s,i}}{X_{s,i} - 1} \right) \]  

(1.55)

\(^{11}\) The term is called the blowing factor in the general case, but is more correctly called a suction factor for the specific case of condensation.
If we take $g_m^*$ to be the value defined for low mass transfer rates in equation (1.16) and the driving force to be defined by equation (1.52) we can rearrange equation (1.55) to be:

$$N = \frac{cD_{12}}{\delta} \ln(1 + B_{ms}) \frac{B_{ms}}{B_{ms}} = g_m^* \Theta B_{ms}$$ (1.56)

where the blowing factor is found to be:

$$\Theta = \frac{\ln(1 + B_{ms})}{B_{ms}}$$ (1.57)

An analogous expression can be derived in terms of mass units by assuming a Couette flow situation as [Mills, 1995, pp. 958]:

$$m^* = \frac{\rho D_{12}}{\delta} \frac{\ln(1 + \mathcal{E}_{ms}) \mathcal{E}_{ms}}{\mathcal{E}_{ms}} \mathcal{E}_{ms} = \left( \frac{m_{s,b} - m_{s,l}}{m_{s,l} - 1} \right)$$ (1.58, 1.59)

Equation (1.57) is derived assuming a constant molar concentration, whereas equation (1.58) assumes a constant mixture density. For an ideal gas the former is generally a better assumption.

The Sherwood number is often used to relate the effective diffusion layer thickness, $\delta$, to the characteristic dimension of the flow, $x$:

$$\frac{1}{\delta} = \frac{Sh_x}{x}$$ (1.60)

Equation (1.60) is exploited in many of the condensation models discussed in the remainder of the thesis.

As a final word it must be noted that this simple one-dimensional case is only an approximation. An attempt to capture the influence of actual multidimensional boundary layer flow has resulted in the derivation of a blowing factor. The relationships derived using this simplified theory do produce acceptable results for many heat and mass transfer problems. For those problems where this representations fails, a correction is usually attempted by defining an alternative blowing factor which is deduced from matching equation (1.56) or (1.58) to experimental data for the problem of interest. This type of correction was defined by Kim and Corradini for condensation on large surfaces [Kim, 1990] (see Appendix A, section A.1.5).

### 1.5.3 Analogies between heat, mass, and momentum transfer

The transfer of heat, mass, and momentum are similar because they are governed by physical laws of identical mathematical form.
\[ q^* = - \left( \alpha + E_H \right) \frac{\partial (\rho c_p T)}{\partial z} \bigg|_{z=0} = h(T_w - T_b) \]  

Fourier's law of conduction \hfill (1.61)

\[ N_n = -\left( D_{12} + E_D \right) \frac{\partial c_n}{\partial z} \bigg|_{z=0} = \frac{8_m}{c} (c_{n,w} - c_{n,b}) \]  

Fick's law of diffusion \hfill (1.62)

\[ \frac{T}{u_b} = -\left( \nu + E_v \right) \frac{\partial (\rho u / u_b)}{\partial z} \bigg|_{z=0} = \frac{J_0}{2} (u_b - u_w) \]  

Newton's law of viscosity \hfill (1.63)

where \( E_H, E_D, E_v \) are the turbulent (or eddy) diffusivities of heat, mass, and momentum respectively. (Eddy diffusivities are calculated based on turbulence modeling - see Appendix C). The transport equations for heat, mass and momentum are also similar. Taking the transport equations in the \( x \)-direction, with constant molecular properties:

\[ \frac{D\bar{T}}{Dt} = \left( \alpha + \frac{\nu}{Pr_t} \right) \nabla^2 \bar{T} + \frac{Q^*}{\rho} \]  

conservation of energy \hfill (1.64)

\[ \frac{Dc_n}{Dt} = \left( D_{12} + \frac{\nu}{Sc_t} \right) \nabla^2 \bar{c}_n + \bar{R}^* \]  

conservation of species \hfill (1.65)

\[ \frac{Du}{Dt} = \left( \nu + \nu_t \right) \nabla^2 \bar{V} + \left( -\frac{1}{\rho} \frac{\partial P}{\partial x} + g_x \right) \]  

conservation of \( x \)-momentum \hfill (1.66)

where the eddy diffusivities of heat and mass are expressed in terms of the eddy diffusivity for momentum - the eddy viscosity. Each equation consists of a convection term (left hand side), a diffusion term (first term on the right hand side), and a source term. Each of these equations can be represented by a generic equation if the variable of interest is put in dimensionless form:

\[ \phi = \frac{T - T_w}{T_b - T_w} = \frac{c_n - c_{n,w}}{c_{n,b} - c_{n,w}} = \frac{u - u_w}{u_b - u_w} \]  

\[ \frac{D\phi}{Dt} = D\nabla^2 \phi + S \]  

\hfill (1.67)

\hfill (1.68)

where \( D \) and \( S \) are the corresponding diffusivity and source terms. In this form it is easy to see that the three processes obey similar physical laws. There are several dimensionless groups that are often used to characterize the relationship between these mechanisms for different fluids. The Prandtl number is the ratio of momentum diffusivity to thermal diffusivity:

\[ \text{Pr} = \frac{\mu / \rho}{(k / \rho c_p)} = \frac{\nu}{\alpha} \]  

\hfill (1.69)
The Schmidt number is the ratio of momentum diffusivity to mass diffusivity:

\[ Sc = \frac{\mu}{\rho D_{12}} = \frac{v}{D_{12}} \]  

(1.70)

And the Lewis number is the ratio of thermal diffusivity to mass diffusivity:

\[ Le = \frac{Sc}{Pr} = \frac{\alpha}{D_{12}} \]  

(1.71)

Reynolds first proposed an analogy between momentum and heat transfer based on experimental observation - he noted that fluid motion in turbulent flow tends to transfer both heat and momentum. The eddies which transfer momentum in turbulent flow also transport heat. Also the resistance to heat transfer is very close to the resistance of momentum transfer in a viscous sublayer of a fluid with Prandtl number close to unity. As this suggests, there is a relation between friction and heat transfer \((f\) is the Fanning friction factor):

\[ \frac{f}{2} = \frac{C_f}{2} = StPr^{0.6} \]  

(1.72)

For a Prandtl number of one, this reduces to the simple Reynolds Analogy:

\[ \frac{C_f}{2} = St = \frac{h}{\rho c_p} \]  

(1.73)

The Stanton number is seen to be the ratio of energy transfer at the wall by convection to energy transported by the free stream. This relationship can be derived by expressing equations (1.61) through (1.63) in dimensionless form as follows:

\[ \Phi \left|_{z=0}^{\partial} \right. = \frac{h}{\rho c_p(\alpha + E_H)} \]  

(1.74)

\[ \frac{\partial \phi}{\partial z} \left|_{z=0} \right. = \frac{(g_m/c)}{(D_{12} + E_D)} \]  

(1.75)

\[ \frac{\partial \phi}{\partial z} \left|_{z=0} \right. = \frac{f u_b}{2(v + E_v)} \]  

(1.76)

Then setting equations (1.74) and (1.76) equal:

\[ \frac{h}{\rho c_p(\alpha + E_H)} = \frac{f u_b}{2(v + E_v)} \]  

(1.77)
If we assume turbulent flow, the molecular diffusivities $\alpha$ and $\nu$ can be ignored relative to the turbulent diffusivities. If we also assume that the turbulent diffusivities are approximately equal, the result is the Reynolds analogy and the definition of the Stanton number:

$$\frac{f}{2} = \frac{h}{\rho c_p u_b} \equiv St$$

(1.78)

A more general form of the convective momentum and heat transfer analogy is: [Mills p. 283]

$$St = \frac{C_f}{2} Pr^{-0.67} \quad \text{laminar flow (} Pr > 0.5 \text{)}$$

(1.79)

$$St = \frac{C_f}{2} Pr^{-0.57} \quad \text{turbulent flow (} 0.7 < Pr < 400 \text{)}$$

(1.80)

For low mass transfer rates, there is also an analogy between convective heat and mass transfer, called the Chilton-Colburn analogy:

$$\frac{St_m}{St} = \left( \frac{Sc}{Pr} \right)^{-2/3}$$

(1.81)

The Schmidt number is the ratio of momentum diffusivity to mass diffusivity - thus equation (1.81) relates the rate of heat transfer to the rate of mass transfer. $St_m$ is the mass transfer Stanton number which is the ratio of mass transfer at the wall to mass transport by the free stream:

$$St_m = \frac{g_m}{\rho u}$$

(1.82)

A “low mass transfer rate” in this case means essentially that the mass transfer is small enough not to disrupt the flow field near the wall. This is an important detail since neither heat nor momentum transfer cause a flow field disruption by making a part of the flow field disappear through the interface. Thus for the analogy to mass transfer to be true, the same such conditions should exist. In reality this is not the case, and the use of a blowing factor or blowing parameter is used to “correct” the analogy for high mass transfer rates.

For low mass transfer rates, the implications of the Chilton-Colburn analogy offer an easy method to find the Sherwood number for a particular situation. Simply replace the Prandtl number with the Schmidt number in the appropriate expression for the Nusselt number and obtain the Sherwood number. For instance, the McAdams heat transfer relation (for turbulent natural convection along a vertical surface) and the associated mass transfer relation are shown below [McAdams, 1954]:

$$Nu = 0.13(Gr Pr)^{1/3} \quad (1.83)$$

$$Sh = 0.13(Gr Sc)^{1/3} \quad (1.84)$$
To give the reader an indication of the molecular properties of the gases involved, the Prandtl number for each pure gas at 300K is listed here: air 0.69; steam 0.86; hydrogen 0.67; and helium 0.7. The Prandtl and Schmidt numbers for three different mixtures are given over a range of temperature and pressure in Table 1-2. The mixtures are steam-air, steam-air-helium, and steam-air-hydrogen. The mixtures with light gas have a 30% molar concentration of light gas in the noncondensable mix. Notice that the Schmidt numbers for mixtures with helium and hydrogen are nearly equal. This indicates that the expected mass transfer rate of steam in the two different mixtures is expected to be similar, lending credibility to the use of helium as a simulant for hydrogen in condensation experiments.

Table 1-2: Prandtl and Schmidt numbers of relevant gas mixtures

<table>
<thead>
<tr>
<th>Condition</th>
<th>Prandtl Number</th>
<th>Schmidt Number</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Steam-Air only</td>
<td>30% He in nc gas</td>
</tr>
<tr>
<td>T (K)</td>
<td>P (MPa)</td>
<td>Xₜ</td>
</tr>
<tr>
<td>300</td>
<td>0.1048</td>
<td>0.0337</td>
</tr>
<tr>
<td>320</td>
<td>0.1186</td>
<td>0.0889</td>
</tr>
<tr>
<td>340</td>
<td>0.1420</td>
<td>0.1914</td>
</tr>
<tr>
<td>360</td>
<td>0.1837</td>
<td>0.3383</td>
</tr>
<tr>
<td>380</td>
<td>0.2570</td>
<td>0.5008</td>
</tr>
<tr>
<td>400</td>
<td>0.3806</td>
<td>0.6451</td>
</tr>
</tbody>
</table>

The Grashof numbers for the same gas mixtures, with the addition of the Grashof number for air only convection, are shown in Table 1-3. The Grashof number is a dimensionless group for natural convection flow which is analogous to the Reynolds number for forced convection flow. The Grashof number is given by the formula:

\[ Gr_x = \frac{g \rho (\rho_i - \rho_s) x^3}{\mu^2} \]  

where \( x \) is the characteristic dimension of the flow, in the particular case of interest, flow along a vertical wall, the characteristic dimension \( x \) is the distance from the top of the wall.

The Grashof numbers in Table 1-3 are raised to the 1/3 power (form used in equation 1.82) and have been normalized to the value for air-only convection with \( T_{bulk} = 300 \text{ K} \) and \( T_{wall} - T_{bulk} = 10 \text{ K} \), \( Gr^{1/3} = 1.154 \times 10^3 \). All values have been calculated for a length, \( x \), of 1.0 meter. Notice that the Grashof numbers are considerably higher for steam-air mixtures compared to air-only convection. The presence of condensing steam leads to higher Grashof numbers because the density change across the boundary layer is not only a function of temperature change across the boundary layer, but also a function of the steam concentration change across the boundary layer. The entries in Table 1-3 also show the influence of the light gases on the Grashof number. The presence of a light gas decreases the density change across the boundary layer, decreasing the buoyancy driving force for natural convection. The decrease in convection driving force is reflected in the smaller Grashof numbers for mixtures with light gases.
Also notice that the Grashof numbers increase for mixtures with steam as the bulk temperature increases with a fixed value of wall subcooling (i.e., fixed temperature difference between the wall and the bulk). This increase in the Grashof number is due to the characteristics of the steam saturation pressure curve. As the temperature and the saturation pressure of steam increase, the difference in saturation pressure for a given value of wall subcooling also increases. That is, the saturation pressure difference of steam at 380 K vs 370 K is larger than the saturation pressure difference for steam at 320 K vs 310 K. Thus the steam concentration change across the boundary layer is greater for a given value of wall subcooling at higher temperatures. This in turn leads to a greater density difference across the boundary layer for steam mixtures at high temperatures.

### Table 1-3: Normalized Grashof numbers of relevant gas mixtures

<table>
<thead>
<tr>
<th>T&lt;sub&gt;bulk&lt;/sub&gt; (K)</th>
<th>P (MPa)</th>
<th>Air only</th>
<th>Steam only</th>
<th>30% He in nc gas</th>
<th>30% H&lt;sub&gt;2&lt;/sub&gt; in nc gas</th>
<th>Air only</th>
<th>Steam only</th>
<th>30% He in nc gas</th>
<th>30% H&lt;sub&gt;2&lt;/sub&gt; in nc gas</th>
</tr>
</thead>
<tbody>
<tr>
<td>300</td>
<td>0.1048</td>
<td>1.00</td>
<td>1.06</td>
<td>0.82</td>
<td>0.83</td>
<td>1.52</td>
<td>1.60</td>
<td>1.24</td>
<td>1.27</td>
</tr>
<tr>
<td>320</td>
<td>0.1186</td>
<td>0.98</td>
<td>1.12</td>
<td>0.85</td>
<td>0.86</td>
<td>1.49</td>
<td>1.62</td>
<td>1.25</td>
<td>1.27</td>
</tr>
<tr>
<td>340</td>
<td>0.1420</td>
<td>1.01</td>
<td>1.27</td>
<td>0.94</td>
<td>0.95</td>
<td>1.53</td>
<td>1.80</td>
<td>1.35</td>
<td>1.36</td>
</tr>
<tr>
<td>360</td>
<td>0.1837</td>
<td>1.11</td>
<td>1.55</td>
<td>1.12</td>
<td>1.12</td>
<td>1.66</td>
<td>2.15</td>
<td>1.58</td>
<td>1.58</td>
</tr>
<tr>
<td>380</td>
<td>0.2570</td>
<td>1.23</td>
<td>1.96</td>
<td>1.41</td>
<td>1.38</td>
<td>1.92</td>
<td>2.69</td>
<td>1.95</td>
<td>1.94</td>
</tr>
<tr>
<td>400</td>
<td>0.3806</td>
<td>1.54</td>
<td>2.51</td>
<td>1.79</td>
<td>1.74</td>
<td>2.30</td>
<td>3.43</td>
<td>2.47</td>
<td>2.43</td>
</tr>
</tbody>
</table>

* Normalized to (Gr<sub>0</sub>)<sup>1/3</sup> = 1.154x10<sup>3</sup>, value for air at 300 K, with T<sub>bulk</sub> - T<sub>wall</sub> = 10 K, x = 1.0 meter.

#### 1.5.4 Property evaluation

The conditions at which transport and thermodynamic properties are evaluated are extremely important in mass transfer calculations. The choice of a specific reference state can have a major influence on the numerical value of the answer. The heat and mass transfer equations require that the Grashof and Prandtl numbers, mixture density, viscosity, conductivity and diffusion coefficient be evaluated at some reference temperature and composition. For low mass transfer rate analyses (where a small compositional variation is assumed over the boundary layer) the mixture properties are generally evaluated at the free-stream composition and the mean boundary layer temperature. For high mass transfer rates, this assumption is clearly inadequate since the composition varies significantly across the boundary layer. Mass transfer texts give some guidance on the choice of properties, generally suggesting that a suitable average be taken (temperature and composition) and all properties be evaluated at that reference state [Mills, 1995]. However, the texts also suggest that the numerical values be compared with experimental data whenever possible to help choose the appropriate average values for individual circumstance. Table 1-4 lists several possible reference states, each state consists of a definition for the average temperature and the average steam mole fraction. The scheme used to evaluate properties in this thesis is scheme number 7. A more detailed treatment of properties is presented in chapter 2 along with a thorough analysis of the sensitivity of the DLM condensation model to changes in the reference state. Table 1-4 has been included here in the discussion of mass transfer section for completeness.
Table 1-4: Possible definitions of the reference state to evaluate transport properties

<table>
<thead>
<tr>
<th>Scheme</th>
<th>Reference Temperature</th>
<th>Reference Steam Mole Fraction</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>$T_b$</td>
<td>$X_{s,b}$</td>
</tr>
<tr>
<td>2</td>
<td>$\frac{T_b + T_i}{2}$</td>
<td>$X_{s,b}$</td>
</tr>
<tr>
<td>3</td>
<td>$\frac{T_b + T_i}{2}$</td>
<td>$\frac{X_{s,b} + X_{i,i}}{2}$</td>
</tr>
<tr>
<td>4</td>
<td>$\frac{T_b + T_i}{2}$</td>
<td>$\frac{P_{\text{sat}}(T_{\text{ref}})}{P_{\text{total}}}$</td>
</tr>
<tr>
<td>5</td>
<td>$\frac{T_b - T_i}{\ln(T_b/T_i)}$</td>
<td>$\frac{X_{s,b} + X_{i,i}}{2}$</td>
</tr>
<tr>
<td>6</td>
<td>$\frac{T_b - T_i}{\ln(T_b/T_i)}$</td>
<td>$\frac{X_{s,b} - X_{i,i}}{\ln(x_{s,b}/x_{i,i})}$</td>
</tr>
<tr>
<td>7</td>
<td>$\frac{T_b - T_i}{\ln(T_b/T_i)}$</td>
<td>$\frac{P_{\text{sat}}(T_{\text{ref}})}{P_{\text{total}}}$</td>
</tr>
</tbody>
</table>

1.6 Outline of Work Presented in this Thesis

This chapter gave a brief explanation as to why this work was carried out. A review of physical phenomena important in containment analysis was also presented. Section 1.3 gave a quick overview of condensation models, while appendix A may be consulted for a detailed review. The chapter rounded out by discussing a few containment codes available for analysis work and presenting a short summary of mass transfer theory. Chapter two gives an in-depth analysis of the modified Peterson condensation model. The model is implemented into Mathcad, compared with other models over a wide range of conditions, and a sensitivity analysis is performed on the model for variations in key properties. Chapter three discussed the numerical simulations completed for turbulent boundary layers. First the goals are discussed, followed by the selection process for a suitable computer code. Next the assumptions and limitations of the analysis are discussed, the benchmark problems are presented, and the “experimental” matrix is set up. Finally the results are presented along with a discussion of their implications for the boundary layer hypothesis in the next chapter. Chapter four presents the goals of the boundary layer hypothesis - basically to develop a boundary layer-type heat transfer model for use in a finite volume containment analysis computer code. The boundary layer model is then implemented in GOTHIC 4.1c, and tested. The results are then discussed. Chapter five wraps up by summarizing the major findings of this work, the original contributions to the field of containment analysis and heat transfer, and gives a list of possible items for further development.
2. CONDENSATION MODEL EVALUATION

2.1 Goals of Model Evaluation

The goals for this chapter are fairly straightforward. First, the approach used to model several different types of condensation surfaces will be presented and justified. This will cover aspects such as surface orientation, material composition, and other simplifications which are used to make the impending analysis tractable. Second, a summary of the literature on the importance and influence of surface orientation and light gas addition will be presented. Third, the method which was used by the author to evaluate several different condensation models will be presented. A numerical comparison of predicted condensation rates for several condensation models is performed for a range of containment conditions. The sensitivity of the different models to changes in key variables is also discussed. Finally, the decision to focus primarily on the diffusion layer model (the Peterson approach) to condensation modeling is presented and justified.

2.2 Heat Sink Modeling in Containment Analysis

There are several types of heat sinks inside a nuclear reactor containment building. Most of these heat sinks will play an important role during a loss of coolant accident (LOCA). Even though individual heat sinks may seem insignificantly small, the sum total of all in-containment sinks will have a profound effect on the peak pressure in a containment building following a LOCA. When performing an analysis of containment performance, it is important to recognize that the condensation rate may differ among heat sinks of various types. Consequently, the method used to model heat transfer to the different heat sinks should be considered carefully. Surface size, orientation, and structural thermal conductivity can all have an effect on the condensation rate. Accordingly, the most appropriate method of modeling heat transfer will differ for different types of heat sinks.

2.2.1 Small fast acting heat sinks

Fast acting heat sinks, such as metal gratings, pumps and piping, and structural steel, have an important influence on the containment pressure immediately following a LOCA. The individual heat sinks are usually small, but collectively they are second only to a suppression pool in effectiveness for limiting the pressure spike immediately following the blowdown. For practical reasons, these components can be modeled as “equivalent thermal masses” when performing a containment analysis. This simple approach is warranted because most fast acting heat sinks are composed of a relatively small mass of high conductivity metal which becomes thermally saturated within the first few hundred seconds after a blowdown.

The key parameter to model correctly for a fast acting heat sink is the total thermal capacity of the component because this determines how much each heat sink contributes to limiting the pressure spike. The next most important parameter to model is the effective surface area available for heat transfer since this directly figures into the rate at which heat is absorbed by the heat sink.
The heat transfer rate to a fast acting heat sink will initially be quite large, and then decrease exponentially as the heat sink temperature approaches that of the containment atmosphere. Since the total amount of energy absorbed by the heat sink is limited by the small thermal capacity of the component and not the condensation rate, the exact condensation model used is not important. For example, in a transient where the peak containment pressure is reached at $t = 1000$ seconds, the consequence of a steel grate becoming thermally saturated at $t = 100$ seconds versus $t = 200$ seconds is not very significant. What is significant is that the total thermal capacity of the grate is felt relatively quickly. It is not imperative that the condensation relations used in these circumstances be extremely accurate, just that they allow a sufficiently high condensation rate for the component to become saturated quickly. Therefore, it is acceptable to use a simple, easily calculated condensation heat transfer coefficient, such as the Uchida relation, when modeling small fast acting heat sinks.

The orientation of a heat sink surface is important to model only when it is needed to determine the condensation rate on the heat sink surface, or when condensation on the heat sink will induce buoyancy forces which may influence the flow in the vicinity of the heat sink. Because the accuracy of the condensation relations is of secondary importance, the orientation of the effective condensation surface can generally be ignored in the calculation. It is then necessary to look at buoyancy forces to determine whether orientation is important. In some cases the effective surface area of the heat sink is small enough that any induced buoyancy force is too small to significantly influence the flow. However, for a heat sink with a large surface area, a substantial buoyancy force may be induced. This buoyancy force will be strongest immediately after the blowdown and decrease rapidly as the heat sink saturates. Once the heat sink is saturated, the buoyancy force will vanish. For heat sinks which saturate within the first few hundred seconds of the transient, the buoyancy induced by these surfaces will most likely be insignificant relative to the turbulent atmospheric mixing produced by the break. Furthermore, these forces will not be sustained long enough to produce a significant effect on the long-term convection patterns within the containment structure. Therefore it is reasonable to conclude that for fast acting heat sinks, detailed modeling of the effective surface orientation is not important for capturing either flow patterns or the condensation rate.

2.2.2 Large surfaces

The second major type of heat sink is the large containment surface. These surfaces, such as walls, floors, pools, and ceilings, generally have a larger gross heat capacity and a lower thermal conductivity than most of the small metallic in-containment components. These traits tend to make the containment structure itself an important, long-term, passive heat sink in a containment analysis. The scale of these surfaces has a profound effect on the circulation within the containment and thus modeling the condensation process itself is important. Large surfaces generally fall into one of two categories - high conductivity or low conductivity. In practical situations the high conductivity surfaces are generally metallic while the low conductivity surfaces tend to be concrete. This difference is very important, as the limiting heat transfer mechanisms for the two are distinct.

---

1 The surface orientation is also important when determining the thickness of the liquid film, which is a factor when determining the overall resistance to heat transfer. However, the thickness of the liquid film is only important for very high condensation rates, thus it is not considered important to this discussion.
Concrete

Large concrete structures have a large heat capacity, and thus do not become thermally saturated quickly. However, the rate at which heat is absorbed by these heat sinks is limited by the low thermal conductivity of the concrete. The concrete surface temperature will quickly approach that of the containment atmosphere and heat will slowly be conducted into the concrete mass. Concrete walls and structures do absorb a significant amount of energy because of their large size, but their effectiveness as passive heat sinks is limited because of their long response times. Condensation will continue to occur on concrete surfaces for a long time after the LOCA because the concrete will continue to absorb heat, although slowly. From a modeling perspective it is not important to use a sophisticated condensation model at the surface of a concrete heat sink because the heat transfer rate will be limited by the low conductivity of the concrete. Therefore the most important parameter to model accurately is the conductivity of the concrete. However, modeling of the condensation process is not as simple as with fast acting heat sinks because it is possible that the heat transfer rate will be high enough for a sufficiently long time to induce significant buoyancy forces near large concrete surfaces. It is important that an analysis capture these buoyancy forces because they may impact global circulation within the containment. However, such a modeling scheme depends primarily on the way in which the fluid region near the heat sink is discretized rather than with the condensation correlation used to predict the heat transfer rate.

Metallic

Large metallic surfaces which do not become saturated quickly deserve special attention. In this case the surfaces may be the same size as the structural concrete surfaces discussed above, but unlike concrete the metal surfaces have the capability to remove heat at an appreciable rate for a relatively long period of time. Examples of such surfaces are an externally cooled steel containment shell (AP600 design), steel walls of an in-containment water pool, or a pool surface (thermal conductivity closer to that of steel than concrete). Modeling condensation on this type of heat sink is very important, because the total amount of heat removed by the heat sink is generally limited by the rate of condensation predicted by the condensation model used at the surface. Physically, the limiting factor in this situation is the buildup of noncondensable gas near the condensation surface which acts to impede the condensation process. Therefore it is appropriate to use an accurate condensation model in this case since the heat removal rate of the structure is primarily dependent on the instantaneous rate predicted by the condensation correlation.

These large surfaces will also induce buoyant forces which will influence the flow field near the heat sink and possibly influence the global circulation in the containment. This circulation can have a direct effect on the condensation rate by sweeping away noncondensable gases and bringing more steam into the proximity of the cool surface. For this reason it is also important to create the model in such a way as to capture these buoyant forces and their effects on the atmosphere. The condensation model and fluid region noding should also take into account the orientation of the surface because the buildup of noncondensable gases at a surface may be affected by the surface orientation. There are generally four condensation surface orientations of interest in containment analysis: vertical, inclined, horizontal facing upward, and horizontal.
facing downward. Vertical and inclined surfaces generally characterize containment domes and walls, while consideration of horizontal surfaces applies to floors, pools and ceilings.

Most large surfaces that fall into the category of important long term heat sinks are vertical or near vertical. On these vertical surfaces there will most likely be a downward flowing boundary layer near the surface. Correctly predicting the heat transfer rate and the momentum balance in this boundary layer are primary objectives of this thesis. A notable special situation occurs for the surface of a water pool. Since the pool surface is horizontal, buoyancy forces will not act to sweep the layer of noncondensable gas away from the cool surface if the gas is heavier than water vapor (as is air at most temperatures). If the atmosphere above the pool is quiescent, the noncondensable layer is expected to increase steadily in thickness, which should cause a decrease in the condensation rate at the pool surface. This phenomenon is important and should be studied, but is much more complex than modeling the boundary layer next to a vertical wall, and is left for future work. Table 2-1 summarizes the three types of heat sinks discussed in this section. For each type of heat sink the parameters which limit the heat transfer rate are identified, and those that are secondary or can be ignored are also listed. To give a more complete picture of the influence of surface orientation on the condensation rate, section 2.3 gives a summary of the experimental work in that area.

Table 2-1: Important parameters for heat sink modeling

<table>
<thead>
<tr>
<th>Type of Heat Sink</th>
<th>Primary (limiting) parameters</th>
<th>Secondary Parameters</th>
<th>Inconsequential Parameters</th>
</tr>
</thead>
<tbody>
<tr>
<td>small, high $k$</td>
<td>$c_p$, $k$, $A_s$, $A_s,_{\text{eff}}$, $k$</td>
<td>$A_s,_{\text{eff}}$, $k$</td>
<td>orientation, condensation model</td>
</tr>
<tr>
<td>large, low $k$</td>
<td>$k$, $A_s$, $k$, $A_s$</td>
<td>total $c_p$</td>
<td>condensation model</td>
</tr>
<tr>
<td>large, high $k$</td>
<td>$A_s$, condensation model</td>
<td>total $c_p$, $k$, orientation</td>
<td></td>
</tr>
</tbody>
</table>

2.3 Surface Orientation and Gas Mixture

This section is included for two reasons. The first is to give the reader a visual and verbal description of the condensation phenomenon on horizontal and vertical surfaces. The second is to present a brief summary of the experimental programs which have been carried out to study the effects of surface orientation and gas mixture on condensation rate. The presence of hydrogen inside containment atmospheres has always been a real concern but it has garnered more attention since the Three Mile Island-2 accident in 1979. The presence of hydrogen is a concern in the present study because the light gas may cause a reduction in the condensation rate, and thus an increase in the overall containment pressure. Because of the nature of systems which rely on natural convection, the interaction between surface orientation and gas mixture is a serious concern. The research in this area has generally been conducted using helium gas as a nonflammable substitute for hydrogen.
2.3.1 Description of condensation

A downward facing horizontal surface of interest would be a ceiling in a compartment of the containment building or the top of a pool enclosure, such as the top of the wetwell in a containment with a suppression pool. Figure 2-1 shows graphically the situation for condensation on this type of surface as it has been reported in the literature [Anderson, 1998; Stein, 1987]. For a wetting surface, a condensate film forms across the horizontal surface and pendant drops form and separate from the film under the influence of gravity. A gas-vapor boundary layer is present beneath the condensate film and the condensation rate is limited by the diffusion of vapor through this boundary layer. Properties of the noncondensable gas mixture are of primary concern. For instance the diffusivity, which governs mass transfer, varies significantly between different gases. The buoyancy of noncondensable gases is also expected to be important because it could cause stratification of the gas layer or induce mixing, depending on the relative molecular weights of the gas and the vapor.

Vertical surfaces will have a condensate film which will flow downward under the influence of gravity. Inclined surfaces will form drops and water ridges in the absence of a complete film if the condensation rate is not high enough to support a complete film. Drops which depart from these ridges (or rolling waves) play a similar role to that of the drops which fall from a horizontal surface, causing a slight increase in the rate of heat transfer over that for a complete condensate film [Anderson, 1998]. The properties of the noncondensable gas mixture are again of primary importance because diffusion and natural convection are the physical processes which limit the rate of condensation.

![Figure 2-1: Film condensation on a horizontal surface.](image-url)
The literature is rather sparse concerning surface orientation and condensation in the presence of a noncondensable gas, but there are a few experimental programs that have looked specifically at orientation and the effect it has on condensation with steam/gas mixtures. Table 2-2 lists the studies of interest and the conditions for which they were carried out. Each study is discussed in turn and then conclusions are drawn where appropriate. Gaps in the data are also pointed out.

The studies presented here are all for experiments using steam as the condensing vapor and helium or air, or both, as the noncondensable gas.

<table>
<thead>
<tr>
<th>Researcher/Surface Finish</th>
<th>Pressure (MPa)</th>
<th>Vel. (m/s)</th>
<th>$X_{\text{nc}}$</th>
<th>$X_{\text{He}}$</th>
<th>$X_{\text{He}/X_{\text{nc}}}$</th>
<th>Presented in Section</th>
</tr>
</thead>
<tbody>
<tr>
<td>Stein, et. al (1985)</td>
<td>0.31-1.24</td>
<td>----</td>
<td>0.006 - 0.37</td>
<td>0</td>
<td>-</td>
<td>0.006 - 0.37</td>
</tr>
<tr>
<td>Cho, et. al (1988)</td>
<td>0.31-1.24</td>
<td>----</td>
<td>0.01 - 0.30</td>
<td>0.01 - 0.3</td>
<td>1.0</td>
<td>0.01 - 0.30</td>
</tr>
<tr>
<td>Huhtiniemi, et. al (1989)</td>
<td>0.1</td>
<td>1 - 3</td>
<td>0.17 - 0.80</td>
<td>0</td>
<td>0.80</td>
<td>0.17 - 0.80</td>
</tr>
<tr>
<td>Huhtiniemi, et. al (1991)</td>
<td>0.1</td>
<td>1 - 2</td>
<td>0.17 - 0.80</td>
<td>0</td>
<td>0.80</td>
<td>0.17 - 0.80</td>
</tr>
<tr>
<td>Pernsteiner, et. al (1992)</td>
<td>0.1</td>
<td>0.53 - 0.72</td>
<td>0.0 - 0.18</td>
<td>0.0 - 0.39</td>
<td>0.0 - 0.49</td>
<td>0.53 - 0.72</td>
</tr>
<tr>
<td>Anderson (1998)</td>
<td>0.1</td>
<td>0.29 - 0.78</td>
<td>0.0 - 0.26</td>
<td>0.0 - 0.32</td>
<td>0.0 - 0.49</td>
<td>0.29 - 0.78</td>
</tr>
<tr>
<td>Anderson (1998)</td>
<td>0.1 -0.3</td>
<td>----</td>
<td>0.26 - 0.78</td>
<td>0.0 - 0.38</td>
<td>0.0 - 0.49</td>
<td>0.26 - 0.78</td>
</tr>
</tbody>
</table>

* 0° is a horizontally downward facing surface, 90° is a vertical surface.
No studies are discussed here for a horizontally upward facing surface.
2.3.2 Experiments of Stein, Cho, and Lambert

The first two studies of interest were performed by Stein, Cho, and Lambert in a very small, pressurized vessel with a horizontal downward facing polished copper condensing plate. These experimental programs attempted to relate the degradation in condensation rate to the amount of noncondensable gas present. The first series of experiments looked at steam-air atmospheres. The steam-air data was successfully correlated using a natural convection approach based on Rayleigh number and employing the heat/mass transfer analogy [Stein, 1985]. This confirmed that natural convection aids in the mass transfer process, as would be expected in this case since air is more dense than steam. The authors also showed that increasing pressure causes an increase in the condensation rate over and above what is expected from simply changing the gas/steam mass ratio at a particular temperature.

Additional experiments were carried out in the same apparatus to look at steam-helium atmospheres [Cho, 1988]. Since helium is less dense than steam, the authors attempted to fit their data to a relationship in the form of a simple one-dimensional diffusion process. This did not correspond to the data, which showed condensation rates as much as four times higher than predicted from the simple diffusion model. Visual observation during the tests showed that some type of convection phenomenon was taking place that increased the mass transfer rate. The authors were unable to systematically quantify this convection reliably. Another difficulty encountered during the steam-helium tests was that data could not be reproduced at high pressures. Much of this problem was blamed on a dropwise condensation regime which often occurred on the polished surface. Dropwise condensation was also seen in the steam-air tests, but the dropwise data was not used when developing the conclusions from those tests. Very little can be concluded from the Stein et al. data, but several observations can be made. The polished surface was very sensitive to contamination, which resulted in a condensation regime that was sometimes dropwise, sometimes filmwise, and sometimes mixed. The tests for steam-air showed that the heat and mass transfer analogy can be used to predict filmwise condensation from a horizontal surface. Finally, these tests imply that under some conditions, the light gas helium may not be as detrimental to condensation as was previously assumed. It must be pointed out that this is not a conclusion, merely an observation. Unfortunately, no tests were performed which examined atmospheres with a mixture of steam, air, and helium.

2.3.3 Experiments of Huhtiniemi and Pernsteiner

Huhtiniemi studied the effect of surface orientation on the condensation rate in the presence of air for a polished aluminum surface [Huhtiniemi, 1989] and a painted aluminum surface\(^2\) [Huhtiniemi, 1991] in forced convection \((v = 1-3 \text{ m/s})\) at atmospheric pressure. The surface orientation ranged from horizontal downward facing to vertical. The surface finish had a noticeable impact on the regime of condensation; the polished surface sometimes reverted to dropwise condensation while the painted surface consistently produced filmwise condensation. It was shown consistently that heat transfer coefficients for film condensation of steam in the presence of air decrease slightly with increasing angle. This small enhancement for horizontal downward facing surfaces over inclined surfaces is attributed to increased steam-gas boundary

\(^2\) The paint is an inorganic zinc paint which is similar to that proposed by Westinghouse for use on the AP600 steel containment shell.
layer mixing caused by pendant droplets falling through the gas boundary layer [Huhtiniemi, 1991].

Pernsteiner later used the same facility to study the effects of adding helium to the steam-air mixture for condensation on a downward facing horizontal surface. (No tests were completed for changes in surface orientation.) He found that the presence of helium in the gas mixture had little or no inhibiting effect on the condensation rate for a fixed molar amount of noncondensable gas, with helium in the range of \( X_{he}/X_{nc} < 39\% \) (4\% > \( X_{he} \) > 16\%). This was somewhat unexpected because the lower density of helium compared to steam should result in some stratification which would displace the steam, moving it farther away from the condensing surface, thus decreasing the condensation rate. To explain his observation, Pernsteiner suggested that, at these helium concentrations, the higher diffusivity of helium relative to air increases steam diffusion through the boundary layer enough to counter the decrease in condensation which would result from stratification. This suggestion is consistent with the earlier conclusion of Siddique that, on a molar basis, hydrogen (and helium) is less inhibiting to condensation than air [Siddique, 1989]. However, it must be remembered that the Pernsteiner studies were carried out in a slightly forced convection regime, and thus the conclusions may not be directly applicable to nearly stagnant atmospheres where the presence of helium may retard natural convection.  

### 2.3.4 Experiments of Anderson

The effect of orientation and helium concentration on condensation for natural convection conditions was studied directly by Anderson [Anderson, 1998]. Two different experimental facilities were constructed as 1/12th scale representations of the AP600. The first was a polycarbonate atmospheric pressure facility which had one horizontal downward facing condensing plate and one vertical condensing plate. A second steel pressurized facility was created with a condensing surface approximating the elliptical upper dome of the AP600 (i.e., horizontal at the top and gradually transitioning to vertical). The condensing plates in both facilities were painted with the same inorganic zinc paint proposed for the AP600 and used in the Huhtiniemi and Pernsteiner experiments.

For steam-air mixtures in the atmospheric facility Anderson found that the average condensation rate was slightly higher on the horizontal plate than on the vertical plate. This trend was consistent for the large data set gathered in both the atmospheric and pressurized facility. However, it must be noted that the natural convection pattern which exists in the Anderson facilities is such that the steam-gas mixture will rise from the injection point near the bottom, come in contact with the horizontal plate first, then move downward along the side of the vessel.

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3 Dehbi performed condensation experiments on the outside of a vertical copper tube in the presence of air and a mixture of air and helium [Dehbi, 1991]. The results indicate that, on a molar basis, the helium-air mixture is slightly more inhibiting to condensation than pure air. The reduction was shown to be less than 10\% in most cases, and within 20\% for all cases. Dehbi suggests that the decreased buoyant effect of the lighter gas mixture is not compensated for by the increase in the diffusivity of the helium mixture, which is inconsistent with the observations of both Pernsteiner and Siddique. Dehbi’s conclusion is supported by the analytical work of Herranz [Herranz, 1998], but Herranz predicts that the inhibiting effect of helium should be within measurement error for helium concentrations in the range \( X_{he}/X_{nc} < 30\% \).
to come in contact with the vertical condensing plate. Thus it is possible that the lower condensation rate seen on the vertical plate is due to the gas mixture being slightly depleted of steam as compared to the gas mixture near the horizontal plate. No experiments were performed where only the horizontal or the vertical plate were tested individually, hence this question cannot be resolved completely from the data published to date.

The effect of helium on the condensation rate for both the atmospheric and pressurized facility in the natural convection regime was studied extensively for helium concentrations in the range $X_{\text{he}}/X_{\text{nc}} < 30\%$. When some helium was substituted for air but the total molar fraction of noncondensable gas remained unchanged, the condensation rate was essentially the same as for the steam-air experiments under the same conditions. For these helium tests the average condensation rate on the horizontal plate was again slightly higher than on the vertical plate. These results were confirmed in the pressurized facility. However, although the average condensation rate for the tests with helium showed little change from the steam-air tests, the variation of local points about the average showed a higher deviation. This was attributed to pockets of light gas that intermittently collected near the edges of the condensation plates.

The negligible effect of helium in concentrations in the range $X_{\text{he}}/X_{\text{nc}} < 30\%$ for condensation at atmospheric pressure has been analytically explained by Herranz [Herranz, 1998]. He shows that the increased diffusivity of the noncondensable mixture balances the decrease in the buoyancy force for helium concentrations in this range. For helium concentrations above about 30\% in the noncondensable mixture, the buoyancy effect dominates, and the heat transfer rate decreases. This effect is slightly more pronounced as the temperature of the steam mixture increases, and thus would be expected to be more pronounced at higher pressures where the saturation temperature of steam is higher. This phenomenon is explored further in section 2.6.

A key conclusion put forth by Anderson is that the total amount of helium present is not as important as the amount of helium relative to the total amount of noncondensable gas. When the helium molar concentration in the noncondensable gas surpasses 40\%, the noncondensable mixture can become less dense than the steam, causing a noncondensable rich stratification layer above the steam mixture. This stratification can reduce the heat transfer rate by as much as 50\% in the affected region. Anderson and Herranz have also evaluated a condensation model against their experimental results [Anderson, 1998; Herranz, 1998]. The model is based on a turbulent natural convection boundary layer diffusion model proposed by Peterson [Peterson, 1993], which has been modified slightly to include the effects of suction and large temperature drops across the boundary layer. They have shown that their model, which accounts for the diffusivity and buoyancy changes which occur with differing air and helium ratios in the noncondensable gas, is quite good at predicting the experimentally measured values of condensation rate. This model is discussed further in section 2.4 and in appendix A.

2.3.5 Summary of the effect of surface orientation

The majority of the recent data published (with helium as a simulant for hydrogen) supports the conclusion that for hydrogen concentrations below the detonation limit, the effect of hydrogen on the condensation rate inside the containment is small. This has been shown for horizontal downward facing surfaces as well as for vertical and inclined surfaces. Furthermore, the rate of
condensation seems to be relatively independent of surface orientation. Therefore, it is plausible to apply a very similar condensation model to both horizontal downward facing surfaces and vertical surfaces without introducing significant error, thereby simplifying a containment analysis. The model which was chosen for work in the present thesis was that proposed by Peterson [Peterson, 1993] and modified by Anderson and Herranz [Anderson, 1998; Herranz, 1998] which will be discussed at length in section 2.4.

2.4 Condensation Models Under Study

This section presents several condensation models taken from the literature and the method used to numerically compare the condensation rates predicted by each for a range of containment conditions. The following models are discussed in this section:

- Uchida [Uchida, 1965]
- Kataoka [Kataoka, 1993]
- Gido & Koestel [Gido, 1983]
- Dehbi [Dehbi, 1991] 4
- Standard Mass Conductance [Mills, 1995]
- Diffusion Layer Model (Peterson implementation) [Peterson, 1993]
- Diffusion Layer Model (Anderson implementation) [Anderson, 1998]
- Diffusion Layer Model (present implementation)

The listed condensation models were programmed into a Mathcad worksheet in a general format which allowed direct numerical comparisons to be performed for specified conditions. Great care was taken to provide consistency between the models which used variables such as heat capacity, conductivity, enthalpy, or mole fraction. The Mathcad worksheet is listed in full in Appendix D. Section 2.4.1 details the exact form of the Diffusion Layer Model that is evaluated, which is the primary condensation model under consideration in this thesis. Section 2.4.2 lists the equations of the other models that are used as a comparison. More on each of these models can be found in Appendix A.

2.4.1 Anderson diffusion layer model

A thorough literature search was performed to determine the current state of condensation modeling and to identify the best model available which could easily be implemented into a finite volume computer code. 5 The overall goal is to improve the capabilities of the finite volume code to predict containment performance for advanced designs which rely solely on natural convection and condensation to control the containment pressure following a loss of coolant accident.

The model which was identified as the most promising candidate for this purpose is that proposed by Peterson [Peterson, 1993]. For simplicity, this approach will be termed the Diffusion Layer Model (DLM), consistent with the terminology of Anderson and Herranz who proposed several modifications to the original model [Anderson, 1998; Herranz, 1998]. A

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4 The Dehbi condensation experiments were performed for condensation on the outside of a vertical tube. A correction factor of 0.8 was used to correct for the effect of curvature in order to create a correlation for flat plate condensation. The correlation that was published, which is used here, is for flat plate condensation.

5 From this point forward, the discussion concerns only condensation on vertical surfaces.
complete discussion of the model’s history is given in Appendix A. The exact form which is used throughout the remainder of this thesis is given below.

In this approach, the condensation and convection processes are assumed to occur in parallel, and both of these processes occur in series with heat transfer through a condensate film which is present on the surface. The entire process is governed by the equation:

$$q_{\text{bulk-wat}} = q_{\text{film}} = q_{\text{cond}} + q_{\text{conv}}$$  \hspace{1cm} (2.1)

The individual heat transfer processes can be expressed as:

$$q_{\text{film}} = h_{\text{film}} (T_i - T)$$  \hspace{1cm} (2.2)
$$q_{\text{conv}} = h_{\text{conv}} (T_b - T_i)$$  \hspace{1cm} (2.3)
$$q_{\text{cond}} = h_{\text{cond}} (T_{r,b} - T_i)$$  \hspace{1cm} (2.4)

The film heat transfer coefficient is evaluated according to a modified Nusselt relation [Herranz, 1998]:

$$h_{\text{film}} = \left[ \frac{h'_{fg} g \rho_1 (\rho_i - \rho_s) k_i^3}{4 \mu_i z (T_i - T_w)} \right]^{1/4} \Psi$$  \hspace{1cm} (2.5)

where a modification to the latent heat is used to correct for condensate subcooling:

$$h'_{fg} = h_{fg} \left[ 1 + 0.68 \frac{c_{pl}(T_i - T_w)}{h_{fg}} \right]$$  \hspace{1cm} (2.6)

and $\Psi$ accounts for the enhancement to heat transfer from waves on the film surface:

$$\Psi = Re_i^{0.04}$$  \hspace{1cm} (2.7)

The convection heat transfer coefficient is expressed by the simple relation:

$$h_{\text{conv}} = \frac{k_m}{x} \cdot \frac{Nu_x}{x}$$  \hspace{1cm} (2.8)

The Peterson approach is unique in that it allows the condensation heat transfer coefficient to be expressed simply as:

$$h_{\text{cond}} = \frac{k_{\text{cond}}}{x} \cdot Sh_x$$  \hspace{1cm} (2.9)

---

6 A slightly different relationship is used in the GOTHIC code to determine the film heat transfer coefficient. A complete discussion of these differences is given in Chapter 4.
This is accomplished through the definition of the condensation conductivity, $k_{\text{cond}}$. The condensation conductivity plays an analogous role in condensation heat transfer to the gas mixture conductivity in convection heat transfer. The condensation conductivity has its origin in a rigorous mass transfer conductance approach. (See the discussion on mass transfer theory in section 1.5) Mass transfer processes are driven by gradients in species concentrations. In the case of condensation in the presence of air, the condensation rate is limited by the rate at which steam can diffuse through the air boundary layer - a mass transfer problem. This diffusion rate is driven by a gradient in steam concentration across the boundary layer. The utility of the Peterson condensation conductivity is that it transforms the driving force from a difference in concentration to a difference in saturation temperatures - thus transforming the mass transfer process into an equivalent heat transfer process. The derivation of the condensation conductivity is given in Appendix B, and it follows directly from the theory of mass transfer presented in section 1.5. The form of the condensation conductivity proposed by Herranz and Anderson and used in this thesis is:

$$k_{\text{cond}} = \frac{h_t^2 C M_t^2 D}{R T_b T_s \phi}$$  \hspace{1cm} (2.10)

The variable $\phi$ is the ratio of the log mean mole fractions of noncondensable gas to vapor:

$$\phi = \frac{X_{g,\text{avg}}}{X_{r,\text{avg}}} = \frac{\ln[X_{g,b} / X_{g,i}]}{\ln[X_{g,b} / X_{g,i}]}$$  \hspace{1cm} (2.11, 2.12)

Now all that remains to complete the approach is to define expressions for the Nusselt and Sherwood numbers. Peterson and Anderson both recommend the use of the McAdams correlation to derive the value of the Nusselt number:

$$N_u_x = 0.13 \left(Gr_x^{1/3} Pr^{1/3} \right)$$  \hspace{1cm} (2.13)

This expression for the Nusselt number has the benefit that it is independent of the characteristic length - thus it may be used to derive both average and local values. The expression for the Sherwood number is arrived at by applying the heat and mass transfer analogy to the McAdams relation to arrive at the expression:

$$S_h_x = 0.13 \left(Gr_x^{1/3} Sc^{1/3} \right)$$  \hspace{1cm} (2.14)

It is then possible to define an effective conductivity in the form:

$$k_{\text{eff}} = k_{\text{cond}} + \left( \frac{Pr}{Sc} \right)^{1/3} k_m$$  \hspace{1cm} (2.15)

The combined condensation and convection heat transfer can then be expressed as:
\[ q_{bi} = \frac{Sh}{x_k} k_{eff} (T_b - T_i) \]  \hspace{1cm} (2.16)

This expression is only technically correct in a saturated atmosphere - where the bulk vapor temperature, \( T_b \), and the saturation temperature, \( T_{sat,b} \), are equal. Anderson and Herranz then propose multiplying the Sherwood number by a suction term to account for the augmentation of heat transfer at high mass transfer rates. The proposed relations are given by:

\[ Sh_s = 0.13 \left( \frac{Gr^{1/3} Sc^{1/3}}{r} \right) \Theta \]  \hspace{1cm} (2.17)

\[ \Theta = \frac{r}{\exp(r) - 1} \]  \hspace{1cm} (2.18)

This diffusion layer model (DLM) will be used to model condensation on large containment surfaces, both horizontal and vertical. The surface orientation is considered when choosing the convection relation which is part of the condensation model. As stated, the relation which was used by Herranz and Anderson for vertical surfaces is the McAdams correlation. For downward facing horizontal surfaces, the leading coefficient is simply changed from 0.13 to 0.14. Because this is such a small change, the McAdams correlation with a leading coefficient of 0.13 will be used here to model natural convection for both vertical and horizontal downward facing surfaces [McAdams, 1954].

The essential equations for the diffusion layer model have been listed, but several other properties must be evaluated in order to determine a value for a heat transfer rate. Such properties include densities in the bulk and at the interface, the latent heat, the conductivity of the gas mixture, the diffusion coefficient for the mixture, and so on. Since evaluation of these physical properties is needed for all of the condensation models compared in this chapter, a complete discussion is presented in section 2.5.

2.4.2 Other condensation models studied

This section simply groups together the equations of the other condensation models which are compared to the diffusion layer model described in section 2.4.1. The model equations are listed and the reader is directed to Appendix A for more details.

**Uchida (air/steam)**

\[
 h = 379 \left( \frac{W_g}{W_s} \right)^{-0.707} 
\]  \hspace{1cm} (2.19)

**Kataoka (air/steam)**

\[
 h = 430 \left( \frac{W_g}{W_s} \right)^{-0.8} 
\]  \hspace{1cm} (2.20)

**Dehbi (air/steam)**

\[
 h = \frac{L^{0.05} \left[ (3.7 + 28.7P) - (2438 + 458.3P) \log_{10} \left( \frac{W_g}{W_s} \right) \right]}{(T_b - T_w)^{0.25}} 
\]  \hspace{1cm} (2.21)
Dehbi (steam/air/helium)

\[ h = \frac{L^{0.05} \left[ (3.7 + 28.7 P) - (2438 + 458.3 P) \log_{10} (W_{he} + W_a) \right]}{(T_b - T_w)^{0.25}} \]

\[ \times \left[ 0.948 - 8.67 W_{he} + 7.36 W_{he} (W_{he} + W_a) \right] \]

Gido & Koestel (natural convection only)

\[ h = 5.25 \left( \frac{u_f}{u_w} \right)^2 \frac{1}{\delta} \frac{u_w C * \left( \rho_{s,b} - \rho_{s,i} \right)}{\rho_i} \left[ \frac{\rho_i h_{fs}}{T_{b}^{sat} - T_w} \right]^{12/7} \frac{\rho_i g^4 L^5}{\mu_i} \]

Standard Mass Conductance Model (including suction) (see section 1.5 for more details)

\[ h = \frac{m^* h_{fs}}{T_b - T_i} \] (2.24)

\[ m^* = \frac{\rho D_{12}}{\delta} \Theta \varepsilon_{ms} \] (2.25)

\[ \Theta = \left( \frac{\ln (1 + \varepsilon_{ms})}{\varepsilon_{ms}} \right) \] (2.26)

\[ \varepsilon_{ms} = \left( \frac{W_{s,b} - W_{s,i}}{W_{s,i} - 1} \right) \] (2.27)

2.5 Property Evaluation

In order to evaluate the heat transfer rate by using any of the condensation models, it is first necessary to evaluate a host of physical properties of the steam, individual noncondensable gases, and finally the gas mixture. A great deal of attention was focused on determining the best and most consistent methods to calculate these properties. The author had some difficulty reproducing results from other researchers and it was thought that some of the discrepancy was in the evaluation of physical properties. For this reason a section on property evaluation has been included with a detailed list of sources of individual property relations. In many places more than one reference is listed. This is because more than one reference was checked to determine if there was agreement within the technical community for evaluation of different properties. In particular, special attention was paid to evaluation of the diffusion coefficient which is used in the diffusion layer model, and the mass conductance model. Slight changes in the diffusion coefficient can have a significant influence on the predicted heat transfer rate.

It is also necessary to determine the specific temperature and gas composition to use when evaluating “average” properties in the boundary layer for use in the diffusion layer model and the mass conductance model. Several texts on heat and mass transfer were consulted, but no “best” method was found. The advice of the texts generally recommends evaluating the boundary layer properties at a suitable average of the bulk and interface states. However, what constitutes a suitable average is not clear in all situations. For low mass transfer rates, the temperature (and
thus concentration) gradient across the boundary layer is small. For this situation most texts recommend evaluating properties at the average of the bulk and interface temperatures, but at the bulk mixture composition. For high mass transfer rates, the composition changes greatly over the boundary layer and this method is not adequate since many properties vary a great deal with concentration. To determine the extent of this problem, a sensitivity study was performed on the different methods used to evaluate average mixture compositions and the effect each different method had on the resulting heat transfer rate.

2.5.1 Steam properties

The properties of steam were the simplest to ascertain. A software program was purchased which had the entire steam tables programmed into a set of formulas [ChemicalLogic, 1996]. From this a set of Excel spreadsheets were created that stored the steam properties as a function of saturation temperature at intervals of 1°C. The following properties were stored: saturation pressure (MPa), liquid and vapor density (kg/m³), liquid and vapor enthalpy (J/kg), liquid and vapor conductivity (W/m-K), liquid and vapor viscosity (kg/m-s), and liquid and vapor specific heat (J/kg-K). These tables were then loaded into the Mathcad worksheet as a set of arrays. A given property was found at a specific temperature by interpolation. Properties could be found for a specified saturation pressure by first determining the corresponding saturation temperature.

2.5.2 Molar concentration and density

The concentration of the gas mixture is needed to determine the condensation conductivity. For the noncondensable gases, the concentration is evaluated using the ideal gas law:

\[ C_{nc} = \frac{P_{nc}}{R_u T} \left[ \frac{kmol}{m^3} \right] \]  \hspace{1cm} (2.28)

where pressure is in Pascals, temperature is in Kelvin, and the universal gas constant is 8314 [J/kmol-K]. The concentration of steam is evaluated as the density divided by the molecular weight.

\[ C_s = \frac{\rho_s}{M_s} \left[ \frac{kmol}{m^3} \right] \]  \hspace{1cm} (2.29)

The concentration of the mixture is simply the sum of the concentration of the two components.

\[ C_{mix} = C_s + C_{nc} \]  \hspace{1cm} (2.30)

The density of the noncondensable gas mixture is calculated by multiplying the noncondensable concentration by the equivalent molecular weight of the mixture.

---

7 It was assumed that the steam was always in a saturated state. This is a valid assumption since the vast majority of reactor accidents under consideration will result in a saturated atmosphere.
\[
\rho_{nc} = C_{nc} M_{nc} \left[ \frac{\text{kg}}{\text{m}^3} \right] \quad M_{nc} = \sum_{i=1}^{n} \frac{X_i M_i}{\sum_{j=1}^{n} X_j} \quad (2.31, 2.32)
\]

where the index \( i \) refers to each of the noncondensable gases in sequence.

The density of the mixture, including steam, is simply the sum of the densities of the two parts:

\[
\rho_{\text{mix}} = \rho_s + \rho_{nc} \quad (2.33)
\]

\subsection*{2.5.3 Specific heat}

The specific heat capacity of steam was evaluated from the steam tables properties discussed in section 2.5.1. The specific heat capacity at constant pressure for each noncondensable gas was evaluated according to a function which was taken from the GOTHIC 4.1c technical manual [George, 1994]. These functions are listed below. The factor of 4186.8 appears in each function to convert from the original units of (BTU / lbm-R) to the desired units of (J / kg-K). Temperature is in Kelvin.

**Air**

\[
c_p = 4186.8 \left[ 0.24438 - 4.20419 \times 10^{-5} T + 9.61128 \times 10^{-8} T^2 - 1.116383 \times 10^{-11} T^3 \right] \quad \left[ \frac{\text{J}}{\text{kg} - \text{K}} \right]
\quad (2.34)
\]

**Hydrogen \((T < 400\text{K})\)**

\[
c_p = 4186.8 \left[ 1.45910 + 1.60057 \times 10^{-2} T - 4.44048 \times 10^{-5} T^2 + 4.21220 \times 10^{-8} T^3 \right] \quad \left[ \frac{\text{J}}{\text{kg} - \text{K}} \right]
\quad (2.35)
\]

**Hydrogen \((T \geq 400\text{K})\)**

\[
c_p = 4186.8 \left[ 3.56903 - 4.8959 \times 10^{-4} T + 6.22549 \times 10^{-7} T^2 - 1.19686 \times 10^{-10} T^3 \right] \quad \left[ \frac{\text{J}}{\text{kg} - \text{K}} \right]
\quad (2.36)
\]

**Helium**

\[
c_p = 4186.8 \left[ 1.2404 \right] \quad \left[ \frac{\text{J}}{\text{kg} - \text{K}} \right]
\quad (2.37)
\]

The specific heat of a gas mixture is a mass weighted average which is calculated according to the relation:

\[
c_{p,\text{mix}} = \sum_{i=1}^{n} W_i (c_p)_i
\quad (2.38)
\]
Because of the level of attention paid to property evaluation, the predictions from these equations for specific heat have been checked against data from two separate references for each gas at several temperatures. Table 2-3 lists comparisons at three selected temperatures within the range of interest. It can be seen that there is excellent agreement for all gases and all of the temperatures.

Table 2-3: Specific heat (J / kg-K) comparison with reference values

<table>
<thead>
<tr>
<th>T (K)</th>
<th>Ref. 1 / Ref. 2</th>
<th>Calc.</th>
<th>% Diff</th>
<th>Ref. 1 / Ref. 2</th>
<th>Calc.</th>
<th>% Diff</th>
<th>Ref. 1 / Ref. 2</th>
<th>Calc.</th>
<th>% Diff</th>
</tr>
</thead>
<tbody>
<tr>
<td>300</td>
<td>1007</td>
<td>1005</td>
<td>-0.20</td>
<td>5190</td>
<td>5190</td>
<td>+0.00</td>
<td>14,320</td>
<td>14,280</td>
<td>-0.28</td>
</tr>
<tr>
<td></td>
<td>1005</td>
<td></td>
<td>+0.00</td>
<td>5200</td>
<td>5200</td>
<td>-0.19</td>
<td>14,780</td>
<td></td>
<td>-3.38</td>
</tr>
<tr>
<td>400</td>
<td>1014.9</td>
<td>1014</td>
<td>-0.09</td>
<td>5190</td>
<td>5190</td>
<td>+0.00</td>
<td>14,480</td>
<td>14,400</td>
<td>+0.21</td>
</tr>
<tr>
<td></td>
<td>1009</td>
<td></td>
<td>+0.50</td>
<td>5200</td>
<td>5200</td>
<td>-0.19</td>
<td>14,400</td>
<td></td>
<td>+0.76</td>
</tr>
<tr>
<td>500</td>
<td>1030.5</td>
<td>1030</td>
<td>-0.05</td>
<td>5190</td>
<td>5190</td>
<td>+0.00</td>
<td>14,510</td>
<td>14,350</td>
<td>+0.00</td>
</tr>
<tr>
<td></td>
<td>1017</td>
<td></td>
<td>+1.28</td>
<td>5200</td>
<td>5200</td>
<td>-0.19</td>
<td>14,510</td>
<td></td>
<td>+1.11</td>
</tr>
</tbody>
</table>

Ref. 1: Touloukian, Thermophysical Properties of Matter, Vol. 6, 1970

2.5.4 Viscosity

The viscosity of steam was derived from the steam table values discussed in section 2.5.1. The relationship used to evaluate the viscosity of the noncondensable gases is that derived by Chapman-Enskog according to the kinetic theory of gases. A brief overview of the theoretical basis is given in Reid [Reid, 1987]:

\[
\mu = 2.669 \times 10^{-6} \frac{\sqrt{MT}}{\sigma^2 \Omega_\mu} \left[ \frac{\text{kg}}{\text{m} \cdot \text{s}} \right] \tag{2.39}
\]

Two unknowns remain in this equation. According to the theory, \( \sigma [\text{\AA}] \) (angstroms) corresponds to the diameter of the gas molecules, which are assumed to be hard, non-interacting spheres. This quantity is unique to each individual gas. The second unknown, \( \Omega_\mu \), is called the collision integral. The collision integral is a modification to the model which accounts for the fact that molecules within the gas do interact. Whereas \( \sigma \) is a constant for each gas, \( \Omega_\mu \) can be expressed as a complex function of temperature. The relation which is used in this thesis to determine the collision integral is that given by Neufeld [Reid, 1987]:

\[
\Omega_\mu = A(T^*)^B + C[\exp(-DT^*)] + E[\exp(-FT^*)] \tag{2.40}
\]

\[
A = 1.16145 \quad B = 0.14874 \quad C = 0.52487 \quad T^* = \left( \frac{\kappa}{\varepsilon} \right) \frac{T}{T_{\text{vis}}}
\]

\[
D = 0.77320 \quad E = 2.16178 \quad F = 2.43787
\]

The dimensionless temperature that is used to evaluate the collision integral is dependent on the quantity \( \varepsilon \). This is termed the characteristic energy and is related to the dimensionless temperature through Boltzmann's constant, \( \kappa \). Together the two quantities (\( \sigma, (\varepsilon / \kappa) \)) are
generally termed the Lennard-Jones potential force constants. These constants are tabulated in several references and are usually deduced from experimentally measured values of viscosity for each gas. These two constants can be used in the evaluation of the viscosity, conductivity, and diffusion coefficients for gases or gas mixtures. The key to using them properly is to remember to always use a given pair (i.e., do not use $\sigma$ from one reference and $\left(\frac{\varepsilon}{k}\right)$ from another). This is especially important when evaluating the diffusion coefficient of mixtures containing water vapor, which will be discussed later. Table 2-6 in section 2.5.6 contains the Lennard-Jones potential constants for the relevant gases and the references from where they were taken.

Finally, the viscosity of the gas mixture is calculated using the Wilke method [Reid, 1987]:

$$\mu_{mix} = \sum_{i=1}^{n} \frac{X_i \mu_i}{\sum_{j=1}^{n} X_j \phi_{ij}}$$

$$\phi_{ij} = \frac{1 + \left(\frac{\mu_i}{\mu_j}\right)^{1/2}\left(M_j / M_i\right)^{1/4}}{\sqrt{1 + M_i / M_j}^{1/2}}$$

The values of predicted viscosity are compared with those given in two separate references to assure that the selected relations give accurate values. Table 2-4 shows this comparison at three temperatures which span the range of interest. The predictions of viscosity are shown to agree very well with those in the selected references. All predictions are within 2%.

<table>
<thead>
<tr>
<th>T (K)</th>
<th>Air</th>
<th>Helium</th>
<th>Hydrogen</th>
</tr>
</thead>
<tbody>
<tr>
<td>Ref. 1</td>
<td>Ref. 2</td>
<td>Calc.</td>
<td>% Diff</td>
</tr>
<tr>
<td>300</td>
<td>18.53</td>
<td>18.45</td>
<td>- 0.43</td>
</tr>
<tr>
<td></td>
<td>18.46</td>
<td></td>
<td>- 0.05</td>
</tr>
<tr>
<td>400</td>
<td>22.94</td>
<td>22.62</td>
<td>- 1.39</td>
</tr>
<tr>
<td></td>
<td>22.86</td>
<td></td>
<td>- 1.05</td>
</tr>
<tr>
<td>500</td>
<td>26.82</td>
<td>26.33</td>
<td>- 1.83</td>
</tr>
<tr>
<td></td>
<td>26.7</td>
<td></td>
<td>- 1.39</td>
</tr>
</tbody>
</table>

2.5.5 Thermal conductivity

According to the kinetic theory of Chapman-Enskog, the thermal conductivity of a monatomic gas at low pressure ($P < 1.0 \text{ MPa}$) is primarily a function of translational motion and is related to the viscosity of the gas according to [Reid, 1987; Mills, 1995]:

$$k' = \frac{5}{2} c_v \mu$$

(2.43)

For an ideal gas, the specific heat at constant volume is given by:

$$c_v = \frac{3}{2} \frac{R}{M}$$

(2.44)

Thus the conductivity of a monatomic ideal gas is given by:

$$k' = \frac{15}{4} \frac{R}{M} \mu \left[ \frac{W}{m - K} \right]$$

(2.45)

For polyatomic gases, such as $H_2$ and air, a correction must be made for the additional contributions to conductivity from rotational and vibrational degrees of freedom. The correction employed here is termed the modified Eucken correction. This correction term is defined as [Mills, 1995]:

$$k^* = 1.32 \left( c_p - \frac{5}{2} \frac{R}{M} \right) \mu$$

(2.46)

The conductivity of a polyatomic ideal gas at low pressure is then given by:

$$k = k' + k^* = \frac{15}{4} \frac{R}{M} \mu + 1.32 \left( c_p - \frac{5}{2} \frac{R}{M} \right) \mu$$

(2.47)

After a bit of algebraic manipulation, the conductivity of polyatomic gases can also be expressed as:

$$k = k' + 0.88 \left(\frac{2}{5} \frac{M}{c_p R_u} - 1 \right) k'$$

(2.48)

This final form was that used in the evaluation of conductivity for both hydrogen and air. The conductivity of a gas mixture is calculated according to the following formula, where the function $\phi_{ij}$ was defined previously as equation (2.41) in the viscosity section:

$$k_{mix} = \sum_{i=1}^{N} \frac{X_i k_i}{\sum_{j=1}^{N} X_j \phi_{ij}}$$

(2.49)

Predictions of thermal conductivity from these equations were compared with data from two separate references for each gas over a range of temperature.

Table 2-5 lists values for three temperatures which span the temperature range of interest and which are representative of the values over the entire range. The difference between the calculated values and the reference values are noticeably greater than with either specific heat or
viscosity. It appears that the chosen relations over-predict the conductivity of air and helium at 300K. Notice especially that the conductivity of helium differs from one reference by almost 6% at 300K and 400K - but agrees very well with the second reference at all three temperatures. The values predicted for hydrogen seem to straddle the reference values. Even with these small discrepancies, it is judged that the predictions for conductivity given by the presented equations are adequate for the work being carried out in this thesis. However, special attention will be paid to the sensitivity of the heat transfer coefficient predictions to fluctuations in thermal conductivity.

### Table 2-5: Thermal conductivity (mW / m-K) comparison with reference values

<table>
<thead>
<tr>
<th>T (K)</th>
<th>Air Ref. 1/2 Calc. Value</th>
<th>% Diff</th>
<th>Helium Ref. 1/2 Calc. Value</th>
<th>% Diff</th>
<th>Hydrogen Ref. 1/2 Calc. Value</th>
<th>% Diff</th>
</tr>
</thead>
<tbody>
<tr>
<td>300</td>
<td>26.14</td>
<td>26.86</td>
<td>+2.75</td>
<td>149.9</td>
<td>157.6</td>
<td>+5.14</td>
</tr>
<tr>
<td></td>
<td>26.20</td>
<td></td>
<td>+2.52</td>
<td>156</td>
<td></td>
<td>+1.03</td>
</tr>
<tr>
<td>400</td>
<td>33.05</td>
<td>33.21</td>
<td>+0.48</td>
<td>179.5</td>
<td>189.9</td>
<td>+5.79</td>
</tr>
<tr>
<td></td>
<td>33.8</td>
<td></td>
<td>-1.75</td>
<td>190</td>
<td></td>
<td>-0.05</td>
</tr>
<tr>
<td>500</td>
<td>39.51</td>
<td>39.19</td>
<td>-0.81</td>
<td>211.4</td>
<td>219.5</td>
<td>+3.83</td>
</tr>
<tr>
<td></td>
<td>40.70</td>
<td></td>
<td>-3.71</td>
<td>222</td>
<td></td>
<td>-1.13</td>
</tr>
</tbody>
</table>

2.5.6 Diffusion coefficient
The evaluation of the binary diffusion coefficient for a pair of gases, or an effective diffusion coefficient for a gas mixture, is of primary importance because it can have a large impact on the condensation rate predicted by the diffusion layer model. A great deal of attention was invested in comparing two different methods available for calculation of the diffusion coefficients, and specifically, the use of the Lennard-Jones constants in the relationships.

The Chapman-Enskog theory predicts a binary diffusion coefficient of the form [Reid, 1987]:

\[
D_{12} = \frac{0.00266 T^{3/2}}{\sqrt{M_{12} \sigma_{12}^2 \Omega_D P}} \left[ \frac{\text{cm}^2}{\text{s}} \right] \quad M_{12} = 2 \left[ \frac{1}{M_1} + \frac{1}{M_2} \right]^{-1} \tag{2.50, 2.51}
\]

where \(M_1\) and \(M_2\) represent the molecular weights of the first and second species, temperature is in Kelvin, and pressure is in Bars. With a little algebraic manipulation, the expression presented in [Mills, 1995] can be arrived at (pressure is in atmospheres):

\[
D_{12} = 1.86 \times 10^{-7} \sqrt{\frac{T^3}{\sigma_{12}^2 \Omega_D P}} \left[ \frac{\text{m}^2}{\text{s}} \right] \tag{2.52}
\]

The collision integral \(\Omega_D\) differs from that defined for viscosity and conductivity, and can be evaluated according to the relationship of Neufeld [Reid, 1987]:

\[
\Omega_D = \frac{A}{(T^*)^6} + \frac{C}{\exp(DT^*)} + \frac{E}{\exp(FT^*)} + \frac{G}{\exp(HT^*)} \tag{2.53}
\]

\[
A = 1.06036 \quad B = 0.15610 \quad C = 0.19300 \quad D = 0.47635
\]

\[
E = 1.03587 \quad F = 1.52996 \quad G = 1.76474 \quad H = 3.89411
\]

\[
T^* = \frac{\kappa}{\epsilon_{12}} T_{abs}
\]

The Lennard-Jones parameters \(\sigma_{12}\) and \(\epsilon_{12}\) can be obtained by the empirical relations [Reid, 1987; Mills, 1995]:

\[
\sigma_{12}^2 = \frac{\sigma_1 + \sigma_2}{2} \quad \epsilon_{12} = \sqrt{\epsilon_1 \epsilon_2} \tag{2.54, 2.55}
\]

This method of calculating diffusion coefficients was derived for dilute, nonpolar, monatomic gases. Errors can occur when the method is used for other types of gases, and several modifications have been proposed. However, the added complexity of these modification are usually only justified when evaluating highly polar, or molecularly complex gases such as hydrocarbons or alcohols. Therefore the simple relations presented here will be used for all of the gases under consideration.

The method used by Anderson and Herranz in their development and testing of the diffusion layer model is that of Wilke-Lee [Anderson, 1998; Herranz, 1998]. This is an empirical method devised by studying a group of 64 different binary gas systems at atmospheric pressure and near-
room temperature for which experimental data were available at the time [Wilke-Lee, 1955]. Essentially, an empirical correction factor for the theoretical equation was devised in order to better predict experimental results. Included in the 64 binary gas systems studied were those of steam-air, steam-helium, and steam-hydrogen. The equation proposed by Wilke-Lee is:

\[
D_{12} = \frac{3.03 - \left(0.98 / \sqrt{M_{12}}\right) \left(10^{-3}\right) T^{3/2}}{\sqrt{M_{12}} \sigma_{12}^2 \Omega_D \rho} \left[ \frac{\text{cm}^2}{\text{s}} \right]
\]  

(2.56)

A comparison of predictions between the theoretical and the Wilke-Lee method was performed for the gas systems of interest. This included comparisons between predictions derived using several different sets of Lennard-Jones force constants.

<table>
<thead>
<tr>
<th>Gas</th>
<th>(M)</th>
<th>(\sigma) (A) (\rightarrow)</th>
<th>(\epsilon) (K) (\rightarrow)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Air</td>
<td>28.96</td>
<td>3.711</td>
<td>78.6</td>
</tr>
<tr>
<td>He</td>
<td>4.003</td>
<td>2.551</td>
<td>10.22</td>
</tr>
<tr>
<td>(H_2)</td>
<td>2.016</td>
<td>2.827</td>
<td>59.7</td>
</tr>
<tr>
<td>(H_2O)</td>
<td>18.02</td>
<td>2.641</td>
<td>809.1</td>
</tr>
<tr>
<td>(H_2O^*) (diffusion)</td>
<td></td>
<td>3.737</td>
<td>32</td>
</tr>
</tbody>
</table>

\* Constants defined for evaluating diffusion coefficients only
\* [Lienhard, 1987]

Table 2-6 lists the values of Lennard-Jones constants for the gases of interest from several different references. Most of the constants are derived from viscosity data, and are in fairly close agreement. The major exception to this is water vapor. Two references, Mills and Lienhard, specifically list separate values of the constants for use in determining diffusion coefficients. Also of note is that all of the values of the force constants listed in the Wilke-Lee reference are noticeably different from the others. These two observations raised questions as to which relationship, and which constants, should be used to derive diffusion coefficients for use in the diffusion layer model. To address this question, a thorough comparison between the predictions using the two models and the several pairs of constants was made using some available experimental data.

The binary diffusion coefficient for steam-air mixtures at atmospheric pressure has been plotted as a function of temperature in Figure 2-3. Predictions from both the Chapman-Enskog and the Wilke-Lee methods have been plotted. In addition, the Lennard-Jones constants from each of the four references listed in Table 2-6 have all been used. The legends in the graphs identify each

\* NOTE: The force constants for air, helium, and hydrogen given by Reid, Mills, and Lienhard are identical. It is only the steam constants which differ among the references. Thus comparing the effect of these different Lennard-Jones constant groups on predictions of steam mixture diffusion coefficients actually only compares the effect of the force constants defined for steam.
curve by both the method used and the force constants used. Each legend entry first identifies the method used for prediction: Chapman (for Chapman-Enskog) or Wilke-Lee. The abbreviation in parentheses refers to the source of the Lennard-Jones force constants: Reid, Mills, Lien (for Lienhard), or W-L (for Wilke-Lee). The values used for steam from Mills and Lienhard are those listed in Table 2-6 as being for diffusion. Experimental data points are plotted using symbols without lines.

The temperature range for comparison is 290-370 K, and was chosen for two reasons. First, it is the range of temperature which is most likely to be encountered during the condensation modeling work presented in the latter chapters of this thesis. (The diffusion coefficient in the DLM is evaluated at an average boundary layer temperature, which is within this range for all probable scenarios.) Second, the experimental data found in the literature all fall within this range. Because the Chapman-Enskog and Wilke-Lee equations both have the same functional dependence on pressure, evaluating the two approaches at a single pressure is sufficient to give an indication of their performance.

The sources of the data points for steam-air mixtures in Figure 2-3 are discussed briefly. Marrero and Mason performed a comprehensive review of diffusion coefficient data in 1972. The points labeled Marrero-Mason eq. are from a curve fit relationship developed from a wide array of steam-air data [Marrero, 1972]. The points labeled Mills eq. are from another curve fit which is given in the Mills text [Mills, 1995]. Not surprisingly the Mills eq. points fall directly on the line predicted by the Chapman relation using the constants proposed by Mills. (The Marrero-Mason curve fit is also included in the Mills text.) Finally, there was one data point each for steam-air systems listed in the references [Reid, 1987], [Wilke, 1955], and [Nelson, 1956]. Figure 2-4 was included to more clearly show the difference between the modeling options. This figure shows the percent difference between the model predictions and the data points from the Marrero-Mason equation.

The first thing that is evident from these graphs is that the Wilke-Lee method consistently predicts diffusion coefficients about 5% higher than the Chapman-Enskog relation for each pair of force constants. The particular combination of the Wilke-Lee method with the force constants from Reid (which are derived from viscosity data) consistently under-predicts the Marrero-Mason data by about 10%. This is the particular combination used by Anderson [Anderson, 1998]. The Chapman-Enskog relation using the constant pairs from Reid predicts an even lower value. The Wilke-Lee method, using the constants from the Wilke-Lee paper, consistently over predicts the data by a few percent. From the graph, the best method seems to be the Chapman-Enskog relation using the constants proposed by Lienhard. (The Wilke-Lee constants for steam and the Lienhard constants for steam diffusion are essentially equal). This combination seems to split the difference between the two sets of data points which occur over the entire temperature range (Marrero-Mason equation and Mills equation). For this reason, the Chapman-Enskog relation, with force constants from Lienhard, will be used to predict steam-air diffusion coefficients in this thesis.
Figure 2-3: Steam-air binary diffusion coefficients at one atmosphere

Figure 2-4: % Difference of steam-air binary diffusion coefficients as compared to Marrero-Mason equation at one atmosphere
The binary diffusion coefficient predictions for steam-helium mixtures are shown in Figure 2-5. The data points are relatively sparse because a search for reference data turned up only two easily accessible independent sources. Schwertz and Brow [Schwertz, 1951] conducted experiments for both steam-helium and steam-hydrogen mixtures. Three data points for each combination were reported. One other data point was given by Lee and Wilke [Lee, 1954].

The first thing that should be gleaned from Figure 2-5 is that the diffusion coefficient for steam in helium is considerably higher than that for steam in air. That said, there is essentially no difference in the predictions from the Chapman-Enskog and Wilke-Lee methods for the steam-helium system. However, there is a substantial difference between the predictions depending on the force constants used. For the steam-helium mixture, the force constants of Reid show the best agreement with the available data. The Reid constants, along with the Wilke-Lee equation, are used by Anderson to evaluate steam-helium diffusion coefficients [Anderson, 1998]. The Reid constants will also be used in this thesis, but with the Chapman-Enskog equation.

The predicted values of the diffusion coefficient for the steam-hydrogen system are shown in Figure 2-6 with several data points from the literature. (It should be noted that there is some indication in the literature that the method used to gather the data of Crider and Winkelman may produce artificially low results [Schwertz, 1951; Crider, 1956].) For all force constant pairs, the Wilke-Lee equation predicts values which are about 5% below those from the Chapman-Enskog equation. The Wilke-Lee equation with the Reid force constants significantly under-predicts all of the experimental values for the diffusion coefficient over the entire temperature range - in fact this combination predicts the lowest values of diffusion coefficient of all the combinations tested. This observation is important since this particular combination would most probably be used if the method employed by Anderson was extended to cover steam-hydrogen mixtures. In light of the discrepancy with the available data, using this combination is not acceptable.

The prediction from the Wilke-Lee equation using the Wilke-Lee constants agrees very well with the one data point for this mixture used by Wilke and Lee in the derivation of their model. This combination predicts values which are right in the middle of the available data. The Wilke-Lee(WL) combination for hydrogen is also seen to predict a diffusion coefficient that is about the same magnitude as the preferred relation (Chapman(Reid)) for the steam-helium system. This result seems to confirm that helium is a good substitute for hydrogen in experimental systems designed to study the effect of light gas on condensation.

The Chapman(Lien) combination predicts a slightly higher diffusion coefficient than the Wilke-Lee(W-L) combination. The Chapman(Lien) combination also predicts values which fall in the midst of the data on the low end, and passes through the single data point at the upper end of the temperature range. These observations point to the Chapman(Lien) combination as being the best to use for a steam-hydrogen mixture.
Figure 2-5: Steam-helium binary diffusion coefficient at one atmosphere

Figure 2-6: Steam-hydrogen binary diffusion coefficient at one atmosphere
2.5.7 Comparison of mixture relations

This section compares different rules for evaluating the specific heat, viscosity, and thermal conductivity of a gas mixture. The research on gas properties conducted for this project resulted in the adoption of the mixture rules which were cited in sections 2.5.3, 2.5.4, and 2.5.5. However, these were not the mixture rules used by Anderson when he compared predictions from the DLM to his experimental data. Instead of the mass fraction weighting recommended for specific heat, or the Wilke rule weighting for viscosity and conductivity, Anderson used a straight mole fraction weighting for all three properties [Anderson, 1998, p. 261]. In order to have confidence in the DLM, it is important to determine how sensitive the DLM is to changes in these mixture rules.

Accordingly, the mixture properties are evaluated according to the two different rules for steam-air, steam-air-helium, and steam-air-hydrogen mixtures. Anderson did not use hydrogen in his modeling, however it is of interest in case anyone wishes to extend his analysis to include this gas. Three separate graphs will be shown for each property. The first shows the values of the mixture property for steam-air-helium mixtures - where the helium has a 0%, 15%, and 30% molar concentration within the noncondensable gas. The second shows the same except with hydrogen in the mixture instead of helium. The third graph shows the percentage error introduced by using the straight mole fraction weighting versus the recommended mixture rule for the specified property. The pressure has no direct effect on the evaluation of the properties, since the relations used to calculate specific heat, viscosity, and conductivity are independent of pressure. For convenience, the comparisons are made at a total pressure of one atmosphere - which allows the mole fraction of steam to vary from essentially zero to near unity over the same temperature range used when studying the diffusion coefficients.

Specific Heat

The literature indicates that specific heat of a gas mixture should be calculated based on a mass fraction weighting of the gas constituent components. This tends to make sense, because the specific heat is in units of energy per unit mass per unit degree (J/kg-K). This mixture rule has the following form:

\[ c_{p,\text{mix}} = \sum_{i=1}^{n} W_i (c_p)_i \]  \hspace{1cm} (2.57)

Anderson instead used a mole fraction weighting, which has the form:

\[ c_{p,\text{mix}} = \sum_{i=1}^{n} X_i (c_p)_i \]  \hspace{1cm} (2.58)

Figure 2-7 and Figure 2-8 show the results of this comparison. It is clear that there is an extreme difference in the value of the heat capacity predicted by the two mixture rules for the cases where there is light gas included in the mixture. However, the steam-air predictions are virtually unaltered. In all cases the value of the specific heat converges to that of pure steam as the limit of 373K is reached. This is expected because as the temperature increases, the saturation
pressure of steam increases and the mixture becomes more enriched with steam. Thus the mixture property converges to the steam value in the limit of all steam (373K at one atmosphere). The mole fraction of steam is plotted on the graphs to help illustrate this.

Figure 2-9 is included to show the percentage difference between the predictions (as compared to the recommended mass fraction mixture rule). The discrepancy between the predictions of the mixture rules is a direct consequence of the vast difference between the mole fraction and mass fraction of the light gases in these conditions. Because hydrogen and helium have such a low molecular weight compared to either air or steam, their contribution to the mass fraction weighted specific heat is relatively small while their contribution to the mole average is much larger. Figure 2-10 shows graphically the difference between mole fractions and mass fractions for the gases in a mixture of steam-air-helium, where the helium has a 30% molar concentration in the noncondensable gas mix. While the mole and mass fractions of steam are nearly equal, the mole and mass fractions for both air and helium differ by quite a bit. These differences are slightly greater for a mixture containing hydrogen.

It is clearly shown that using a straight mole fraction mixing rule for specific heat introduces significant errors into the specific heat predictions. The effect of this error on the prediction of the heat transfer coefficient from the DLM will be examined in section 2.6.1.

Figure 2-7: Specific heat mixture rule comparison for steam-air-helium mixtures (1 atm.)
Figure 2-8: Specific heat mixture rule comparison for steam-air-hydrogen mixtures (1 atm)

Figure 2-9: Error in mixture specific heat from using a mole fraction mixing rule (1 atm.)
Viscosity
The literature indicates that the viscosity of a gas mixture should be calculated based on a function of the mole fractions and molecular weights of the gas constituent components. The Wilke mixture rule, which was presented in section 2.5.4 and is used in this thesis, has the following form:

\[ \mu_{mix} = \sum_{i=1}^{n} \frac{X_i \mu_i}{\sum_{j=1}^{n} X_j \phi_{ij}} \quad (2.59) \]

\[ \phi_{ij} = \frac{\left[1 + \left(\mu_i / \mu_j\right)^{1/2} \left(M_j / M_i\right)^{1/4}\right]^2}{\sqrt{8 \left(1 + M_j / M_i\right)^{1/2}}} \quad (2.60) \]

Anderson used a simple mole fraction weighting in his evaluation of the DLM, which has the form:

\[ \mu_{mix} = \sum_{i=1}^{n} X_i \mu_i \quad (2.61) \]

As in the case of specific heat, a comparison between these two mixture rules was undertaken. Figure 2-11 shows the case for steam-air-helium mixtures. Very little difference is seen between the two rules. However, in Figure 2-12 for steam-air-hydrogen mixtures, there is a noticeable difference in prediction. These observations make sense, upon referencing Table 2-4 for the values of viscosity. Helium and air have nearly equal viscosity values, while hydrogen has a significantly lower viscosity than either helium or air. Figure 2-13 shows the percent error introduced into the mixture calculation by the simple mole fraction rule. A study of this effect on the heat transfer predictions from the DLM will be carried out later in the chapter.
Figure 2-11: Viscosity mixture rule comparison for steam-air-helium mixtures (1 atm.)

Figure 2-12: Viscosity mixture rule comparison for steam-air-hydrogen mixtures (1 atm.)
Figure 2-13: Error in mixture viscosity from using a mole fraction mixing rule (1 atm.)

Thermal Conductivity

The literature indicates that the thermal conductivity of a gas mixture should be calculated using the same rule as for viscosity. The Wilke mixture rule, which was presented in section 2.5.5 and is used in this thesis, has the following form:

\[
\phi_{ij} = \frac{1 + \left( \frac{\mu_i}{\mu_j} \right)^{1/2} \left( \frac{M_j}{M_i} \right)^{1/4}}{\sqrt{8 \left( 1 + M_i / M_j \right)^{1/2}}} \quad (2.63)
\]

\[
k_{mix} = \sum_{i=1}^{n} X_i k_i \quad (2.62)
\]

Anderson used a simple mole fraction weighting in his evaluation of the DLM, which has the form:

\[
k_{mix} = \sum_{i=1}^{n} X_i k_i \quad (2.64)
\]

A comparison of the predictions from these two mixture rules was carried out. Figure 2-14 and Figure 2-15 show that there is a marked difference between the mixture conductivity calculated by the two rules. The mole fraction rule consistently predicts much higher values of conductivity for mixtures with either helium or hydrogen. Figure 2-16 clearly shows that the largest error is for prediction of helium mixtures. At first it may seem that the hydrogen mixture should be the one with the largest error, since hydrogen has a much higher thermal conductivity than helium. Both mixture rules do predict a higher mixture conductivity for the hydrogen mixtures, but it is actually the low value of hydrogen viscosity relative to air (which is used in the Wilke rule) which helps to reduce the discrepancy between the two rules. Again a sensitivity analysis of the DLM to changes in mixture conductivity values will be presented later in this chapter.

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Figure 2-14: Conductivity mixture rule comparison for steam-air-helium mixtures (1 atm.)

Figure 2-15: Conductivity mixture rule comparison for steam-air-hydrogen mixtures (1 atm.)
Figure 2-16: Error in mixture conductivity from using a mole fraction mixing rule (1 atm.)
2.6 Diffusion Layer Model Sensitivity Analysis

Section 2.5.7 explored the variation in the calculation of individual mixture properties when alternate mixture rules were employed. This section explores the error introduced into the overall heat transfer coefficient predicted by the DLM as a result of the differences in the calculation of individual properties. In other words, the sensitivity of the DLM to changes in the mixture properties of specific heat, viscosity, thermal conductivity, diffusion coefficient, and various combinations, is determined.

A thorough sensitivity analysis was performed which compared predictions of the DLM convection (eq. 2.8), condensation (eq. 2.9), and total heat transfer coefficients (eq. 2.2) for the range of conditions described in Table 2-7. The baseline values of the heat transfer coefficient were calculated using the mixture rules and diffusion coefficient as outlined in sections 2.5.1 - 2.5.6, which are the implementation procedures recommended in this thesis. These baseline values were then compared to predictions calculated when employing the straight mole fraction mixture rules for specific heat, viscosity, and thermal conductivity. HTC predictions were compared when varying only one rule, in order to isolate the effect of each mixture property on the overall heat transfer coefficient. A comparison was also made between the baseline values and those calculated when using the mole fraction mixture rules for all three properties concurrently. The sensitivity of the DLM to the diffusion coefficient is also determined by comparing baseline HTC values with those calculated when employing the diffusion coefficient as calculated by Anderson. Finally, the combined effect of using all mole fraction mixture rules, and the Anderson diffusion coefficient, is calculated.

<table>
<thead>
<tr>
<th>Variable</th>
<th>Minimum</th>
<th>Maximum</th>
</tr>
</thead>
<tbody>
<tr>
<td>Pressure (Bar)</td>
<td>1</td>
<td>5</td>
</tr>
<tr>
<td>$T_{wall}$ (K)</td>
<td>305</td>
<td>345</td>
</tr>
<tr>
<td>$T_{bulk}$ (K)</td>
<td>310</td>
<td>440</td>
</tr>
<tr>
<td>$X_s$</td>
<td>0.05</td>
<td>0.9</td>
</tr>
<tr>
<td>$X_{He} / X_{nc}$</td>
<td>0.0</td>
<td>0.3</td>
</tr>
<tr>
<td>$X_{H_2} / X_{nc}$</td>
<td>0.0</td>
<td>0.3</td>
</tr>
</tbody>
</table>

The mixture properties in the last section were plotted as a function of temperature at one atmosphere, which was equivalent to plotting the properties as a function of steam mole fraction, which increases with steam saturation temperature. Since the properties of the individual gases are independent of pressure and only weakly dependent on temperature, this indicates that the properties of the mixture are primarily a function of the relative amounts of the constituent components, as would be expected. Thus in this section, it is instructive to plot the dependent variables directly as a function of steam mole fraction. The dependent variable will be the percent difference between the HTC prediction with the specific changes as compared to the baseline values. The particular conditions used to illustrate the DLM sensitivity are those of a volume which is initially filled with a noncondensable gas mixture of specified makeup (0 or 30 molar % helium or hydrogen) at one atmosphere and 300K. The total pressure is calculated as...
the partial pressure of the noncondensable gas at the bulk temperature added to the saturation pressure of the steam at the bulk temperature. The condensing surface is held constant at 345 K.

### 2.6.1 Sensitivity to specific heat

Turning now to the evaluation, the mixture specific heat is used only in the calculation of the contribution to the heat transfer coefficient. Recall from Figure 2-9 that using a mole fraction weighting for the mixture specific heat will significantly over-predict the property, by over 100% in some cases involving hydrogen. Figure 2-17 shows the change in the convection HTC and the total HTC as a function of the steam mole fraction when the mole fraction mixing rule is used (eq. 2.58) as compared to using the correct mixture rule (eq. 2.57). The graph clearly shows that the large over-prediction in the mixture specific heat will cause a substantial over-prediction in the predicted convection heat transfer coefficient. However, as the convection contribution to the overall heat transfer is quite small, the total heat transfer coefficient varies by less than 5% in all cases. Thus it is concluded that the DLM is quite insensitive to specific heat values calculated by different mixture rules.

![Figure 2-17: DLM sensitivity to changes in mixture specific heat](image-url)
2.6.2 Sensitivity to viscosity

The viscosity of the mixture is used in the calculations for both convection and condensation heat transfer. The results of the analysis showed that these two contributions change by equal amounts differences in the mixture viscosity definition, thus only the results for condensation will be presented since the condensation component is overriding when determining the overall heat transfer. Recall from Figure 2-13 that using a mole fraction weighting for mixture viscosity (eq. 2.61) can slightly over-predict the property for helium mixtures and will significantly under-predict the property for hydrogen mixtures. Figure 2-18 shows the change in the condensation HTC and the total HTC as a function of the steam mole fraction when the mole fraction mixture rule is used (eq. 2.61) as compared to using the correct mixture rule (eq. 2.59). The graph clearly shows that the DLM predictions are only slightly affected by the errors in the mixture viscosity. However, as the steam mole fraction approaches unity, the total HTC error is noticeably less than the condensation HTC error. This is primarily due to the influence of the condensate film. For a fixed wall temperature, as the bulk steam fraction gets extremely high (and thus the rate of mass transfer increases significantly), the resistance of the condensate film becomes more important in limiting the total heat transfer coefficient. Thus, even though the condensation HTC difference from baseline is essentially the same for all values of steam mole fraction, the error in the total HTC decreases.

Figure 2-18: DLM sensitivity to changes in mixture viscosity
2.6.3 Sensitivity to thermal conductivity

The mixture thermal conductivity is used when calculating the convection contribution to heat transfer. Recall from Figure 2-16 that using a mole fraction weighting for mixture conductivity (eq. 2.64) will significantly over-predict the property for mixtures with either helium or hydrogen. Figure 2-18 shows the change in the convection HTC and the total HTC as a function of the steam mole fraction when the mixture conductivity is calculated according to a simple mole fraction weighting (eq. 2.64) as compared to the correct weighting (2.62). The graph clearly shows that the DLM convection HTCs are significantly over-predicted for mixtures with hydrogen or helium, by 20% or more. However, the total heat transfer coefficient is over-predicted by less than 1.5% in all cases. Thus, even though the convection HTC differs from baseline values considerably, the overall DLM is considered to be relatively insensitive to changes in the thermal conductivity of the gas mixture.

Figure 2-19: DLM sensitivity to changes in mixture conductivity
2.6.4 Sensitivity to all gases concurrently

The effect of each mixture rule has been quantified on the predictions of the DLM. For completeness, the effect of the error introduced by using mole fraction mixture rules for all three properties (specific heat, viscosity, thermal conductivity) concurrently is quantified. Figure 2-20 shows the change from baseline for the convection and total heat transfer coefficients. (Notice that the curve for convection HTC for a 30% hydrogen mixture has been divided by two - i.e., the actual value of the difference is approximately 70%. The values for the curve have been divided by two in order to expand the scale of the graph.) Figure 2-20 shows that the error in the convection HTC can be quite significant. However, the sensitivity of the total HTC to using these mixture rules is less than 5% for most mixtures. The exception to this is for a mixture with a significant amount of hydrogen, where the error can be above 5%.

It does appear that the sensitivity of the model changes significantly with the addition of light gas, thus a more in-depth analysis of this phenomenon is presented later in section 2.6.8.

![Figure 2-20: DLM sensitivity to change in all mixture rules concurrently](image)

Figure 2-20: DLM sensitivity to change in all mixture rules concurrently
2.6.5 Sensitivity to diffusion coefficient

The sensitivity of the DLM predictions to the value of the diffusion coefficient was also studied by comparing the baseline values with those predicted by using the diffusion coefficient methodology of Anderson. The baseline values of the HTCs were calculated using the Chapman-Enskog equation (2.51) and the Lennard-Jones potential force constant pairs identified in section 2.5.6. That is, the values for air, helium and hydrogen are those derived from viscosity units [Reid, 1987]. For steam-air and steam-hydrogen mixtures, the force constants used for steam were those defined for diffusion in Lienhard [Lienhard, 1987]. For steam-helium mixtures, the viscosity values for steam are used [Reid, 1987]. The Anderson values were calculated using the Wilke-Lee equation and the force constants for steam, air, and helium derived from viscosity [Anderson, 1998]. Note that Anderson did not calculate values for the diffusion of steam-air-hydrogen mixtures. The hydrogen mixture comparison in this section is a comparison between baseline values, and those calculated using the Wilke-Lee equation with force constants from Reid for all gases.

Figure 2-21 shows the results of this analysis. When using the Anderson method for calculating diffusion coefficients, the DLM under-predicts the baseline values by around 5% for all mixtures. Again the trend is seen that the total HTC error decreases as the steam mole fraction approaches unity because the resistance to the total heat transfer from the liquid film becomes more significant. This 5% discrepancy, while relatively minor, is cause for concern since the DLM implemented by Anderson compared very favorably to his experimental data. This point will be addressed in more detail when the overall suitability of the model is discussed at the end of this chapter.

![Figure 2-21: DLM sensitivity to changes in diffusion coefficient](image-url)
2.6.6 Sensitivity to changes in gases and diffusion coefficient

Finally, the difference between the values calculated using the physical property relations presented in this thesis and those used in the work of Anderson is determined. That is, the baseline properties are calculated according to the logic of the present author, and compared to those values calculated according to the logic of Anderson (which use mole fraction weighting for specific heat, viscosity, and conductivity, and the Wilke-Lee relation for diffusion coefficient). The result is presented in Figure 2-22. Only the difference in the total heat transfer coefficient is shown. However, the difference is shown for five different noncondensable gas mixtures instead of three. In general, the discrepancy in the definition of the diffusion coefficient is overriding, as most of the curves show under-prediction of the Anderson method compared to that of Mattingly. However, the hydrogen mixtures are much more affected by the errors in prediction of specific heat, viscosity, and conductivity in concert. Thus these two errors tend to cancel out in the case of the 30% hydrogen mixture.

![Figure 2-22: DLM predictions using logic of Anderson compared to that of Mattingly](image)

2.6.7 Sensitivity to X_{avg} and T_{avg}

To complete the sensitivity analysis of the model to changes in variable definitions, the sensitivity of the DLM to the definitions of the average temperature and steam mole fraction will be explored. There are several options for defining each of these variables. The different options are presented in Table 2-8. Figure 2-23 shows the DLM sensitivity to the definitions of the average steam mole fraction, X_{s,avg}. This is the mole fraction of steam which is used to evaluate the properties in the boundary layer. The graph shows that the model is quite sensitive to this
variable. The most error is introduced when using $X_{s,\text{avg}}^4$, which is simply the mole fraction of the bulk mixture. This option is sometimes recommended for evaluating low-mass transfer rate diffusion, but it is not recommended for high-mass transfer rates - Figure 2-23 illustrates why this is the case.

<table>
<thead>
<tr>
<th>Baseline</th>
<th>$T_{\text{avg}} = -\frac{T_b - T_i}{\ln(T_b / T_i)}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$T_{\text{avg}}^2$</td>
<td>$T_{\text{avg}} = \frac{T_b + T_i}{2}$</td>
</tr>
<tr>
<td>$T_{\text{avg}}^3$</td>
<td>$T_{\text{avg}} = T_b$</td>
</tr>
</tbody>
</table>

Table 2-8: Possible definitions for $T_{\text{avg}}$ and $X_{s,\text{avg}}$

<table>
<thead>
<tr>
<th>Baseline</th>
<th>$X_{s,\text{avg}} = \frac{P_s(T_{\text{avg}})}{P_{\text{total}}}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$X_{s,\text{avg}}^2$</td>
<td>$X_{s,\text{avg}} = \frac{X_{s,b} + X_{s,i}}{2}$</td>
</tr>
<tr>
<td>$X_{s,\text{avg}}^3$</td>
<td>$X_{s,\text{avg}} = \frac{X_{s,b} - X_{s,i}}{\ln(X_{s,b} / X_{s,i})}$</td>
</tr>
<tr>
<td>$X_{s,\text{avg}}^4$</td>
<td>$X_{s,\text{avg}} = X_{s,b}$</td>
</tr>
</tbody>
</table>

Figure 2-23: DLM sensitivity to alternate definitions of $X_{s,\text{avg}}$ compared to baseline

Figure 2-24 shows the model sensitivity to the definition of the average temperature. The DLM is much more sensitive to variations in the definition of the average steam mole fraction than in the definition of average temperature. On one level this makes sense, because the individual properties of the gases vary only slightly with temperature, but mixture properties vary much more with changes in the relative amounts of constituent gases. However, for all of the cases in Figure 2-24 the average steam mole fraction is calculated using the baseline equation, which is dependent on the average temperature. Thus when using $T_{\text{avg}}^3$, the value of $X_{s,\text{avg}}^4$ is the same value as the bulk steam mole fraction, which is the same as $X_{s,\text{avg}}^4$. Clearly the variation in
properties with temperature overrides the under-prediction which would normally be caused by only using $X_{s,\text{avg}}$. A close look at the properties shows that an increase in the temperature of the boundary layer tends to increase the heat transfer rate. This is especially the case with the diffusion coefficient which increases according to $T_{\text{avg}}^{3/2}$. This cancellation of effects is not of concern here, because the bulk temperature should never be used when evaluating average properties in the boundary layer. What is really of interest here is that the predictions of the model do not change much when the $T_{\text{avg}}$ definition is changed from the baseline (log mean) value to $T_{\text{avg}}$ (arithmetic mean). Thus, the DLM is seen to be insensitive to the definition of average temperature in the boundary layer.

![Graph](image)

**Figure 2-24: DLM sensitivity to alternate definitions of $T_{\text{avg}}$ compared to baseline**

### 2.6.8 Sensitivity to light gas concentration

The presence of a light gas, such as helium or hydrogen, in the noncondensable mixture will cause a decrease in the density of the gas mixture. Figure 2-25 shows why this phenomenon is important. This figure plots the density of pure air, steam, helium, and hydrogen, as well as the mixture density for five different combinations, at one atmosphere. Steam is assumed to be in the saturated state, thus as the temperature increases (and the total pressure remains constant), the mole fraction of steam increases.

For a given noncondensable gas mixture, the density driving force is found by subtracting the gas mixture density at the bulk temperature from the density at the interface temperature - both values can be obtained by following a single curve on Figure 2-25 from one value of temperature.
to the other. Thus, the average slope of the particular curve between two different temperatures is indicative of the density driving force. Figure 2-25 clearly shows that the addition of light gas not only decreases the density of the mixture, but also decreases the slope of the curves compared to the steam-air curve slope, and thus the driving force. The density difference decreases with the decreasing molecular weight of the light gas (i.e., hydrogen is more detrimental than helium) and with the increasing concentration of a particular light gas.

Also notice that a 30% concentration of hydrogen in the noncondensable gas will result in a noncondensable mixture which is nearly the same density as pure steam. In fact, for a 40% concentration of hydrogen in the noncondensable gas, or a 44% concentration of helium in the noncondensable gas, the molecular weight of the noncondensable gas becomes equal to the weight of the steam. At this point the assumption of the noncondensable gas being heavier than steam (used to derive the diffusion layer model) breaks down and a stratified atmosphere is expected to develop. As the possibility of stratification is a very real concern in reactor accidents, the ability of the model to accurately represent the decrease in heat transfer at the onset of stratification is desirable. The DLM will be shown to produce the correct trends.

Figure 2-25: Density of gas mixtures at 1 atmosphere with helium or hydrogen present

The impact of light gases on the density driving force is more easily seen by comparing Grashof numbers for mixtures with different concentrations of light gas. Figure 2-26 shows curves of normalized Grashof numbers raised to the 1/3 power for pure air, steam-air, and steam-air-hydrogen mixtures (data is taken from Table 1-3). The Grashof numbers in Figure 2-26 have been normalized to the value of the Grashof number for air-only convection with $T_{\text{bulk}} = 300$ K, $Gr_x^{1/3} = 1.154 \times 10^3$. All values have been calculated for a length, $x$, of 1.0 meter and $(T_{\text{bulk}} - T_{\text{wall}}) = 10$ K. As mentioned previously, the presence of a light gas decreases the density change across the boundary layer, decreasing the buoyancy driving force for natural convection. The decrease
in convection driving force is reflected in the smaller Grashof numbers for mixtures with hydrogen as compared to the steam-air mixture at the same conditions. This is clearly shown in Figure 2-26. Notice also that the Grashof numbers are considerably higher for steam-air mixtures compared to air-only convection. The presence of condensing steam leads to higher Grashof numbers because the density change across the boundary layer is not only a function of the temperature change across the boundary layer, but also a function of the steam concentration change across the boundary layer.

![Figure 2-26: Normalized Grashof numbers of steam-air and steam-air-hydrogen mixtures](image)

Specific attention has been paid to the effect that light gases have on the predictions of the DLM. Anderson showed in his work that the heat transfer predictions change with helium content: they first increase and then decrease, resulting in a predicted heat transfer coefficient that does not change significantly until the concentration of helium in the noncondensable mixture is higher than about 30%. The discrepancies in the way in which the mixture properties are calculated in this thesis necessitates a re-evaluation of this conclusion. Also, since Anderson did not investigate the effect of hydrogen on the DLM, it was necessary to look carefully at hydrogen effects as well.

As a first step, the analysis of Anderson (i.e., using Anderson’s mixture rules and diffusion coefficient) was re-created for \( P = 1 \text{ atm}, \ T_{\text{bulk}} = 90 \text{C} (363.15 \text{K}) \) and \( T_{\text{wall}} = 30 \text{C} (303.15 \text{K}) \) and shown in Figure 2-27. While the exact numerical results for convection differ somewhat from those published by Anderson, the conclusion for helium addition is essentially the same. For helium concentrations in the noncondensable gas below 30%, the decrease in the heat transfer...
coefficient of condensation is less than the margin of error in his experimental data (~ 10-15%). Because the condensation component comprises most of the heat transfer, the influence of the total heat transfer coefficient follows closely that of the condensation component. Figure 2-27 shows that with Anderson’s methodology, the convection HTC first increases and then decreases for increasing concentrations of either helium or hydrogen. By contrast, the condensation HTC always decreases with an increase in light gas concentration.

![Figure 2-27: Light gas effects on DLM predictions of Anderson and Mattingly for P=1 atm., T_{bulk} = 363.15 K, T_{wall} = 303.15 K](image)

These results indicate that the total HTC may be more sensitive to helium than indicated by the Anderson analysis. Also, it is interesting to note that the physical conditions of Figure 2-27 are not those encountered in a PWR - i.e., there is a partial pressure of noncondensable gas of only 0.31 Bars (1/3 atmosphere). These conditions may in fact occur in a BWR, where the drywell may in fact be purged of noncondensable gases - however the condensation models evaluated here are most likely to be used in a PWR-type containment, such as the Westinghouse AP600. Thus an analysis was done to determine the model predictions for various PWR containment conditions. This analysis assumed a volume initially filled with the specified noncondensable gas mixture at a pressure of 1 atmosphere (1.01325 Bar) and T_{initial} = 310 K. Three separate bulk conditions were considered and the results are shown in Figure 2-28. In all cases, the wall temperature is 30 K below that of the bulk.

Figure 2-28 shows that the total heat transfer coefficient predicted by the DLM is much less sensitive to light gas for low temperature, low pressure situations. As the temperature and pressure increase, the presence of a light gas significantly degrades the total heat transfer.
coefficient. This is consistent with the observations of Anderson and Herranz [Anderson, 1998; Herranz, 1998]. The present analysis also shows that hydrogen is slightly more inhibiting than helium. The conclusion drawn from this analysis is that at a 30% helium or 30% hydrogen concentration within the noncondensable gas, the decrease in the heat transfer should be noticeable, and is not insignificant. However the 10% decrease for the case of 30% helium in the noncondensable mixture is still within the experimental uncertainty of Anderson, thus it is not certain that such a decrease would appear in the experimental data.

![Graph](image)

**Figure 2-28:** HTC change with helium or hydrogen for different $T_{\text{bulk}}$, $\Delta T=30K$

Anderson also indicated that the detrimental effect of the presence of light gas also changes with a change in the wall temperature. To determine this effect, the wall temperature was varied for each bulk condition studied. Figure 2-29 shows the percent change in the total heat transfer coefficient predicted for wall temperatures at 10 K and 30 K below the bulk condition for mixtures containing various amounts of hydrogen in the noncondensable mixture. The graph shows that the decrease in heat transfer coefficient is most extreme for small temperature differences across the boundary layer. That is, as the mass transfer rate increases (increasing $\Delta T$), the DLM becomes less sensitive to the presence of hydrogen. However, as the bulk temperature increases, the mitigating effect of the decreasing wall temperature becomes less and less. The same trend was seen for helium mixtures (graph not shown).
2.6.9 Summary of sensitivity analysis

In this section the influence of several parameters on the predictions of the diffusion layer model (DLM) were quantified over the range of conditions specified in Table 2-7. The results show that the convection HTC is very sensitive to changes in the specific heat and the thermal conductivity of the gas mixtures, but relatively unaffected by changes in viscosity. The condensation HTC is most sensitive to changes in the diffusion coefficient and the presence of light noncondensable gases. The sensitivity of the total HTC follows very closely that of the condensation component, as should be expected since condensation accounts for the vast majority of heat transfer in the cases studied. The DLM is very insensitive to the definition used for the average temperature in the boundary layer, but is extremely sensitive to the definition of the average steam mole fraction in the boundary layer. The sensitivity of the model to different concentrations of light gas was studied extensively. The total heat transfer coefficient decreases noticeably with even small concentrations of light gases, but decreases sharply for light gas concentrations in the noncondensable mix greater than 30%. It was also shown that the sensitivity to light gas is very much a function of how the mixture properties are evaluated.

Table 2-9 summarizes the results of the sensitivity analysis on the definition of individual properties. Each property studied is listed in the first column, with the baseline definition listed in the second column. The third column shows the alternate definitions of the property that were studied. The fourth column shows the maximum discrepancy in the property value between the two definitions. The fifth column shows the maximum change in the total heat transfer coefficient predicted by the DLM when using the alternate definition of the particular variable.
Table 2-9: DLM sensitivity to changes in particular variables

<table>
<thead>
<tr>
<th>Prop.</th>
<th>Baseline definition</th>
<th>Variation</th>
<th>Maximum Change in Property</th>
<th>Maximum Change in Total HTC</th>
</tr>
</thead>
<tbody>
<tr>
<td>$T_{avg}$</td>
<td>$T_b - T_i \over \ln(T_b / T_i)$</td>
<td>$T_b + T_i \over 2$</td>
<td>0.2 %</td>
<td>0.04 %</td>
</tr>
<tr>
<td>$X_{s,avg}$</td>
<td>$P_s(T_{avg}) \over P_{total}$</td>
<td>$X_{s,b} + X_{s,i} \over 2$</td>
<td>39 %</td>
<td>10 %</td>
</tr>
<tr>
<td></td>
<td>$X_{s,b} - X_{s,i} \over \ln(X_{s,b} / X_{s,i})$</td>
<td>$X_{s,b}$</td>
<td>9 %</td>
<td>2.5 %</td>
</tr>
<tr>
<td>$c_{p,mix}$</td>
<td>$\sum W_i (c_p)_i$</td>
<td>$\sum X_i (c_p)_i$</td>
<td>250 %</td>
<td>2.5 %</td>
</tr>
<tr>
<td>$\mu_{mix}$</td>
<td>$\sum X_i \mu_i \over \sum X_i \phi_{ij}$</td>
<td>$\sum X_i \mu_i$</td>
<td>-13 %</td>
<td>3.4 %</td>
</tr>
<tr>
<td>$k_{mix}$</td>
<td>$\sum X_i k_i \over \sum X_i \phi_{ij}$</td>
<td>$\sum X_i k_i$</td>
<td>40 %</td>
<td>1 %</td>
</tr>
<tr>
<td>$D_{12}$</td>
<td>$1.86 \times 10^{-7} \sqrt{T^3 \left( \frac{1}{M_1} + \frac{1}{M_2} \right) \over \sigma_{12} \Omega_n P}$</td>
<td>$\left[ 3.03 - \left( \frac{0.98 / \sqrt{M_{12}}}{\sqrt{M_{12} \sigma_{12}^2 \Omega_D P}} \right) \right] (10^{-3}) \over T^{3/2}$</td>
<td>-10 %</td>
<td>-6 %</td>
</tr>
</tbody>
</table>

* When the variation definitions are used for $c_p$, $\mu$ and $k$ concurrently, the maximum change in the DLM is 7%, which occurs for a mixture containing 30% hydrogen in the noncondensable gas.
2.7 Comparison Between Models and Data

This section presents and compares the predictions from the following models over a range of containment conditions:

1. Uchida
2. Kataoka
3. Dehbi
4. Gido-Koestel natural convection
5. Standard mass conductance model, low-mass-transfer-rate formulation (see chapter 1)
6. Standard mass conductance model, high-mass-transfer-rate formulation (see chapter 1)
7. Peterson Diffusion Model
8. DLM (present implementation of the diffusion layer model)

The predictions from these models will be compared to published experimental data from the University of Wisconsin-Madison (UW) and MIT. The UW data base comprises the largest, consistent set of experimental values for the range of conditions encountered in advanced containment analysis. The experimental facilities used to gather the data were constructed specifically to mimic the AP600 dimensions, and were painstakingly designed to reduce the errors associated with measurement. As a result the standard deviation of the experimental data is less than 20% in almost all cases and less than 15% in most cases. In addition, both atmospheric and pressurized tests were completed. The atmospheric tests are unique in that they encompass the conditions which are encountered in a BWR drywell following a LOCA - i.e., most of the noncondensable gases have been ejected from the atmosphere. Also, the UW experiments included tests which were performed with helium present in the atmosphere.

The UW facilities use flat plates as condensing surfaces, and the wall temperature was significantly below 100 °C in most cases. The experiments were designed to gather data for significant natural convection driving forces, i.e., high wall subcooling. The UW data were gathered in two experimental facilities. One is an atmospheric facility with one horizontal condensing plate and one vertical condensing plate. The heat transfer coefficients measured on the vertical plate were nearly identical to those measured on the horizontal plate for all experiments. Each experimental heat transfer coefficient value used here for comparison to the model predictions is the average heat transfer coefficient from both the vertical and horizontal plates. The second UW experimental facility is a pressurized facility which was designed to mimic the dimensions of the Westinghouse AP600 domed containment. In this facility, the condensing surface gradually transitions from a horizontal downward facing surface to a vertical surface. The measured values of the heat transfer coefficients were nearly identical along the entire surface for most of the experiments. Each value of the heat transfer coefficient used here for comparison to model predictions is the average heat transfer coefficient for the entire surface.

The second data set used for comparison is a new data set that has been developed at MIT [Liu, 1999]. The data is for condensation on the outside of a 4.0 cm outside diameter, 2.0 meter long vertical smooth tube. The tube assembly is representative of a tube in a condenser system where boiling tube-side water acts as the heat sink for shell-side steam condensation. As a result of this setup, the outside tube temperature is slightly higher than 100 °C. This results in a significantly
lower convection driving force than was present in the UW experiments, and as such, these data represent a completely different set of physical conditions. These data exist for steam-air and steam-air helium mixtures at pressures above one atmosphere. Since the data are for condensation on the outside of a tube, the heat transfer is augmented slightly due to the effect of curvature. In order to use these data here for comparison to the predictions of the DLM, a factor of 0.8 was used to transform the measured values of heat transfer coefficient for a tube to those useful for comparison to a flat plate situation. The value of 0.8 was chosen based on the previous work of Dehbi, who used this value to modify his measurements for tube condensation in order to define a flat plate condensation correlation (see next paragraph).

Finally the predictions of the DLM are compared to those of the Dehbi correlation. Dehbi performed condensation experiments with a setup similar to that of Liu [Dehbi, 1991]. Steam was condensed on the outside of a vertical tube. In this case, the tube temperature was held significantly below 100 °C by circulating subcooled water on the inside of the tube. There are two Dehbi correlations, one for steam-air mixtures, and another for steam-air-helium mixtures at pressures between 1.5 - 4.5 atmospheres. Both are used in this evaluation. As mentioned above, Dehbi used a factor of 0.8 to account for the effect of curvature on the heat transfer coefficient value. The correlations which are published, and which are used here, have this factor included and are meant to be used for condensation on a flat plate.

The model comparisons will be presented in a series of graphs. In addition to directly comparing the different condensation models, the graphs are also used to deal with the issue of which suction factor to use with the current implementation of the diffusion layer model (DLM). Several different forms of the suction factor have been proposed by different researchers, and two have been presented by Anderson and Herranz in different publications. The effect of each suction factor on the overall results is a special concern because the suction factor is in essence a correction factor to the DLM for high mass transfer rates. The three suction factors which are evaluated here are defined as:

\[ \Theta_1 = \frac{X_{nc,i}}{X_{nc,b}} \quad \Theta_2 = \frac{\ln(r + 1)}{r} = \frac{X_{nc,i}}{X_{nc,\text{avg}}} \quad \Theta_3 = \frac{r}{\exp(r) - 1} \]

where the value of \( r \) is defined as:

\[ r = \frac{X_{s,i} - X_{s,b}}{1 - X_{s,i}} \]

In the following graphs, the three suction definitions are delineated by using the symbols “T1”, “T2”, and “T3”, for Theta1, Theta2, and Theta3.

---

9 T2 was published in [Anderson, 1998], T3 was published in [Anderson, 1997]
2.7.1 Steam-air mixtures

Figure 2-30 shows some selected experimental data and the predictions of several different models plotted as a function of the air-to-steam mass fraction ratio. This ratio is used as the primary function in the Uchida correlation. The data presented were gathered by Anderson in the UW atmospheric facility and published in his Ph.D. thesis [Anderson, 1998]. CEB stands for Coolant Energy Balance, and HFM stands for Heat Flux Monitor - two independent experimental methods use to gather heat flux data. The total pressure in the facility is one atmosphere, which results in the partial pressure of air being considerably less than one atmosphere. The figure shows that the Uchida correlation significantly over-predicts the condensation rate. This limitation of the Uchida model, which is generally thought to be conservative, was analyzed and explained by Peterson [Peterson, 1996]. Anderson later published a graph very similar to Figure 2-30 which also proved this point. Figure 2-30 is included here to test the current implementation of the DLM and to reiterate the point that the Uchida correlation is not applicable for use in an atmosphere where the partial pressure of noncondensable gas is less than one atmosphere - such as that in a BWR drywell following a LOCA.

Also note that the Kataoka and Dehbi models significantly over-predict the experimental data. This is expected of the Kataoka model since it has the same functional form as the Uchida relation. The Dehbi model is used here to predict heat transfer under conditions that are outside of the range of Dehbi’s experiments, which were for pressures of 1.5 - 4.5 Bar. This graph seems to indicate that using the Dehbi relation outside the range for which it was developed is not acceptable. The Peterson relation is essentially the DLM with no suction term - and it slightly under-predicts the data. The DLM with the suction factor \( T_3 \) agrees quite well with the data, as does the standard high-mass-transfer-rate conductance model [Mills, 1995].

![Figure 2-30: Model comparison to steam-air data from the atmospheric facility](image-url)
Although Figure 2-30 is instructive, the data are quite sparse, and the conclusions drawn from them are therefore of limited value. To give a better indication of model performance, the predictions are compared to the UW steam-air data from both the atmospheric and the pressurized facility in Figure 2-31. Here the plot is of calculated versus experimental values. For each experiment, the test conditions were used as input into the condensation models. For each test, the predictions of the models are plotted as the ordinate while the average measured heat transfer coefficient for the test is on the abscissa. The dark diagonal line has a slope of unity to clearly show where the experimental and calculated values are equal. The black dashed lines encompass the 20% error envelope about the diagonal.

Figure 2-31 shows more convincingly that the Uchida and Kataoka models are likely to significantly over-predict the experimental values. This is not the case for the highest heat transfer rates, but is true for the majority of data points on the graph. The Dehbi predictions also over-predict most of the experimental values. Thus the conclusions that these models should not be used in BWR situations (where the partial pressure of noncondensable gas is less than one atmosphere) seems to be a sound one.

The DLM with suction options T2 and T3 are shown to agree fairly well with the data. Suction option T2 consistently gives higher heat transfer values. Comparison of these two options suggests that while the predictions of T2 may be better overall, most of the error results from an over-prediction of the heat transfer coefficient, whereas the errors for the T3 option result in under-predictions (option T1 will be discussed later). When using these heat transfer predictions to evaluate a containment system, it is imperative that errors occur primarily on the side of caution - which in this case would indicate that suction option T3 should be used.

The values for the Peterson diffusion model are shown to consistently under-predict the data (recall that the Peterson model is the DLM with no correction for high mass transfer rates), which is why Anderson and Herranz developed their extensions to the model. The standard mass conductance model, for both high-mass-transfer-rates (H-R) and low-mass-transfer-rates (L-R) also significantly under-predict the experimental data for high mass transfer rates, but do agree quite well with the data at the low end. Finally, the Gido-Koestel natural convection model shows a severe under-prediction in all cases. The reason for this is quite simple. The Gido-Koestel model was developed for very large surfaces, and includes a dependence on the length of the surface of $L^{5/7}$. The models here are all evaluated for a length of 2 meters. The Gido-Koestel predictions (and the Dehbi predictions) will increase noticeably for larger surfaces. However, the Gido-Koestel model is also used in conjunction with a forced convection model - thus it is relatively unlikely that the total heat transfer prediction from the Gido-Koestel logic will be as low as that indicated here.

---

10 Notice the error bars which have been included for two data points, one at the low end and one at the high end. The error bars represent an average standard deviation of 15% in the UW data.
To look more closely at the suction parameter effect on the DLM, the model is compared to steam-air data at pressures greater than one atmosphere. Figure 2-32 compares model predictions with steam-air data from the UW pressurized facility. The pressure ranges from 1.5 to 3.06 Bar. The figures show predictions for the DLM with all three options for suction, the Peterson model (DLM with no suction), and predictions from Dehbi. Clearly, the suction option T1 is not useful, as it causes severe over-predictions compared to the data and the other models. Again the Peterson formulation is seen to under-predict the experimental data. The Dehbi correlation and the DLM with suction option T3 agree quite well, but seem to under-predict the data by about 15-20%. The suction option T2 also under-predicts the data, but to a lesser degree than T3.

Figure 2-33 shows all of the models compared to the UW pressurized steam-air data. Here the Uchida and Kataoka models are shown to predict conservative results. The conditions under which these data were taken are typical of PWR atmospheres following a loss of coolant accident, i.e., there is a partial pressure of noncondensable gases that is slightly greater than one atmosphere. As was seen in Figure 2-31, the standard mass conductance models and the Gido-Koestel models all under-predict the experimental data.
Figure 2-32: Suction effect / data comparison for steam-air mixtures, $P = 1.5 - 3.0$ Bar

Figure 2-33: Model comparison to UW pressurized steam-air data, $P = 1.5 - 3.0$ Bar
The DLM, Dehbi, and Uchida models are compared to both the UW data and the MIT data in Figure 2-34. The comparison has been limited to these three models in order to keep the graph readable. The DLM is shown to predict heat transfer coefficients which agree fairly well with the data of both experiments, but does seem to significantly under-predict the MIT data in the upper end. The DLM also agrees very well with the predictions of the Dehbi relation for the conditions of the UW data which bolsters the confidence in the DLM predictions and the UW database. It is interesting to notice that the Dehbi relation does not consistently agree with the new MIT data, tending to over-predict the data at low values for the heat transfer coefficient and under-predict for high values. Recall, however, that the Dehbi data and the new MIT data are gathered under different conditions. In this light, the discrepancy between the Dehbi relation and the MIT data is concluded to be a result of using the Dehbi relation in another situation outside its range of applicability. As expected, the Uchida relation is shown to consistently under-predict the data from both experiments.

![Figure 2-34: Model comparison to UW & MIT steam-air data, P = 1.5 - 4.5 Bar](image)

**2.7.2 Helium mixtures**

Predictions from the different models will now be compared to experimental data with helium in the noncondensable mixture. Figure 2-35 shows the predictions of the models against the experimental UW steam-air-helium data taken at a total pressure of one atmosphere with a helium molar concentration of 30% in the noncondensable gas ($X_{He}/X_{nc} = 0.3$). The data were gathered by Anderson in both the atmospheric and pressurized facilities and published in his thesis [Anderson, 1998]. As in the helium-free case, the Dehbi, Uchida, and Kataoka models tend to over-predict the experimental data. The Uchida and Kataoka models were not intended to
be used for mixtures in which light gases are present, this is another reason why they should not be used for this case. The Dehbi model is again being used outside of the range of conditions for which it was derived. The DLM with suction option T2 over-predicts data at the low end of the spectrum and under-predicts data at the high end. The suction option T3 agrees quite well with the data at the low-end of the spectrum, over-predicts the experimental data in the range of 200-300 W/m²-K, and under-predicts the data at the high end quite appreciably. The Peterson model significantly under-predicts the data, as do the remaining models. The DLM (T3) option seems to be the most acceptable compromise of the models which are compared in Figure 2-35 for the present conditions.

Figure 2-35: Model comparison to UW steam-air-helium data (1 atm.) (X_{He}/X_{nc}= 0.3)

Figure 2-36 shows the comparison of model predictions to data from both UW and MIT for steam-air-helium mixtures at pressurized conditions. The DLM is again shown to predict heat transfer coefficients which agree well with the data of both experiments. In fact, the agreement between the DLM and the data is better in this case than the case without helium. The Dehbi relation for steam-air-helium predicts heat transfer coefficients which agree well with the UW data, but not with the MIT data. The discrepancy between the Dehbi relation and the MIT data is again because of using the Dehbi relation outside its range of applicability. The predictions of the Uchida relation are shown for comparison, and again under-predict the data from both experiments.
2.7.3 Hydrogen mixtures

No tests were performed by Anderson, Dehbi or Liu with hydrogen in the noncondensable mix. Instead, helium was used as a nonflammable simulant for hydrogen. Because a consistent set of data for hydrogen mixtures does not exist, several conclusions will be drawn from the observations presented in section 2.6.8. (Recall that section 2.6.8 determined the sensitivity of the DLM to the presence of both helium and hydrogen.)

Intuitively, the presence of hydrogen is expected to hamper the condensation process slightly more than the presence of helium - mainly because it is less dense and thus causes a decrease in the density driving force. Figure 2-27 and Figure 2-28 both compare the predictions of the diffusion layer model for mixtures containing helium or hydrogen. In both graphs it is shown that the presence of hydrogen degrades heat transfer slightly more than the presence of the same molar concentration of helium. This degradation effect is more severe as the concentration of hydrogen increases. For a hydrogen concentration in the noncondensable gas of less than about 30%, the decrease in heat transfer is only slightly more than that caused by the presence of an equal amount of helium. Thus for most containment conditions of interest here, it is expected that helium is in fact a good substitute of hydrogen.

The diffusion layer model is deemed to be a good model to use for cases where hydrogen is expected to be present since the DLM does in fact predict that hydrogen will have a significant impact on the results, and shows trends which are both qualitatively valid and quantitatively useful.
2.8 Conclusions and Model Selection

Several goals were accomplished in this chapter. First, a discussion of condensation on different surfaces was presented. The conclusion was that for a wetting surface, the difference between the condensation rate on a vertical versus a horizontal surface is extremely small - thus a vertical model may be used when modeling condensation on the dome and walls of a large containment building. Next, the combined effects of light gas and surface orientation were presented. To date, the majority of experimental evidence suggests that for low-to-moderate concentrations of light gases, the degradation of heat transfer on all surfaces is quite small. However, it was later shown that the diffusion layer model does in fact predict a degradation in condensation when light gases are present.

In section 2.4 the condensation models which are evaluated were summarized. The full details of the models may be found in appendix A or in chapter 1. Section 2.5 set forth the methodology which was used to calculate all of the physical properties that were needed to implement the condensation models being studied. For completeness the methodology for property evaluation is spelled out specifically in Table 2-10. The evaluation of mixture properties, especially of diffusion coefficients, was the major difference between the implementation of the DLM in this thesis and that by Anderson. The force constants that were used for evaluation of the physical properties are listed in Table 2-11. Notice that there are different values of the constants used for steam when evaluating diffusion coefficients. These values were chosen in section 2.5.6 after comparing predictions for diffusion coefficients using the different force constant pairs to the available experimental data.

<table>
<thead>
<tr>
<th>Property</th>
<th>Definition</th>
</tr>
</thead>
<tbody>
<tr>
<td>$T_{avg}$</td>
<td>$\frac{T_b - T_i}{\ln(T_b / T_i)}$</td>
</tr>
<tr>
<td>$c_{p,mix}$</td>
<td>$\sum W_i (c_p)_i$</td>
</tr>
<tr>
<td>$k_{mix}$</td>
<td>$\sum \frac{X_i k_i}{\sum X_j \phi_{ij}}$</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Property</th>
<th>Definition</th>
</tr>
</thead>
<tbody>
<tr>
<td>$X_{s,avg}$</td>
<td>$\frac{P_s (T_{avg})}{P_{total}}$</td>
</tr>
<tr>
<td>$\mu_{mix}$</td>
<td>$\sum \frac{X_i \mu_i}{\sum X_j \phi_{ij}}$</td>
</tr>
<tr>
<td>$D_{ij}$</td>
<td>$1.86 \times 10^{-7} T^3 \left( \frac{1}{M_i} + \frac{1}{M_j} \right)$ $\frac{\sigma_{ij}^2 \Omega_n P}{\sigma_{12}^2}$</td>
</tr>
</tbody>
</table>
Different property mixture rules were used by Anderson, who proposed the modifications to the original Peterson diffusion model, thus a study of the effect of using these mixture rules was undertaken. An extensive sensitivity analysis of the diffusion layer model was completed in section 2.6. The model is sensitive to changes in the definition of the diffusion coefficient - which is also different in the present work from that used by Anderson. Results of the sensitivity analysis are summarized in Table 2-9. The sensitivity of the DLM to the presence of light gases is clearly shown in Figure 2-27, Figure 2-28, and Figure 2-29. Hydrogen and helium cause a significant degradation of heat transfer - especially at concentrations greater than 30% in the noncondensable mixture. The degradation increases with increasing pressure and saturation temperature, and the effect of hydrogen is more pronounced than that of helium.

Finally the many condensation models under study were numerically compared to the experimental data sets of Anderson (UW) and Liu (MIT). These data sets cover both BWR and PWR typical conditions with total pressures ranging from 1 to 4.5 Bars. The data sets also includes both steam-air and steam-air-helium data. The DLM is shown to agree very well with the correlation of Dehbi for conditions where the Dehbi correlation is valid. In scenarios where the total pressure is held at 1 atmosphere (the noncondensable gas fraction is less than one atmosphere) the Uchida and Dehbi models significantly over-predict the experimental data, but the DLM does not. Finally, the DLM takes into account the presence of light gases in a way which is physical and which results in the light gas having an appreciable effect on the rate of heat transfer. This result helps reduce the generic concern over whether this heat transfer correlation will account for the degradation of condensation caused by light gases. Based on this comparison, and the other analyses in this chapter, it is determined that the DLM with the suction option T3 is the best condensation model currently available for evaluating advanced containment designs.

A final note is included to specifically draw attention to the difference between the DLM as implemented here and as implemented previously by Anderson. There are considerable differences in the way in which the mixture properties are evaluated for the two researchers. The recommended relations for deriving physical properties are given here in Table 2-10 and Table 2-11. The relations that are used differently by Anderson are given in Table 2-12. The fourth
column of this table shows the difference in the value of each property when calculated by the two definitions. The fifth column of the table shows how much this difference impacts the heat transfer coefficient predicted by the DLM. The numbers in this table may seem small, but the cumulative effect of their influence is important. The overall effect of the Anderson implementation is to decrease the sensitivity of the DLM to the presence of light gases. In other words, the DLM predicts less of a decrease in condensation rate due to the presence of hydrogen or helium when using the Anderson implementation scheme. Unfortunately, there are no experimental data available to compare against the DLM predictions for steam-air-hydrogen mixtures.

Table 2-12: Difference between implementation of Mattingly and Anderson

<table>
<thead>
<tr>
<th>Prop.</th>
<th>Mattingly</th>
<th>Anderson</th>
<th>Maximum Change in Property</th>
<th>Maximum Change in HTC</th>
</tr>
</thead>
<tbody>
<tr>
<td>$c_p$</td>
<td>$\sum W_i (c_p)_i$</td>
<td>$\sum X_i (c_p)_i$</td>
<td>250 %</td>
<td>2.5 %</td>
</tr>
<tr>
<td>$\mu$</td>
<td>$\mu_{mix}$</td>
<td>$\mu_{mix}$</td>
<td>-13 %</td>
<td>3.4 %</td>
</tr>
<tr>
<td>$k$</td>
<td>$k_{mix}$</td>
<td>$k_{mix}$</td>
<td>40 %</td>
<td>1 %</td>
</tr>
<tr>
<td>$D_{12}$</td>
<td>$1.86 \times 10^{-7} \sqrt{\left[ \frac{1}{M_1} + \frac{1}{M_2} \right]} \left{ \frac{3.03 - \left(0.98 / \sqrt{M_{12}} \right)\left(10^{-3}\right) T^{3/2}}{\sqrt{M_{12} \sigma_i^2 \Omega_D P}} \right}$</td>
<td>$\left[ \frac{3.03 - \left(0.98 / \sqrt{M_{12}} \right)\left(10^{-3}\right) T^{3/2}}{\sqrt{M_{12} \sigma_i^2 \Omega_D P}} \right]$</td>
<td>-10 %</td>
<td>-6 %</td>
</tr>
</tbody>
</table>
3. CFD ANALYSIS OF TURBULENT BOUNDARY LAYERS

This chapter deals with the physics and practical simulation of turbulent boundary layer condensation. A computational fluid dynamics (CFD) package was used to simulate boundary layers and carry out analyses aimed at determining the boundary layer width for various conditions. Section 3.1 presents the reasons for using CFD and the specific goals of the CFD analyses. Section 3.2 discusses the criteria which were used to select a commercial CFD package. Section 3.3 presents the form of the transport equations and turbulence models which are solved, and the types of boundary conditions used for the various problems. Section 3.4 presents some benchmark problems that were studied to assure that the CFD code was performing adequately. Section 3.5 presents the matrix of CFD runs completed in the course of the study and discusses the results from individual runs. Finally section 3.6 presents the conclusions drawn from the CFD studies.

3.1 Goals of the CFD Analysis

The main objective of this thesis is to improve the way in which finite-volume computer codes (which use relatively large computational volumes) calculate condensation heat transfer. This goal is narrowed by taking the first step of concentrating on one prominent condensation phenomenon, a downward flowing natural convection turbulent boundary layer. Improved modeling of this type of boundary layer is the subject of chapter 4. One important parameter used in the improved condensation modeling is the width of the boundary layer. This width is determined from a side calculation and used as input into the new heat transfer methodology (see chapter 4).

The CFD analyses discussed in this chapter are used as a way to determine the width of the boundary layer in a condensing environment for different atmospheric conditions. While this type of numerical approach can be used to determine a vast array of other boundary layer characteristics, only the width and profile of the most important parameters in the boundary layer are studied here. CFD calculations are also extremely expensive and therefore ill suited to be used in conjunction with a containment analysis code while the simulation is being performed. Instead, the CFD calculations are used to lend credibility and support to a much simpler method to estimate boundary layer profiles and thickness which can easily be employed in finite-volume containment analysis codes. The simple method chosen for this purpose is the well-known integral method for natural convection of air on a vertical plate, as presented in Rohsenow and Choi [Rohsenow, 1961]. The equation for estimating the boundary layer width is:

$$\frac{\delta}{x} = 0.565 \text{Gr}_x^{-0.1} \text{Pr}^{-3/15} \left[ 1 + 0.494 \text{Pr}^{2/3} \right]^{0.1}$$  \hspace{1cm} (3.1)

where \( \delta \) is the thickness of the boundary layer and \( x \) is the distance from the leading edge.

The \( x \) subscript on the Grashof number signifies that the characteristic length in the Grashof number calculation is this same distance \( x \).
According to the integral method, the temperature and velocity profiles within the boundary layer are given by the equations:

\[
\frac{T - T_m}{T_0 - T_m} = \left[ 1 - \left( \frac{y}{\delta} \right)^{1/7} \right]
\]

\[
u_x = \Gamma \left( \frac{y}{\delta} \right)^{3/4} \left( 1 - \frac{y}{\delta} \right)^4
\]

(3.2, 3.3)

The parameter \( \Gamma \) used in the velocity profile has the dimensions of velocity and is given by:

\[
\Gamma = 1.185 \frac{V}{x} Gr_x^{0.5} \left[ 1 + 0.494 Pr^{2/3} \right]^{0.1}
\]

(3.4)

where \( V \) is the kinematic viscosity, \( x \) is the distance from the leading edge, and the characteristic length used in calculating the Grashof number is again the distance \( x \).

These equations give results for air that agree well with experimental data for turbulent natural convection boundary layers [Rohsenow, 1961]. However, using these relations to calculate the characteristics of a steam-air boundary layer, with steam-condensation, is beyond the scope of their design and should be justified. On closer inspection, there are several factors that do support this extension of their purpose. The properties of steam do not deviate much from those of an ideal gas at the temperatures and pressures of interest (\( P = 1 \) to 5 atmospheres, \( T = 300 \) to 410 K). The Prandtl number of steam-air mixtures at conditions of interest is between 0.69 and 1.0, not much different from that of pure air which is nearly constant at 0.69. The kinematic viscosity of a steam-air mixture at these conditions varies from that of pure air by less than 10%. Also, a steam-air boundary layer is expected to be more narrow than a pure air boundary layer, thus these equations should overestimate the layer thickness and essentially bound the true layer.

The reason why the steam-air layer is expected to be more narrow than a pure air layer is found by inspecting the integral method relations more closely. Natural convection boundary layers decrease in width for increasing driving force, i.e., an increase in the density difference across the boundary layer which in turn increases the Grashof number. For an air layer, this density difference is due only to the change in temperature across the boundary layer. For a steam-air mixture, the density difference is also a function of the concentration change of steam across the boundary layer. For a steam-air boundary layer where the steam is condensing on the cool side of the boundary layer, the density difference across the boundary layer is significantly greater than that due to the temperature change alone (This is shown in Figure 2-25).

To lend more credibility to the choice of using the integral method equations to determine boundary layer characteristics, the predictions from the integral method will be compared to some CFD simulation results. It is prudent then to discuss what is considered a reasonable agreement between the two methods. First, the boundary layer is expected to be on the order of centimeters in width for the surfaces considered in this thesis. This is considerably less than the one to two meter width of normal cells used in finite-volume computer codes such as GOTHIC.
Because of this large difference in characteristic size, a reasonable agreement of a factor of two in boundary layer thickness between the two methods is considered to be reasonable. This choice may at first seem somewhat arbitrary. However, since the boundary layer characteristics are only one aspect involved in showing the utility of the improved heat and mass transfer approach presented in chapter 4, it is only necessary to have a first order estimate of the boundary layer width and parameter profiles to prove the point. A clear distinction between laminar and turbulent boundary layers will also be shown, and the factor of two error in the turbulent boundary layer width will still be shown to be considerably larger than the width of a laminar boundary layer.

Another aspect in the determination of what constitutes agreement are the particular variables chosen for comparison. The total width of the boundary layer is a somewhat arbitrary boundary and not of much use. In the integral method, the momentum and thermal boundary layers are assumed to be equal in width. In the CFD calculations this ideal condition is not expected since the real fluid mixture does not have a Prandtl number of unity. The boundary layer profiles for comparison are thus not straightforward. The velocity profile of the integral method will be compared directly with the velocity profile from the CFD cases. The temperature profile from the integral method will be compared with the predicted temperature profile from a CFD case with air convection and with the steam profile for cases where condensation is occurring. The reason for this is that the CFD simulations will have profiles for steam fraction and temperature - which will be different. However, the steam profile accounts for the vast majority of energy transport and therefore this profile is indicative of the total energy of the flow.

Finally, since the boundary layer profiles are expected to be steep near the wall and taper off considerably near the edge, it is deemed adequate to only capture about 80% of the profile in determining the "effective" boundary layer width. That is, we are concerned with predicting the width over which the "interesting changes" occur. For natural convection, the "interesting change" is the section of the boundary layer over which the thermal profile changes dramatically. In the present case, we are attempting to capture the width over which 80% of the change takes place between interface values and free stream values,

$$0.8 = \frac{T - T_m}{T_0 - T_m} = \left[1 - \left(\frac{\gamma}{\delta}\right)^{1/7}\right]$$

For velocity, the effective width is considered to be the width over which the velocity parallel to the surface approaches 80% of the free stream value. Restated, the goals of the CFD are to predict the 80% mark for both the thermal and momentum thickness. Table 3-1 below summarizes the goals for the CFD analysis.
Table 3-1: Goals of the CFD analysis

- Confirm that the integral method can be used to reasonably predict 80% of the width of the thermal boundary layer
- Confirm that the integral method can be used to reasonably predict 80% of the width of the momentum boundary layer
- Show the distinct difference between a laminar and turbulent boundary layer profile
- Show the difference between an air and steam boundary layer

3.2 Selection and Overview of the CFX Computer Code

In order to carry out the CFD analyses, a suitable CFD code was needed. There are several commercial computer codes available to perform computational fluid dynamics simulations. The codes that were investigated for possible use in this study are listed below:

- FLUENT - by Fluent Inc., [FLUENT, 1997]
- GASFLOW - by Los Alamos National Laboratory, [Wilson, 1992]

3.2.1 Selection of a CFD computer code

Prior to purchasing a code, each of the four codes listed above was examined to determine if it was capable of performing the necessary calculations and had the characteristics desired by the author. The desired characteristics are summarized in Table 3-2 along with the characteristics of each code. This table represents the ability of the available code version at the time the selection was made and is not meant to represent the capabilities of the codes presently available.

Table 3-2: Codes investigated for CFD analysis

<table>
<thead>
<tr>
<th>Desired characteristics / requirements</th>
<th>ADINA</th>
<th>CFX</th>
<th>FLUENT</th>
<th>GASFLOW</th>
</tr>
</thead>
<tbody>
<tr>
<td>Graphical pre/post-processing</td>
<td>X</td>
<td>X</td>
<td>X</td>
<td></td>
</tr>
<tr>
<td>Compressible &amp; incompressible flow</td>
<td>X</td>
<td>X</td>
<td>X</td>
<td>X</td>
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<tr>
<td>Multi-species flow with mass transfer</td>
<td>X</td>
<td>X</td>
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<td>X</td>
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<tr>
<td>Turbulence models</td>
<td></td>
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<tr>
<td>low-Reynolds-number K-ε model</td>
<td>X</td>
<td>X</td>
<td></td>
<td>X</td>
</tr>
<tr>
<td>Wilcox K-ω model</td>
<td>X</td>
<td>X</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Transient &amp; steady-state capabilities</td>
<td>X</td>
<td>X</td>
<td>X</td>
<td>X</td>
</tr>
<tr>
<td>Thorough written documentation</td>
<td>X</td>
<td>X</td>
<td>X</td>
<td></td>
</tr>
<tr>
<td>Large commercial following</td>
<td>X</td>
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<tr>
<td>Compatibility with present computers</td>
<td>X</td>
<td>X</td>
<td>X</td>
<td>X</td>
</tr>
<tr>
<td>Education discounted price</td>
<td>X</td>
<td>X</td>
<td>X</td>
<td></td>
</tr>
<tr>
<td>Technical support</td>
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<td>X</td>
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</tr>
</tbody>
</table>
In general, the CFD code must have the ability to calculate a two-dimensional, compressible, transient, multi-species, turbulent flow. A graphical pre-processor is desired to greatly increase the ease with which the studies can be undertaken. Also, a turbulence model that is suitable for calculations within the boundary layer is required. Only two turbulence models in wide use are able to meet this requirement; one is a low-Reynolds-number turbulence $K$-$\epsilon$ model and the other is the $K$-$\omega$ model. The normal $K$-$\epsilon$ model which uses wall functions, is not suited for this task, since the boundary layer can not be resolved numerically with this approach. Some comments on each code are listed below.

**ADINA**
The ADINA suite of computer codes consists of ADINA, ADINA-F, and ADINA-T. The main code, ADINA, stands for Automatic Dynamic Incremental Nonlinear Analysis, and was originally written to calculate stress distribution in solid materials such as steel or concrete. The code was developed at MIT by J.K. Bathe, a professor of mechanical engineering. The ADINA-T code was developed later to study heat transfer in solids and the ADINA-F code was developed to simulate fluid flow and heat transfer. The codes use a finite-element formulation and come with a graphical pre-processor to aid in meshing and a post-processor to visualize numerical results. ADINA R&D, Inc., allows the codes to be used free of charge by any member of the MIT community after signing a licensing agreement. However, the no-charge license does not include technical support from the code distributor. One advantage of the ADINA system was that the author previously used ADINA-T during his master of science thesis work on radiation heat transfer. Ultimately the ADINA system of codes was chosen as part of a backup plan because the treatment of mass transfer is somewhat simplified and may not be robust enough to accurately predict the condensation boundary layers which will be studied in this analysis. The ADINA code is also not as well known or accepted in the CFD community as the more popular codes FLUENT and CFX.

**CFX & FLUENT**
The CFX and FLUENT codes met all of the requirements and desires for the CFD analysis. Both codes use a finite-volume formulation and are well known in the CFD community. The boundary conditions for the CFD analyses in this thesis are more complex than those generally encountered in run-of-the-mill CFD studies. In order to implement these complex boundary conditions, the user must be able to write source code which can then be integrated into the main flow solver. Both FLUENT and CFX have this essential capability. FLUENT Inc. has a good working relationship with MIT and has been supplying codes for student work here for several years. At the time of this comparison, the CFX code had the added advantage of the $K$-$\omega$ turbulence model. The CFX code was ultimately chosen over FLUENT in order to do a bit of comparison and to expand on the experience of the research team.

**GASFLOW**
GASFLOW grew out of a code called HMS, or Hydrogen Mixing Studies, which was developed at the Los Alamos National Laboratory. The code uses a finite-volume formulation for solving the transient, three-dimensional, compressible, Navier-Stokes equations for multiple gas species. The two main disadvantages of this code are the lack of a low-Reynolds-number $k$-$\epsilon$ model
which is essential to correctly simulate the boundary layer, and the lack of a graphical preprocessor which makes for difficult mesh generation. The GASFLOW code is not as well developed, or as well known within the CFD community as FLUENT or CFX. Finally, user training for the GASFLOW code would have involved a trip to Los Alamos, NM, which was much more inconvenient than traveling to Pennsylvania or New Hampshire.

### 3.2.2 Overview of the CFX-4.2 code

The version of CFX which was used for the analyses in this thesis was CFX-4.2, which was released in January 1998. The CFX suite of codes obtained by MIT consists of the pre-processor, CFX-Build; the solver, CFX-4 Solver; and the post-processor, CFX-Visualize.

CFX uses a finite-volume formulation to solve the continuity equations for mass, momentum, energy, and species. The code has several options to handle incompressible and compressible fluids. There is a straightforward incompressible formulation where buoyancy is modeled using the Boussinesq approximation. The Boussinesq formulation in CFX-4.2 can accommodate buoyancy forces resulting from changes in temperature or species ratios. The CFX code also has a weakly-compressible option where the fluid is treated as compressible, however the speed of sound is assumed to be infinite. This assumption is stated to be applicable to fluid flows with Mach numbers below 0.3 - which is appropriate for a natural or mixed convection boundary layer. With the weakly compressible option, the density of the fluid in each cell is calculated from the ideal gas law according to the mass fraction of the fluid components.

The turbulence models available in CFX-4.2 are the standard K-ε model, an RNG K-ε model\(^1\), the Launder and Sharma low-Reynolds-number K-ε model, and the Wilcox K-ω model [CFX-4.2, 1997]. The low-Reynolds-number K-ε model and the K-ω model are both appropriate for use in resolving boundary layer flows - which means that they can both be integrated through the laminar sublayer without causing numerical instabilities.

### 3.3 Simulation Specifics

This section discusses the equations of motion, the assumptions, and the limitations of the computer code and simulations that will be performed in this chapter. This discussion was placed in a separate section because it applies to both the benchmark problem of section 3.4 and the analyses of section 3.5.

#### 3.3.1 Assumptions and limitations

The biggest assumption that will be made while performing these CFD studies is that the phase change from steam to liquid water can be modeled using boundary conditions without actually forcing the code to simulate the phase change and track the liquid. This is accomplished by treating the condensing wall as a pseudo-boundary where the mass fraction of steam and the velocity normal to the wall are prescribed assuming that the wall actually represents the surface

---

\(^1\) RNG stands for Re-normalized Group, this is a modified version of the standard K-ε model for high velocity flows and is not suitable for near-wall modeling.
of a saturated liquid film. This approach has been adapted from the approach used by Fedorov et al. in simulating evaporation from a liquid film [Fedorov, 1997].

The limitation of this assumption is that the liquid film is not modeled directly by the CFD code, thus the resistance to heat transfer of the film is not calculated. In cases where the condensation rate is very high, the liquid film may be a factor in limiting the heat transfer rate, but in most practical cases the presence of the liquid film will have little effect on the condensation rate. Since the primary reason for carrying out these simulations is to determine the dynamics of the boundary layer, the lack of the liquid film is deemed an acceptable limitation.

The CFX-4.2 program also uses the assumption that the molecular diffusivities are constant and dependent only on the background fluid (i.e., constant viscosity, thermal conductivity, and diffusion coefficient of air without regard to steam content). This assumption is valid for turbulent flows where the effective diffusivities produced by turbulent eddies far outweigh the contributions of the molecular terms. However, the present analyses are performed using the low-Reynolds-number turbulence model where the turbulence is damped out near the solid boundary, thus this assumption may not be valid. To combat this problem, the molecular properties of the steam-air mixture will be calculated in advance based on the boundary conditions used to represent the condensation interface (cold wall). These calculated values for viscosity, thermal conductivity, and molecular diffusion coefficient will then be input into the code as the properties of the fluid. This will assure that the near-wall region, which is the only region to require accurate molecular properties, will be represented correctly.

The last assumption used is that of a weakly compressible fluid. This assumption means that the density of the steam-air mixture in each cell is calculated based on the ideal gas law taking into account the relative amounts of steam and air present. Through the ideal gas law, the local temperature of the mixture is also taken into account, but the local pressure is not. Instead a constant reference pressure is used. In effect what this means is that the density changes used to determine buoyancy driving forces are based on temperature and concentration - with no concern for the small fluctuations in pressure which occur along the wall due to the weight of the fluid above the cells of concern. This assumption is often used when modeling ideal gases where simply using the Boussinesq approximation for buoyancy is inadequate. In all other aspects, the fluid is essentially considered to be incompressible. The exact form of the equations will be discussed in the next section.

### 3.3.2 Flow equations and turbulence models

The CFX-4.2 computer code solves the conservation equations for mass, momentum, energy, and species on a rectangular grid using the finite-volume method. The equations can be solved for fully compressible, weakly compressible, or incompressible fluids. The code has several options for modeling turbulence, the one used here is the low-Reynolds-number $K$-$\varepsilon$ model of Launder and Sharma [Launder, 1974]. Two additional equations are solved for these turbulence quantities.

Appendix C reviews the conservation equations and several turbulence models in detail. The reader is referred to the appendix if more detail on this subject is desired. For ease of reference,
the Reynolds averaged, incompressible, time dependent equations of motion are given below in index notation. In order, the equations are for the conservation of mass, momentum, and energy:

$$\frac{\partial U_i}{\partial x_i} = 0$$  \hspace{1cm} (3.6)

$$\rho \left( \frac{\partial U_i}{\partial t} + u_j \frac{\partial U_i}{\partial x_j} \right) = - \frac{\partial P}{\partial x_i} + \frac{\partial}{\partial x_j} \left[ (\mu + \mu_T) \left( \frac{\partial U_i}{\partial x_j} + \frac{\partial U_j}{\partial x_i} \right) \right] - \frac{2}{3} \rho \delta_{ij} \frac{\partial K}{\partial x_j} + (\rho - \rho_0) g_i$$  \hspace{1cm} (3.7)

$$\rho \left( \frac{\partial H}{\partial t} + u_i \frac{\partial H}{\partial x_i} \right) = \left( \frac{\partial p}{\partial t} + u_i \frac{\partial p}{\partial x_i} \right) + \frac{\partial}{\partial x_i} \left( \left( \frac{\mu}{Pr} + \frac{\mu_t}{Pr_t} \right) \frac{\partial H}{\partial x_i} \right) + \Phi$$  \hspace{1cm} (3.8)

Recall that $Pr = \frac{c_p \mu}{k}$ and $Pr_t = \frac{v}{k/\rho c_p} = \frac{v}{\alpha}$, which is the ratio of momentum to thermal diffusivities, $Pr_t$ is the turbulent Prandtl number, and $\mu_t$ is the turbulent eddy viscosity. The turbulent Prandtl number is used to relate the eddy viscosity to the transport of heat.

Several simplifications are made to make the calculations more tractable. The first assumption was already discussed, that of a weakly compressible fluid. This means that the pressure changes throughout the flow domain are assumed to be small, and only a constant reference pressure is used to calculate physical properties. As a consequence of this, the density is considered constant except when calculating the buoyancy term in the momentum equations where it is calculated from the ideal gas law. This treatment of density allows the code to capture the change in density due to concentration difference as well as temperature difference. The density equation is:

$$\rho = \frac{P_{ref} M}{RT}$$  \hspace{1cm} (3.9)

where $P_{ref}$ is the reference pressure, $M$ is the effective molecular weight of the gas mixture, $R$ is the universal gas constant, and $T$ is the absolute temperature.

The final consequence of assuming a weakly compressible fluid is that the pressure work term on the right hand side of the energy equation is assumed to be zero. Another simplification to the energy equation is to ignore the kinetic energy contribution to the total enthalpy. Thus the enthalpy solved for in the energy equation becomes the static enthalpy, which is a function of pressure and temperature only. The viscous dissipation term, $\Phi$, is also ignored. These last two assumptions are valid since the fluid moves very slowly in natural convection boundary layers and the air-steam mixture has a very small viscosity.
The turbulence model used is the low-Reynolds-number $K$-$\varepsilon$ model of Launder and Sharma with an added term, $G$, to include contributions due to buoyancy\(^2\). The transport equations for $K$ and $\varepsilon$ are listed below.

\begin{align}
\rho \frac{\partial K}{\partial t} + \rho U_j \frac{\partial K}{\partial x_j} &= \left[ \mu_i \left( \frac{\partial U_i}{\partial x_j} + \frac{\partial U_j}{\partial x_i} \right) - \frac{2}{3} \rho K \delta_{ij} \right] \frac{\partial U_i}{\partial x_j} - \rho \varepsilon + \frac{\partial}{\partial x_j} \left[ \left( \mu + \frac{\mu_t}{\sigma_K} \right) \frac{\partial K}{\partial x_j} \right] - \varepsilon_0 + G \\
\rho \frac{\partial \varepsilon}{\partial t} + \rho U_j \frac{\partial \varepsilon}{\partial x_j} &= C_{\varepsilon_1} f_1 \frac{\varepsilon}{K} \left[ \mu_i \left( \frac{\partial U_i}{\partial x_j} + \frac{\partial U_j}{\partial x_i} \right) - \frac{2}{3} \rho K \delta_{ij} \right] \frac{\partial U_i}{\partial x_j} - C_{\varepsilon_2} f_2 \frac{\rho \varepsilon^2}{K} + E \\
&+ \frac{\partial}{\partial x_j} \left[ \left( \mu + \frac{\mu_t}{\sigma_\varepsilon} \right) \frac{\partial \varepsilon}{\partial x_j} \right] + C_{\varepsilon_3} \frac{\varepsilon}{K} G
\end{align}

(3.10)

where $\varepsilon_0$ is the value of $\varepsilon$ at the wall, and the turbulent viscosity is given by:

$$\mu_t = C_{\mu} f_\mu \frac{K^2}{\varepsilon}$$

(3.12)

The remaining constants and functions are defined below:

$$G = \frac{\mu_t}{\rho Pr_t} \frac{\partial \rho}{\partial x_i}$$

$$f_\mu = \exp \left( -3.4 \left[ 1 + \frac{Re_t}{50} \right]^2 \right), \quad f_1 = 1, \quad f_2 = 1 - 0.3 \exp(-Re_t^2)$$

(3.13)

$$\varepsilon_0 = 2\mu \left( \frac{\partial \sqrt{K}}{\partial x_i} \right)^2, \quad E = 2 \frac{\mu \mu_t}{\rho} \left( \frac{\partial U}{\partial x_i} \frac{\partial U}{\partial x_i} \right)^2, \quad Re_t = \frac{\rho K^2}{\mu_\varepsilon}$$

$$C_{\varepsilon_1} = 1.44, \quad C_{\varepsilon_2} = 1.92, \quad C_{\varepsilon_3} = 1.44, \quad C_\mu = 0.09, \quad \sigma_{\mu_t} = 1.0, \quad \sigma_\varepsilon = 1.3$$

3.3.3 Modeling mass diffusion

One additional equation is required in order to model the mass transfer of water vapor. The code uses a single fluid to represent the gas phase. In this case, the fluid is made up of a mixture of steam and air. The mass fraction of steam is treated as a scalar quantity that obeys an advection-
diffusion equation. The mass fraction of air, also called the *carrier fluid* or *background fluid* is found by subtracting the steam mass fraction from unity. The steam species concentration conservation equation is

\[ \rho \frac{\partial m}{\partial t} + \rho u_i \frac{\partial m}{\partial x_i} = \frac{\partial}{\partial x_i} \left( \mu \frac{m}{Sc} + \mu_t \frac{\partial m}{\partial x_i} \right) + m^* \]

where \( m \) is the mass fraction of steam, and \( m^* \) is a source term which is zero in the present case.

Recall that \( \mu/Sc = \rho D \), where \( Sc \) is the Schmidt number, \( \mu \) is the viscosity and \( D \) is the binary diffusion coefficient of the steam air mixture. \( Sc_t \) is the turbulent Schmidt number which is generally taken to be equal to the turbulent Prandtl number.

### 3.3.4 Boundary conditions

The boundary conditions used in the analyses here are generally of four types: inlets, pressure boundaries, walls, or symmetry planes. Each will be described further. An inlet is a two-dimensional plane where all quantities are specified. That is, the three components of velocity may be specified along with temperature, steam mass fraction, \( K \), or \( \varepsilon \). For incompressible or weakly compressible flow, the fluid pressure at an inlet is extrapolated from downstream. For fully compressible flows, the inlet pressure must be specified. Mathematically, inlets are Dirichlet boundary conditions for most variables.

A pressure boundary is a two-dimensional plane where a pressure is prescribed and the CFD code calculates the velocity profile through the boundary. Pressure boundaries may have a constant pressure along the entire plane, or a pressure profile may be specified along the plane. The normal gradients of velocity, temperature, \( K \), \( \varepsilon \), and steam fraction are set to zero at pressure boundaries. This is equivalent to a fully-developed flow assumption.

A wall boundary condition is a two-dimensional surface which is similar to an inlet except that no mass flow is allowed through the boundary. A zero normal velocity condition is enforced at the wall. The velocity components in directions other than normal to the wall may be specified. Temperature, heat flux, \( K \), \( \varepsilon \), mass flux of steam, and steam fraction may all be prescribed at the wall.

Symmetry boundary conditions are generally used to trick the solver into thinking that there is a larger computational domain than there actually is. A symmetry boundary is a two-dimensional plane where the conditions placed on the variable is one of reflection. This condition is used when a surface is to be described where there is no net gain or loss of mass, momentum, or energy from a wall type boundary condition. That is, no friction losses, conduction losses, or diffusion losses occur when a fluid is reflected from a symmetry boundary.

These four boundary conditions will be used in various combinations to describe the computational domain for the boundary layer studies. Each computational domain used will be described with a drawing which shows the location and type of the boundary conditions.
3.3.5 Convergence criteria and accuracy

One of the problems associated with numerical simulations is the determination of convergence. For the cases at hand, the run is defined to have achieved convergence when all parameters of interest change by less than 5% during the last 100 iterations of a steady-state calculation. Other criteria may be specified which will allow for more accurate answers to be obtained, but this criteria is judged to be adequate since these CFD cases are used simply to confirm the shapes of profiles within a turbulent mixed convection boundary layer.

To aid convergence and minimize numerical diffusion, all CFD studies are run with the CFX code in double precision mode. In addition, the most accurate linear equation solver, the multi-grid option, is used for the velocity, mass continuity, enthalpy, and steam mole fraction equations. The advection-diffusion equations are solved using either the QUICK method or a MUSCL scheme. The QUICK scheme (quadratic upwind differencing) is third-order accurate for advection and second-order accurate for diffusion. The MUSCL schemes are second order accurate upwind schemes which have been modified to reduce overshoots in predictions, i.e. reduce numerical diffusion.

3.4 Benchmark Problem

Prior to simulating the boundary layers of interest in this thesis, it was necessary to develop some knowledge about how to approach simulations of this type. That is, it was necessary to establish that the computer code and operator can correctly predict the phenomena needed to carry out this study. As a learning tool, a benchmark problem was chosen from the literature which requires the simulation of similar phenomena to those being studied. The chosen problem is one on turbulent heat and mass transfer in an asymmetrically heated, vertical parallel-plate channel [Fedorov, 1997]. This problem has mixed convection flow with an evaporating water film along a vertical flat plate, which is very similar to the condensation problem being studied. The problem is shown in Figure 3-1.

![Figure 3-1: Benchmark CFD problem](image)
Two important assumptions which were applied and reported for this benchmark problem will also be used in this thesis. First is that a low-Reynolds-number K-ε turbulence model can be used to predict simultaneous heat and mass transfer with reasonable accuracy. And second is that a boundary condition may be used to simulate the presence of a liquid water film. The mass transfer rate of steam at the film (for condensation or evaporation) is given by the equation:

\[ m = \frac{\rho D}{(1 - W_i)} \left. \frac{\partial W}{\partial y} \right|_{y=0} \]  

(3.14)

where \( D \) is the binary diffusion coefficient, \( W \) is the mass fraction of steam, and \( W_i \) is the mass fraction of steam at the condensate interface.

Equation (3.13) is the mass transfer equivalent of equation (1.40) which was derived for the molar flux at an interface. Equation (3.13) forms the basis for modeling suction at the condensate interface.

### 3.5 CFD Analyses

The studies in this section will concentrate on characterizing the boundary layer profiles of steam, temperature and velocity as compared to those predicted by the integral method (equations 3.1 - 3.4). Due to time considerations, simulating a pure natural convection boundary layer was foregone in favor of simulating a mixed convection boundary layer. By choosing a mixed convection flow field, the amount of the flow field outside the boundary layer that must be simulated is reduced considerably. Also, by simulating mixed convection, the choice to simulate steady-state results is more meaningful. For a pure natural convection boundary layer, a large cavity would need to be simulated where there is effectively a large reservoir of air and steam at the bulk conditions. A transient analysis would then be required as a steady-state analysis would result in the cavity being brought down to the conditions imposed at the condensing wall. However, the thermal boundary layer for mixed and pure natural convection should be nearly the same size, thus simulating a mixed convection case will suit our purpose.

![Figure 3-2: Problem specification for CFD analysis of boundary layers](image)
As a result of simulating a mixed convection boundary layer, the velocity profiles predicted by the CFD code are expected to differ from those predicted by the integral method. In the mixed convection case, the velocity maximum is expected to be lower and the profile more flat compared to the natural convection case. However, the distance over which the velocity profile approaches the free stream value should still give an indication of the boundary layer width, i.e., the width over which the interesting phenomenon (density change due to condensation) is occurring. Recall that the goal of the CFD studies is to confirm that about 80% of the important phenomena occur in a relatively small part of the boundary layer. The width of this small but important part of the boundary layer will later be estimated using the integral method.

All of the studies reported here are for the following conditions which are indicative of those encountered in containment analyses:

- $T_{\text{bulk}} = 390$ K
- $T_{\text{film}} = 360$ K
- $P_{t} = 3.112$ Bar

Three main areas are explored. The first objective will be to compare the temperature profile and velocity profile for an air-only convection boundary layer with those of the integral method. This will help to assure that the results of the CFD code are close to physical. The second task is to look at the steam and velocity profiles for a condensing situation. The third goal is to establish grid independence.

Figure 3-3 shows the normalized temperature profiles for the air-only mixed convection study. The integral method is used to predict the first two curves. The first is for a laminar profile, the second is for a turbulent profile. The third curve is the normalized temperature profile predicted by the CFD code for the mixed convection study. The temperature profiles are shown to be in good agreement. The integral method is a good indicator of boundary layer width. What is more important for the present study is that the point at which 80% of the temperature change takes place (2-3 cm) differs by only slightly between the integral method and the CFD study.

Figure 3-4 shows the profiles of the downward velocity component. The integral method laminar and turbulent predictions are shown as well as the velocity profile predicted in the CFD study. The velocity profiles differ substantially. This is not unexpected because of the CFD simulation being for mixed convection with a background velocity of -0.2 m/s. The velocity profiles are expected to be somewhat flattened due to the mixed convection regime, and that is what is predicted in Figure 3-4. Notice that the total boundary layer width predicted by the integral method is about 14 cm. Most of the boundary layer flow occurs in the half of the boundary layer closest to the wall. The CFD predictions also show that most of the flow occurs close to the wall. At about 10 cm, the CFD predictions show that the velocity in the boundary decreases to that of the background fluid.
Figure 3-3: Normalized temperature profiles for air-only convection

Figure 3-4: Velocity profiles for air-only convection
Figure 3-5 shows the predicted normalized steam profiles for mixed convection boundary layers compared to the normalized temperature prediction of the integral method. The CFD profiles are in fairly good agreement with the integral method predictions for turbulent boundary layers. (The CFD predictions for three different mesh densities were compared and show close agreement.) Notice that the steam boundary layer without suction is larger than that predicted when the suction velocity is modeled. The predicted boundary layer width of the integral method is about 12 cm. The CFD calculations predict boundary layers wider than this, but all predictions show a 80% change in concentration in less than 4 cm, 1/3 of the boundary layer width predicted by the integral method.

Figure 3-6 shows the velocity profiles predicted by the integral method for turbulent natural convection of air and the CFD calculations for mixed convection condensation of steam. The integral method predictions are based on a Grashof number which is modified to take into account the added driving force of steam condensation. The CFD simulation predicts a velocity maximum at the same location as the integral method. Also, the CFD results show the velocity passing through the background velocity value of -0.2 m/s at a distance of 11 cm from the wall, very close to the 12.5 cm predicted width of the natural convection boundary layer by the integral method. As expected the velocity maximum in the mixed convection case (CFD) is less and the profile more flat than in the pure natural convection case (integral method). Thus it appears that the integral method can be used to predict the width over which the phenomena occur that influence the local boundary layer flow.

![Normalized scalar profiles for condensation](image)

**Figure 3-5: Normalized scalar profiles for condensation**
3.6 Conclusions from the CFD Analysis

The integral method for turbulent natural convection boundary layers was compared to CFD predictions for mixed convection boundary layers. The CFD predictions were for air convection, and steam-air convection with condensation. The goal of using the integral method to reasonably predict the width over which 80% of the change occurs in the thermal boundary layer was shown to have been achieved. For both condensing and non-condensing scenarios, the integral method predicts a scalar profile (either temperature or steam) which closely matches that of the CFD studies. Therefore it is concluded that the integral method may be used to estimate the thickness of the turbulent thermal boundary layer - including estimating the width over which 80% of the change in steam concentration takes place.

For the momentum boundary layer the conclusion is similar. For the cases under study, namely that of a mixed convection boundary layer, it is concluded that the width predicted by the integral method does bound the momentum boundary layer width in which most of the boundary layer flow is contained and the width over which the phenomena occur which influence the local flow field.
4. **Boundary Layer Hypothesis**

The goal of this chapter is to propose and justify a modification for finite-volume containment analysis codes which will increase their ability to accurately predict the condensation rate in an advanced containment system while also capturing the natural phenomena which will affect overall containment system performance. The key to achieving this goal is to change the way in which these codes implement heat and mass transfer and to specialized the finite-volume mesh adjacent to a vertical condensing surface. Section 4.1 presents the hypothesis as originally devised at MIT and the changes proposed in the current research. Section 4.2 discusses particular details of how the boundary layer hypothesis has been implemented into the GOTHIC finite-volume containment analysis code (version 4.1c) [George, 1994]. Section 4.3 demonstrates the utility of the boundary layer approach by presenting some illustrative results for an idealized scenario. Section 4.4 discusses the attempts made to find suitable experimental data to use in benchmarking the hypothesis. Finally section 4.5 summarizes by outlining the cases where this modification is useful and presents ideas for an experiment to more thoroughly demonstrate the utility of the approach.

4.1. **Introduction and Assumptions**

4.1.1. **Original concept and justification**

The boundary layer concept was originally devised and applied by Gavrilas as a way to capture the downflow of cool air near the externally cooled shell of a large PWR containment [Gavrilas, 1995]. Gavrilas used the GOTHIC 3.4e computer code as a tool in the design process of a passively cooled containment for a large rating PWR. The proposed containment was cooled along the lower part of the shell by an external water moat. In order for this cooling system to operate effectively following an accident, the atmosphere had to remained relatively well mixed. The GOTHIC code was the tool used to predict the state of the atmosphere and the overall containment performance.

Gavrilas surmised that a natural convection boundary layer would develop adjacent to the large vertical surfaces of the proposed containment shell. Cooling of the air-steam mixture at the cool shell would cause steam to condense onto the surface, and the remaining cool mixture to become more dense than the surrounding gas. As a result, the cool, steam-depleted gas mixture would flow down along the surface. Because of this, it was possible that a cool air-rich layer would build up on the floor of the containment building. If the mixing forces were not strong enough, it was possible that the cool air could continue to steadily increase in thickness, resulting in stratification of the containment atmosphere. This phenomenon would effectively isolate the moat at the bottom of the containment from the hot steam-rich atmosphere at the top resulting in a failure to cool the containment as desired.

In order to show convincingly that this would not happen, Gavrilas first had to show that GOTHIC was capable of predicting such a phenomenon should it occur. Gavrilas showed that GOTHIC was able to predict a downward flowing boundary layer if a narrow computational volume was used to capture the flow near the cool surface. This approach was necessary for two reasons. First, the size of the computational volumes normally used in a containment analysis.
code are on the order of meters in width. Such large cells are a consequence of the immense size of containment structures, which generally have in excess of 25,000 m$^3$ of free volume. A boundary layer flow stream is at most several tens of centimeters across, which is a much smaller scale. Gavrilas pointed out that this narrow flow stream would be completely overwhelmed by the momentum in the remainder of a normal large computational volume and essentially be lost. The only way to capture the flow dynamics of what is occurring at the wall is to have a cell which is of the same scale as the phenomena at the wall, effectively isolating the boundary layer motion from that of the bulk fluid.

The second reason this small cell was necessary is related to properly modeling the consequences of steam condensation. Physically, the condensation process results in steam diffusing through the gas mixture and condensing onto the cool surface. It is well understood that the condensation/diffusion process only affects the gas mixture very close to the wall. This results in a thin layer of gas where the steam concentration changes from the bulk concentration to the interface concentration, which is immediately adjacent to the condensing surface. This thin layer comprised the diffusion boundary layer, and is on the same scale as the momentum boundary layer, several tens of centimeters in width. It is the decrease in steam concentration, and the accompanying decrease in gas mixture temperature, which results in the density increase in the boundary layer and the natural tendency of the mixture very near the condensing surface to move downward. By having a narrow near-wall computational volume, this decrease in steam concentration in the gas mixture very close to the condensing surface can be captured by the simulation code. Using a normal size computational volume at the condensing surface would result in a very small decrease in the steam concentration of the cell due to its large size. Without a significant decrease in steam concentration of the cell near the condensing surface, it would be impossible to model a cool, steam-depleted downflow of air. The flow in a large cell may still be downward, but the steam content would be incorrectly averaged over a large volume and thus not represent an air rich stream.

It is common practice in any fluid simulation to concentrate the computational cells in the areas where there are steep gradients in the properties being simulated. This practice is also common with finite-volume codes such as GOTHIC. The problem arises when heat and mass transfer calculations are considered. In most finite-volume codes, including GOTHIC, heat transfer between a fluid and a solid surface is calculated explicitly from correlations using the properties of the surface and the fluid in the cell immediately adjacent to the surface. The fluid temperature that is required by these correlations is the bulk temperature, i.e., the temperature outside of the thermal boundary layer. When narrow computational volumes are utilized which are approximately the same width as the thermal boundary layer, the temperature in the cell adjacent to the surface is not representative of the bulk conditions. In essence, the wrong temperature is being used to calculate heat transfer. If this problem goes uncorrected, using small computational cells in this manner may result in additional errors instead of increased resolution and accuracy in of the solution. This was a problem associated with the first work performed in this area.
4.1.2. Previous Work

As already mentioned, the boundary layer method was devised and implemented by Gavrilas [Gavrilas, 1995]. The specifics of the previous work are discussed here. The code version used was GOTHIC 3.4e. Gavrilas proposed using a boundary layer cell in her analyses but was unable to modify the source code to implement the necessary changes in heat transfer logic. Instead she devised a workaround to accomplish the desired results.

The first step in the process is to estimate the maximum width of the boundary layer in order to determine near-wall volume sizes for computer input. For this task Gavrilas employed the laminar boundary layer width equation for air derived using the integral method, as presented by Eckert [1950]:

\[
\frac{\delta}{x} = \left[ \frac{336 (Pr+5/9)}{Pr^2} \right]^{1/4}
\]  

(4.1)

The boundary layer in most containment applications is expected to be turbulent. However, the use of the laminar relation was justified in part because it was expected to bound the velocity maximum for turbulent boundary layers. Using this method, the width of the boundary layer at the bottom of a large containment shell was estimated. The near-wall computational volume was then set to this width for all vertical locations, i.e., if a maximum boundary width of 15 cm was predicted for a 60 meter surface, then all boundary layer cells were set to 15 cm regardless of the width of the boundary layer at the particular elevation.

Once the maximum boundary layer width and the computational cell size were determined, correction factors for the errors in temperature were calculated. Recall that the heat and mass transfer is calculated from correlations based on properties which are taken from the near-wall cell. In the present situation the near-wall cell has been sized to capture the boundary layer and the properties in this cell may not represent bulk properties, as the correlations require. Gavrilas devised a workaround which was used to correct for this. She proposed a multiplication factor which was calculated based on the proportion of the cell which was taken up by the boundary layer. Recall that the boundary layer cells are the same width regardless of their elevation. However, the boundary layer increases in width as it proceeds down the wall. Thus the boundary layer near the top of the shell will consume only a small part of the boundary layer cell width. The remainder of the cell will be occupied by the bulk region. As one proceeds down the wall, a larger and larger portion of the boundary layer cell will be occupied by boundary layer flow. Gavrilas noted that if the boundary layer consumed a large part of the cell then the properties in the cell would no longer represent bulk properties, and the heat transfer rate predicted by the correlations would be wrong.

Gavrilas surmised that the property of primary importance was the temperature difference between the near-wall cell and the wall, because the code calculates heat transfer from a heat transfer coefficient and a temperature difference between the fluid and the surface. The Gavrilas workaround was to define a multiplier for the heat transfer coefficient to correct for the decrease in the near-wall cell temperature due to a cell temperature partly reflecting the boundary layer
temperature. The workaround was derived according to the assumptions shown graphically in Figure 4-1. The different temperatures which are considered are shown clearly, along with the temperature differences of interest. The temperature difference which the condensation model requires is that between the bulk and the wall. Since this is not the temperature difference that is calculated by the code, a correction factor was determined. To do this, Gavrilas assumed that there was a linear temperature profile between the bulk temperature and the wall temperature. Thus, the average “actual” boundary layer temperature would be the average of the two, i.e.,

$$T_{BL} = \frac{T_{bulk} + T_{w}}{2} = \left( \frac{T_{w} + T_{bulk} - T_{w} - T_{w}}{2} \right)$$ \hspace{1cm} (4.2)

The temperature calculated by GOTHIC in the near-wall cell depends on the proportion of the cell occupied by the boundary layer and the bulk. If equation (4.2) is assumed to be correct, then the calculated temperature of the near-wall cell should be:

$$T_{cell} = \frac{(\tau - \delta)T_{bulk} + \delta T_{BL}}{\tau}$$ \hspace{1cm} (4.3)

The error in the calculated temperature difference can then be calculated as a function of the calculated temperature difference and the required temperature difference.

$$\tau \Delta T_{calculated} = (\tau - \delta)\Delta T_{required} + \delta \frac{\Delta T_{required}}{2}$$ \hspace{1cm} (4.4)

$$\Delta T_{calculated} = \frac{(2\tau - \delta)}{2\tau} \Delta T_{required}$$ \hspace{1cm} (4.5)

It then follows that the required temperature difference can be recovered:

$$\Delta T_{required} = \frac{2\tau}{(2\tau - \delta)} \Delta T_{calculated} = M \Delta T_{calculated}$$ \hspace{1cm} (4.6)

$$M = \frac{2\tau}{2\tau - \delta}$$ \hspace{1cm} (4.7)

The multiplier, $M$, can then be applied to the heat transfer coefficient calculated in GOTHIC to correct for the reduced temperature of the near-wall cell as compared to the bulk mixture. This multiplier was calculated for each boundary layer cell and put into function tables in the GOTHIC code which are used to alter the values of the heat transfer coefficient at each surface location. For more detail on this methodology see the original thesis [Gavrilas, 1995]

Several proposed changes have been applied to this general type of approach. They are described in the next section.
4.1.3. Proposed methodology

The present work on the boundary layer hypothesis follows directly on the previous work by Gavrilas and has been pursued using the input and advice from the author of the original hypothesis. The major aspiration of this section is to propose and justify a set of modifications for finite-volume containment analysis codes which will increase the ability of the codes to accurately predict the performance of advanced containment system which rely on natural processes for cooling and pressure control. Specifically, there are two goals which must be accomplished to realize this aspiration. These goals are:

- to accurately predict the condensation rate in a given situation,
- to capture the cool steam-depleted boundary layer flow adjacent to a vertical surface.

The first goal, predicting the correct condensation rate, is not achieved by simply choosing a condensation model which is accurate and applicable to the situation under study. The chosen condensation model must also be implemented into the code logic, and utilized by the analyst, in a manner which is consistent with the physical assumptions used to derive the model. The second goal is somewhat more challenging, as most containment analysis codes were not designed to resolve boundary layer flow. Achievement of the second goal is possible if the first goal is attacked in a particular fashion. In other words, if the condensation model is implemented into the containment analysis code in a specific way, the code is able to predict both the downward flowing cool boundary layer and the correct condensation rate. This section outlines the methodology employed to achieve this.

The condensation model which is used to achieve the above stated goals must meet three criteria. First, it must be accurate for a wide range of conditions. Second, it must be consistent with the
physical assumptions employed, i.e. the condensation model must be physically consistent with the assumption of a downward flowing boundary layer. And third, the condensation model must also be readily integrated into the containment analysis code. A thorough literature review was performed to assess the applicability and usefulness of the available condensation models for containment analysis in general, and use in the boundary layer hypothesis in particular (Appendix A). The diffusion layer model (DLM), originally proposed by Peterson, was chosen as the most appropriate model for this study for three reasons [Peterson, 1993]. First, the DLM is more general and accurate than the empirical model of Uchida, which is widely used in containment analysis [Peterson, 1996]. Second, a modified version of the DLM has been verified against experimental data from facilities which are representative of advanced containment designs [Anderson, 1998]. Third, the DLM is physically consistent with the assumption of a downward flowing boundary layer, and is compatible with the formulation and logic used in the boundary layer hypothesis and the GOTHIC code. Specifically, when using the GOTHIC code with the specified noding strategy, the correct properties (temperature, pressure, etc) are supplied to the DLM without the use of a correction factor. (See chapter 2 for a thorough analysis of the DLM, including comparison with experimental data.)

In order to achieve the second goal, predicting the downward flowing boundary layer, the computational mesh adjacent to the surface must be sufficiently fine to capture this phenomenon. This requires choosing computational volumes which are on the same scale as the boundary layer flow. However, most finite-volume codes calculate heat and mass transfer from the fluid to a solid surface based on the properties of the fluid in the near-wall cell. In the present case, using the properties in the near-wall cell to calculate the condensation rate will result in significant errors. The errors arise because condensation models, including the DLM, are based on bulk properties. Cells which are narrow enough to capture boundary layer flow will not contain bulk properties, but boundary layer properties. Herein lies the reason why containment codes are not well suited for capturing boundary layer flow and the reason for the Gavrilas multiplier (equation 4.7).

The solution to this problem is straightforward in theory, but extremely complex in practice. The containment code must be modified such that bulk properties are used to calculate condensation rates even with these small near-wall cells, but the heat and mass must still removed from the near-wall cell. This in turn requires an assumption of how many cells will encompass the boundary layer. For the work completed in this thesis, two computational cells were used to resolve the boundary layer, thus the properties in the cell twice removed from the wall are assumed to represent bulk properties. Figure 4-2 shows how this was implemented logically.
The next task is to specify a way to determine the width of the boundary layer, and hence determine the width of the boundary layer cells. The combined width of the two cells should be chosen such that the majority of the boundary layer flow is contained within the cells, and such that about 80% of the change in steam concentration between the bulk and the interface occurs within the cells. The width of the inner cell is based on a different criterion. The inner cell must be specified small enough such that the cell becomes depleted of steam. This is necessary in order for the code to calculate a cool air region. The width of the second cell is then the width of the inner cell subtracted from the width of the boundary layer.

To estimate the total width of the boundary layer, the integral method for turbulent natural convection was employed. The specific equations used are those given by Rohsenow and listed as equations (4.8-4.11) [Rohsenow, 1961]. The width of the near-wall cell, $\delta_1$, is specified to be 5% of the total width predicted by equation 4.8. The width of the second boundary layer cell, $\delta_2$, is specified to be 45% of the total width predicted by equation 4.8. This results in capturing only 50% of the total boundary layer width in the two near wall cells. This is considered satisfactory since the phenomena of interest (steam concentration change, velocity maximum, majority of boundary layer mass flow) are all contained within this distance.

The turbulent boundary layer equations are:

$$\frac{\delta_t}{x} = 0.565 \text{Gr}_x^{0.1} \text{Pr}^{-8/15} \left[ 1 + 0.494 \text{Pr}^{2/3} \right]^{0.1} \quad (4.8)$$

where $\delta_t$ is the thickness of the boundary layer and $x$ is the distance from the leading edge.

The $x$ subscript on the Grashof number signifies that the characteristic length in the Grashof number calculation is this same distance $x$. According to the integral method, the temperature and velocity profiles within the boundary layer are given by the equations:
The parameter $F$ used in the velocity profile has the dimensions of velocity and is given by:

$$F = \frac{1.185 \, \frac{v}{x} \, Gr_{x}^{1/2} \left[ 1 + 0.494 \, Pr^{2/3} \right]^{0.1}}{\sqrt{\frac{T_{0} - T_{w}}{T_{0} - T_{w}}}} \left[ 1 - \left( \frac{y}{\delta_{L}} \right) \right]^{1/2} \quad (4.9)$$

$$u_{x} = \Gamma \left( \frac{y}{\delta_{L}} \right)^{1/2} \left( 1 - \frac{y}{\delta_{L}} \right)^{4} \quad (4.10)$$

where $v$ is the kinematic viscosity, $x$ is the distance from the leading edge, and the characteristic length used in calculating the Grashof number is again the distance $x$.

The laminar boundary layer width associated profiles according to the integral method are [Rohsenow, 1961]:

$$\frac{\delta_{l}}{x} = 3.93 \, Gr_{x}^{1/4} \, Pr^{-1/2} \left[ 0.952 + Pr \right]^{1/4} \quad (4.12)$$

$$\frac{T_{0} - T_{w}}{T_{0} - T_{w}} = \left( 1 - \frac{y}{\delta_{L}} \right)^{2} \quad (4.13)$$

$$u_{x} = \Gamma \frac{y}{\delta_{L}} \left( 1 - \frac{y}{\delta_{L}} \right)^{2} \quad (4.14)$$

$$\Gamma = \frac{5.17 \, \frac{v}{x} \, Gr_{x}^{1/2} \left( 0.952 + Pr \right)^{-1/2}}{\sqrt{\frac{T_{0} - T_{w}}{T_{0} - T_{w}}}} \quad (4.15)$$

To illustrate the profiles given by the integral method equations, two figures have been included. Figure 4-3 shows the velocity profile for a distance of 5, 10, and 30 meters down a vertical surface. Both the laminar and turbulent profiles are shown. Figure 4-4 shows the temperature profiles which correspond to the velocity profiles in Figure 4-3. The primary utility of these figures is to show that for a turbulent boundary layer, most of the changes in the temperature profile, and most of the flow, are contained within the 50% of the boundary layer which is closest to the wall. Because of this, the combined width of the laminar layer and turbulent layer cells in GOTHIC will be defined to be 50% of the turbulent boundary layer width predicted by the integral method (i.e. 50% of the value predicted by equation (4.8)).

In order to further justify the use of these equations for predicting boundary layer profiles, a computational fluid dynamic (CFD) study was performed to determine the characteristics of a steam-air boundary layer. This study is detailed in chapter 3. For illustration, the results of one study are included here. Figure 4-5 shows the CFD results for a steam condensation boundary layer developed at a distance 2.5 meters down a vertical wall. The dimensionless steam profile has been plotted along with the dimensionless temperature profile predicted by equation (4.9). The agreement between the CFD predictions and the integral method is quite good. It is therefore concluded that the integral method is an applicable tool for determining the width of the
Figure 4-3: Velocity profiles from the integral method for laminar and turbulent natural convection boundary layers along a vertical flat plate.

Figure 4-4: Temperature profiles from the integral method for laminar and turbulent natural convection boundary layers vertical flat plate.
boundary layer cells used in GOTHIC. Figure 4-6 illustrates how the boundary layer cells are stacked along the vertical surface. The cells are smallest at the top of the surface and get progressively wider in order to follow the development of the actual boundary layer. Figure 4-6 is not drawn to scale and may be slightly misleading. The bulk cells are many times larger than the boundary layer cells, this is not adequately represented by the figure. This process of noding finely at the wall to capture the downward flow at a cool surface is common practice. The methodology proposed here is a way to choose the near-wall volume widths based on physical grounds and in a manner which is consistent with the heat and mass transfer logic of the code.

Figure 4-5: Comparison of CFD predictions to those of the integral method
4.2. Implementation into the GOTHIC code

The implementation of the boundary layer hypothesis and the DLM into the GOTHIC source code required substantial changes to the heat transfer algorithm existing in the code. Essentially, the heat transfer logic was modified such that the fluid properties used for determining the heat transfer rate at a particular thermal conductor (solid conducting boundary) were not required to be those of the cell in which the conductor is located. Instead, three options were programmed into the code which allowed the user to specify using the properties of 1) the cell where the conductor is located, 2) one cell to the “west” (GOTHIC coordinates) of the conductor cell, or 3) two cells to the “west” of the conductor cell. These three options were programmed ONLY for use with the DLM. Choosing a different condensation model in GOTHIC (i.e., Uchida or Gido-Koestel) will automatically use properties in the cell where the conductor is located.

This implementation requires that the user define any surfaces employing the boundary layer hypothesis be located on the “east” side of the simulation volume. This particular strategy for modifications to the code was chosen to reduce the amount of time required to debug the code changes. Another time saving strategy was to implement the DLM only for steam-air mixtures. That is, the DLM implementation into GOTHIC assumes that there is only a single noncondensable gas, air. The implementation of the DLM can be generalized easily in theory to include any other combination of gases which GOTHIC already allows. However, implementing this strategy in the GOTHIC source code is not trivial and should probably be left to the code developers.

Another implementation trick is that of the condensate film. The GOTHIC code has an algorithm for calculating heat transfer through a condensate film. However, this algorithm proved to be incorrect for the current situation. Instead, alternate heat transfer relations for a wavy laminar or a turbulent falling liquid film were used [Mills, 1995]. These relations are
slightly different from the simple Nusselt relation for heat transfer in the liquid film which was used in the evaluation of the DLM in chapter 2 (see equations in Appendix D).

The interfacial heat transfer relations in GOTHIC were disabled in the computational cells where the DLM was being used. Without this modification, the GOTHIC code would predict condensation (from the DLM) and evaporation (from the interfacial heat transfer) within the same cell. Other problems with interfacial heat transfer occur at the bottom of the simulated test volume. In the distributed parameter formulation of GOTHIC (the type used here), a basic assumption is that any free liquid in a computational cell is present as a liquid film on any surfaces in the cell. This assumption is maintained UNTIL a certain thickness of liquid is predicted and suddenly the code interprets the free liquid to be a pool of water. Interfacial heat transfer for pools obeys completely different relations than the heat transfer on vertical surfaces. This transition occurs rapidly within GOTHIC in the cells at the bottom of the volume, where the condensate collects. When the transition from a film to pool occurs in the GOTHIC logic, the liquid pool suddenly starts to evaporate at a very high rate. The effect is similar to suddenly removing the cover from a boiling pot of water. The burst of water vapor that is released completely disrupts the atmosphere and destroys any stratification that previously existed. Physically, re-vaporization of condensate at the bottom of a containment vessel does exist and should be accounted for when simulating an accident scenario. However, the method by which the GOTHIC code suddenly switches from one mode of heat transfer to another is not physical, and must be corrected in order to predict physical results. To solve this situation in the present work, the code was forced to ignore all pools. That is to say, the logic was altered such that no pools were recognized.

Another modification is the condensing temperature of the steam. The condensate temperature should be at or below the temperature at which the steam condenses. However, the GOTHIC algorithm assumes that the condensate temperature is that of the saturation temperature of the cell in which the condensing surface is located. While implementing the DLM, the condensate temperature was changed to be set equal to the interface temperature of the film calculated in the DLM. Without this change, the condensate which pooled at the bottom of the containment vessel was hot and immediately vaporized - resulting in a nonphysical situation and a difficulty in simulation.

One other detail that must be mentioned concerns the calculation of wall friction. Friction along surfaces in GOTHIC is modeled in an inconsistent manner, i.e., as a wall is covered in liquid, the shear between the wall and the vapor is ramped to zero, but shear between the liquid and the vapor is not ramped up at the same time. This results in "frictionless" flow in the near-wall cell for some situations, and a significantly higher velocity than is expected in reality. This problem was overcome in the present work by forcing the code to calculate wall friction for the vapor in all circumstances. This is equivalent to assuming that the vapor in the near-wall cell is always in contact with a non-moving surface, i.e., that the liquid condensate film is not moving. Another friction related problem is that the frictional drag between the vapor and the wall is calculated based on the assumption of flow inside a smooth tube with a Reynolds number calculated using the hydraulic diameter of the cell. Instead, the friction for vapor in the near-wall cell should be changed to be consistent with the assumption of flow along a flat plate, and also to incorporate
the influence of wall roughness which will be encountered in real situations. The fixes required for these two friction problems are complex, and upon consultation with the code developers, were not attempted. More recent versions of the GOTHIC code have been corrected for the problems outlined in this section.

4.3. GOTHIC Illustrative Testing and Results

The best way to prove that the boundary layer hypothesis is useful and has been correctly integrated into the GOTHIC computer code is to complete an illustrative test case. An idealized test case has been devised and is shown schematically in Figure 4-7. This case is representative of the situation which exists in advanced containment designs. The case consists of a large volume with a cooled wall along one side, which is initially filled with air at one atmosphere. The test case scenario is that steam is injected into the volume in a violent manner, causing a rapid increase in pressure and producing a well-mixed atmosphere. Subsequent to reaching the specified pressure, the steam release is reduced to a plume. The plume is released at 11.5 meters above the floor to establish a situation where stratification should develop.

The test case was simulated using the GOTHIC computer code. Two variations were used. The first run consisted of simply noding the volume with equally spaced nodes. No specialized noding was employed at the cold wall, and the normal heat transfer algorithm was used in conjunction with the DLM condensation model. In the second case, the boundary layer hypothesis was employed. A series of narrow near-wall nodes were used along with the modified heat transfer algorithm in GOTHIC. The results are shown in Figure 4-8. For the “normal” run, the atmosphere is predicted to be relatively uniform and well mixed. There is a slight decrease in steam content at the very bottom of the volume, but the decrease is not significant. The results for the case which employs the boundary layer hypothesis is strikingly different. A very clear decrease in steam concentration is evident below the plume elevation. The steam content decreases steadily toward the bottom of the volume. As a result of the higher steam content in the top of the volume, the condensation rate is 25% above that predicted in the run with a well-mixed atmosphere.

A second test case was run for a concrete containment structure (wall, floor, and ceiling). Instead of a constant temperature wall, as the cooling surface, top, right side, and bottom of the test volume were bounded by 100 cm thick concrete walls. The Initial temperature of the concrete was set to 45 C. As expected, the total condensation rate decreases exponentially with time as the concrete surface heats up quickly, but relatively little energy is absorbed due to the low thermal conductivity. However, in the initial few thousand seconds of the transient, a slight stratification layer did develop below the break location. This layer is a result of condensation on the concrete floor and does not arise due to a large downflow of air in the boundary layer adjacent to the wall. Figure 4-9 shows the steam concentration for the concrete case at two different times following the blowdown. Since the boundary layer does not account for the stratification in this case, utilizing the boundary layer hypothesis is not a good use of computer resources.
Figure 4-7: Schematic of test case to illustrate the utility of the boundary layer hypothesis

Figure 4-8: Steam concentration and temperature profiles predicted by GOTHIC for the test case shown in figure 4-7
4.4. Attempts to verify BLH against available experimental data

4.4.1. Westinghouse Large Scale Test

To evaluate the utility of the boundary layer hypothesis for use in actual simulations, the GOTHIC code should be used to simulate experimental data where accurate predictions require the code to predict boundary layer flow. A search for available experimental data identified the Westinghouse Large Scale Test (LST) as a candidate. The LST configuration is shown in Figure 4-10. The LST data are useful for two major reasons; the test is large, and has an externally cooled shell. The cooling of the shell is established by an evaporating water film which flows along the outside of the containment vessel, and assures a high rate of condensation. This high rate of condensation leads to the presence of a cool boundary layer at the shell, which may lead to stratification. Also, the results from the LST experiments do predict significant stratification [Kennedy, 1996].

However, there are several problems associated with simulating this experiment with GOTHIC. First, the test was constructed with large gutters to collect condensate around the perimeter of the test vessel. These gutters introduce significant complications into the development of an adequate-noding scheme. If the noding around the gutters is not highly specialized, the benefits of the boundary layer hypothesis will be mute because the gutters will cause very significant mixing in the region immediately surrounding them. Second, the shell is cooled by an evaporating external water film. Modeling this evaporating film is not possible with the current...
version of GOTHIC. In the analysis of the LST, and the design of the AP600, Westinghouse allocated considerable resources to the development of a GOTHIC version which was capable of modeling this film. And finally, most of the data from these tests are proprietary to Westinghouse and have not been released into the free literature. The only test data that is available in the literature are for a few shake-down runs which were performed without the external water film. Because of the lack of external cooling, the data from these runs are not very useful.

![Figure 4-10. Large Scale Test cross section](adapted from [Kennedy, 1996] with additional assumptions made by the author)

### 4.4.2. University of Wisconsin-Madison facility

A research group at the University of Wisconsin-Madison carried out an entire series of experiments which were used to establish a condensation database for analyzing condensation models [Anderson, 1998]. The experiments cover a wide range of experimental conditions. The DLM was benchmarked against this database (see chapter 2). The UW facilities were also constructed specifically to mimic the aspect ratio of the AP600. However, the facilities were also specifically designed to produce a well-mixed atmosphere - by having a steam injection system at the bottom of the facility. This limits the usefulness of the data as far as benchmarking the boundary layer hypothesis. In the future, these facilities might be modified to allow injection of steam at a higher elevation. This may produce data useful for benchmarking purposes.
4.4.3. LACE and HEDL Tests

There are two other data sets that were investigated to determine if they could be useful in benchmarking the boundary layer hypothesis. The LWR Aerosol Containment Experiments (LACE) program investigated aerosol distribution in containment atmospheres during severe accident sequences [Bloom, 1986]. The tests were performed in the Containment System Test Facility (CSTF) at the Hanford Engineering Development Laboratory (HEDL). The CSTF consists of a large vessel 20.4 meters in height, 7.6 meters in diameter with a free volume of 850 m$^3$. The CSTF was originally designed to mimic a PWR ice condenser containment system. This type of facility should be well suited for performing experiments which could be used to benchmark the boundary layer hypothesis.

A preliminary investigation of the LACE tests resulted in the conclusion that the tests did in fact result in a stratified containment atmosphere, but that the stratification was a result of the test setup, not from the buildup of air on the containment floor [Wolf, 1999]. The steam injection point is elevated considerably from the bottom of the vessel, and the blowdown does not create a well mixed atmosphere at the beginning of the transient. The gas mixture in the bottom of the containment vessel does not become inundated with hot steam, but remains relatively cool throughout the tests. This type of result is not helpful in the present situation.

There were also containment stratification experiments performed with hydrogen and helium in the CSTF [Bloom, 1983] which were later simulated using a containment analysis code [Manno, 1983]. These experiments were performed for containment accident scenarios where steam and either hydrogen or helium were injected into the vessel to simulate a severe accident situation. Stratification was shown in some situations. However, the stratification was a result of the light gas accumulating at the top of the volume, not from cool air accumulating at the bottom. Also, air blowers were installed in the CSTF to increase circulation between the upper and lower elevations of the vessel. The results of these experiments are not useful because of the forced mixing of the atmosphere.

4.5. Boundary Layer Hypothesis Summary

4.5.1. Utility of the boundary layer hypothesis

To assess the performance of advanced containment designs, it is necessary to use a computer code which is capable of predicting natural convection and thermal stratification. The ability of the GOTHIC code, which normally utilizes a coarse finite-volume mesh, to predict thermal stratification may, in certain situations, depend on resolving boundary layer flow adjacent to the condensing surface. To achieve this, the meshing strategy must employ relatively small computational cells near the surface. This was identified by Gavrilas, who proposed a noding strategy consisting of a single narrow near-wall cell and an associated heat transfer model [Gavrilas, 1995]. These concepts are extended in this chapter, in which the boundary layer hypothesis is proposed and tested. The boundary layer hypothesis consists of: 1) utilizing two near-wall computational cells; and 2) employing an appropriate condensation model. In order to implement the boundary layer hypothesis in GOTHIC, the source code was modified to include the chosen condensation model and to extend the computational algorithm to allow the
condensation model to be implemented correctly. Details of this implementation strategy are given in section 4.2. The methodology was tested by simulating an illustrative test case with GOTHIC. The simulation employing the boundary layer hypothesis resulted in stratification being predicted. When the case was repeated using “normal” heat transfer options available in the GOTHIC code, stratification was not predicted. This test case, and the GOTHIC results, are discussed in section 4.3.

The utility of the boundary layer hypothesis is only recognized for certain physical situations where a boundary layer develops, and where the boundary layer may have an impact on the overall performance of a containment system. In the present context, the boundary layer hypothesis was developed to capture the downflow of cool air in the boundary layer adjacent to a tall vertical condensing surface. This particular situation is considered important because the air which flows down along the cool surface may collect at the bottom of the containment vessel and result in a stratified atmosphere, with cool air at the bottom and warm steam at higher elevations. A stratified atmosphere may be detrimental, or beneficial, to certain types of passive cooling systems. In order to determine the effectiveness of these systems, the ability to predict stratification resulting from the presence of a boundary layer is essential.

Other advanced containment designs forego an externally cooled steel shell and instead have a single or double wall concrete containment vessel. Cooling systems in such containment designs often employ a set of internal condensers or a thermosyphon [C.S. Byun, 1998; M. Leiendecker, 1998]. In this situation, the boundary layer hypothesis may not add significantly to the reliability of results. The cooling capabilities of concrete are significantly inferior to those of steel because concrete has a much lower thermal conductivity ($k_{\text{steel}} = 50 \text{ W/m-K}$; $k_{\text{concrete}} = 1.4 \text{ W/m-K}$) [Mills, 1995]. Although the heat capacity of a concrete containment structure is large, the low thermal conductivity effectively limits the rate at which heat is absorbed by the concrete. (A thorough discussion on this topic and how different types of containment heat sinks should be modeled is presented in section 2.2.) Because the condensation rate at a concrete surface will be relatively low, the boundary layer that develops adjacent to the surface may be insignificantly small for most of the duration of the transient. It is probably a waste of computer resources to attempt to resolve the boundary layer using the boundary layer hypothesis in this situation. However, when modeling a passive condenser system, or a thermosyphon at the bottom of the wall, the boundary layer hypothesis may be useful. It may be possible to alter the noding strategy of the boundary layer hypothesis to effectively resolve the boundary layer adjacent to the thermosyphon surfaces. Resolving velocities near these surfaces may increase the ability of the GOTHIC code to predict the natural circulation within the larger atmosphere which is induced by condensation occurring at the surfaces.

Discussion would not be complete without drawing attention to the drawbacks of the boundary layer hypothesis. Implementing the hypothesis requires that additional computational cells be used in a GOTHIC simulation. This increases the run time of the simulation. Also, the vast difference in size between the bulk cells and those employed near the condensing surface results in numerical stability difficulties. These difficulties are overcome by using very small time steps, which also increase the time to complete a simulation. Choosing the width of the near-wall cells to some extent requires knowledge of the temperatures of the wall and atmosphere during the
simulation. Luckily the width of a turbulent boundary layer predicted by the integral method does not vary significantly with temperature. Choosing an average bulk temperature which is expected to be occur and an average wall temperature that is expected are sufficient to choose the initial cell sizes. After a first attempt at the simulation is completed, the widths of the near-wall cells can be adjusted based on observed conditions and the simulation may be repeated. Adding this “fine-tuning” phase to the simulation work also increases the time to complete a given simulation. However, the increase in reliability of the results should more than outweigh the added computational time required. A flowchart for choosing near-wall cell sizes is shown in Figure 4-11.

Figure 4-11: Flowchart for implementing the boundary layer hypothesis

4.5.2. Proposed design for an appropriate benchmark experiment

Locating experimental data that would be useful in benchmarking the boundary layer hypothesis proved to be a difficult task as discussed in section 4.4. Currently, the most appropriate experimental data for this purpose is that from the Westinghouse Large Scale Test [Kennedy, 1996]. However, the useful data is proprietary and has not been released into the open literature. As an alternative, a simple, small scale test may be carried out at the university level. The considerations for such an experiment are presented here.

An experiment which will produce data applicable for benchmarking the boundary layer hypothesis is one which exhibits the same characteristics as the idealized test case shown in Figure 4-7. The experiment should have a relatively large volume-to-surface ratio to assure that
the entire volume is not influenced by the condensation process at the wall (i.e., bulk conditions are not directly tied to those at the wall). Second, the test vessel should be sufficiently tall to assure that a turbulent boundary layer develops. A vessel which is 3 to 4 meters in height should be sufficient. Third, the experiment should start with a quiescent atmosphere, followed by a rapid blowdown phase in which the pressure is increased and the atmosphere is thoroughly mixed. This should be followed by a phase in which either a slow cooldown (no steam injection) is allowed to proceed, or a case where a steam plume is injected to maintain a high pressure and allow development of steady-state conditions. At steady-state, the rate of steam injection exactly equals the rate of condensation, and can be used to determine the total heat being removed from the vessel. To determine the effect that light gas has on the final state of the system, helium or hydrogen should be injected in controlled amounts for several tests. The test with light gases can then be compared direction to those for similar conditions with steam-air only. Finally, the test must be adequately instrumented to determine the following properties:

- total pressure,
- bulk temperature as a function of elevation,
- bulk steam fraction as a function of elevation,
- light gas fraction as a function of elevation,
- near-wall temperature and steam fraction as a function of elevation,
- near-wall velocity at several elevations.

With data from an experiment similar to that described above, the modified GOTHIC code which employs the boundary layer hypothesis can be adequately verified.
5. CONCLUSIONS AND FUTURE WORK

The main focus of this thesis is to advance the analysis techniques which are used to evaluate and predict the performance of passive nuclear reactor containment systems. The current analysis techniques rely heavily on computerized tools to simulate phenomena such as circulation and condensation inside the containment vessel. The analyst has benefited from advances in computer speed in recent years, making detailed, computationally intensive, simulations possible. This increased level of detail allows the modeler to resolve small changes in buoyancy or mass concentration within the containment structure. This resolution is necessary for predicting the performance of passive containment systems since most passive systems rely on buoyancy differences or other small gradients to provide the driving force for operation. However, greater detail is not the only advance needed to predict passive system performance. The models which are implemented in the computational tools must be used in a manner which is consistent with their derivation. Choosing the correct phenomenological models and properly implementing them, using the appropriate level of resolution, is the key focus of this project.

5.1 Physical Phenomena in Containment Analysis

Condensation is the primary means of removing heat and limiting the pressure increase following a loss of coolant accident (LOCA) inside any nuclear reactor containment vessel. Modeling condensation on surfaces and in passive systems is not always a straightforward task. One main complication arises immediately, that of a noncondensable gas. A noncondensable gas acts to severely hinder the condensation process. Whereas condensation of pure steam is generally limited by the resistance to heat transfer of the condensate film, condensation in the presence of a noncondensable gas is diffusion limited. While the steam/gas mixture moves toward the cool surface, only the steam changes phase to liquid, leaving the noncondensable gas to collect at the interface. This gas buildup forms a diffusion boundary layer. In order for the steam to condense, it must first diffuse through this noncondensable boundary layer, causing a decrease in the condensation rate. Because the noncondensable gas builds up at the interface, a very small concentration of noncondensable gas in the bulk atmosphere can cause a severe decrease in condensation rate.

Figure 5-1 illustrates the situation for a flat vertical wall. At the outer limits of the boundary layer, the partial pressures of steam and air are in equilibrium with the local atmospheric conditions. As one moves through the boundary layer toward the condensate film, the steam partial pressure decreases while the air partial pressure increases. At steady state, the partial pressure of air at the interface reaches an equilibrium condition where the amount of air being carried to the interface by the incoming steam-air mixture exactly equals the amount of air diffusing away. The condensation rate is limited by the amount of steam that can diffuse or convect through the air layer. Steam diffusion is driven by the steam partial pressure gradient between the bulk conditions and the interface, whereas steam convection is a result of fluid motion within the boundary layer. A suitable condensation model which represents these phenomena must be employed to accurately predict the condensation rate on large surfaces inside
the containment. Choosing such a model was the basis for the condensation literature review which is discussed in chapter 2.

![Condensation in the presence of air on a vertical wall.](Adapted from Collier, 1981.)

The GOTHIC computer code was chosen to complete the studies in this thesis because it is capable of predicting the complex interaction between condensation and natural convection. However, even though the code can predict these fundamental phenomena, it is not ideally suited for predicting stratification in passively cooled containment systems. This shortcoming is a result of the code utilizing large finite-volumes in the computational mesh. These large volumes do not allow the computer code to capture phenomena that occur on a much smaller scale. One such small-scale phenomenon is the cool, downward flowing, steam depleted boundary layer that develops adjacent to a vertical condensing surface. Predicting this boundary layer is essential for the analysis of advanced containment designs which have an externally cooled steel shell, such as the Westinghouse AP600. This boundary layer plays a vital role in determining whether the atmosphere will remain well mixed, or stratify, following the blowdown phase of a loss of coolant accident.

### 5.2 Condensation Model Evaluation

The following condensation models were compared during the course of this thesis:

- Uchida [Uchida, 1965]
- Kataoka [Kataoka, 1992]
- Gido & Koestel (natural convection only) [Gido & Koestel, 1983]
- Dehbi [Dehbi, 1991]
- Standard Mass Conductance [Mills, 1995]
- Diffusion Layer Model (original Peterson approach) [Peterson, 1993]
- Diffusion Layer Model (Anderson implementation) [Anderson, 1998]
- Diffusion Layer Model (present implementation)
The listed condensation models were programmed into Mathcad in a general format which allowed direct numerical comparisons to be performed for specified conditions. Great care was taken to provide consistency between the models which used variables such as heat capacity, conductivity, enthalpy, or mole fraction. The form and equations of the DLM and two other models, Uchida and Dehbi, will be summarized briefly.

These three condensation models, the DLM, Uchida, and Dehbi, were considered to be the most appropriate models to use when modeling condensation in containment analysis. Predictions from these models were compared directly to experimental data for a range of containment conditions. A discussion of this comparison follows the sensitivity analysis.

5.2.1 DLM sensitivity analysis

The Uchida and Dehbi models are purely empirical and the sensitivity to different variables is readily seen from their constituent equations. The sensitivity of the DLM to different variables is not as easily established. The DLM sensitivity to key variables was determined to justify its designation as a general model, i.e., applicable for the entire range of containment conditions. Also, the implementation details of the DLM in computer codes can vary greatly due to differences in the way in which property values are defined. Such differences exist between the current implementation of the DLM and that used by Anderson in verifying the DLM against experimental data [Anderson, 1998]. The discrepancy between the two implementation strategies also underscored the necessity of determining the sensitivity of the DLM to key parameters.

First, the sensitivity of the DLM to the exact definition of the following properties was determined: mixture specific heat, mixture conductivity, mixture viscosity, binary and mixture diffusion coefficient, average boundary layer temperature and average steam mole fraction. In addition, the sensitivity of the DLM predictions to the presence of both helium and hydrogen gas was studied. This last point is crucial for helping to justify the DLM for use in containment analysis codes. The Anderson evaluation and benchmarking of the DLM did not include studying how the DLM predictions changed when hydrogen was a component of the noncondensable gas mixture.

Hydrogen and helium sensitivity will be discussed first. Figure 5-2 shows the sensitivity of the DLM to changes in the concentration of light gas in the noncondensable mixture. The graph is for a scenario where steam has been injected into a volume which initially contained the specified noncondensable mixture at one atmosphere and 300K. The atmosphere is assumed to be saturated (i.e. \( T_{\text{bulk}} = T_{\text{sat}} \)). The graph shows the percent change in the total heat transfer coefficient caused by the light gas addition as compared to the value without the light gas present. The abscissa in Figure 5-2 is the ratio of the mole fraction of light gas to the total mole fraction of noncondensable gas. It can be seen that the DLM does predict a decrease in condensation rate with an increasing light gas content. Hydrogen is predicted to have a more pronounced affect on the heat transfer rate than helium. Above a light gas concentration of 30% in the noncondensable mix, the heat transfer is seen to decrease sharply. This rapid decrease in heat transfer is due to the decrease in the buoyancy driving force with increasing light gas content. The light gas decreases the average density of the noncondensable gas mixture, which
also decreases the difference between the molecular weights of steam and the noncondensable mixture.

Figure 5-3 shows the effect that the wall subcooling has on the heat transfer coefficient. The driving force for condensation increases as the wall temperature decreases relative to the bulk temperature. The DLM captures this physical phenomenon. The curves in Figure 5-3 show that the DLM is more sensitive to the presence of light gases when the wall subcooling is small. Even though a large degree of wall subcooling is expected in situations of high condensation rates, such as in the AP600, this will not offset the decrease in condensation caused by the presence of hydrogen. The ability of the DLM to capture this complex physical interaction bolsters the argument that it is a general model capable of capturing all relevant influences.

Figure 5-2: Sensitivity of DLM predictions to hydrogen and helium, \((T_{\text{bulk}}-T_{\text{wall}}=30\text{K})\)
Figure 5-3: Sensitivity of DLM to wall temperature for steam-air-hydrogen mixtures

Table 5-1 presents the results of the sensitivity analysis performed to determine the changes in the DLM predictions brought about by changes in the way key mixture properties are defined. The sensitivity analysis was completed by comparing the properties and the predictions from the DLM over the range of conditions encountered in most containment accident scenarios. The first column lists the mixture properties that were studied. The second column, labeled Baseline definition, contains the definitions for the properties that were determined from the literature to be correct. The baseline definitions are used throughout this work. The third column, Variation, shows the other possible definitions which have been encountered in the literature. The fourth column, Maximum change in property, shows the maximum change in the particular property that is predicted when using the specified variation definition as compared to the baseline definition. Finally, the fifth column, maximum change in HTC, shows the maximum change in the total heat transfer coefficient predicted by the DLM when the alternate property definition is used.

From Table 5-1 it is clear that there are significant differences in the mixture properties when alternate definitions for these properties are used. Most notable are the definitions for the average steam mole fraction, the specific heat and the thermal conductivity. The average steam mole fraction being evaluated here is the definition which is used to determine average properties in the boundary layer. The average steam mole fraction has such a large influence on the DLM because it impacts the evaluation of all other mixture properties. It is clear from Table 5-1 that evaluation of the average steam mole fraction is extremely important. The third variation listed for the average steam mole fraction, that of the bulk steam mole fraction, is often used when
performing a first order estimate of heat transfer. The analysis performed here clearly shows that this method of estimation will significantly over-predict condensation rates.

<table>
<thead>
<tr>
<th>Table 5-1: DLM sensitivity to changes in particular variables</th>
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<td>Prop.</td>
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<td>-------</td>
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<tr>
<td>$T_{avg}$</td>
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<tr>
<td>$X_{s,avg}$</td>
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<td>$c_{p, mix}$</td>
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<td>$\mu_{mix}$</td>
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<td>$k_{mix}$</td>
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<td>$D_{ij}$</td>
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The errors in the properties of specific heat, viscosity, and conductivity are encountered primarily when hydrogen or helium is contained in the gas mixtures. Using the incorrect definitions for these mixture properties will result in a significant over-prediction of these properties. Taken separately, the errors in each of these property definitions are seen to impact the DLM predictions only slightly. However, when all three properties (specific heat, viscosity, and thermal conductivity) are evaluated incorrectly, the impact on the DLM predictions is not insignificant (maximum change in HTC of about 7%).
The DLM is also shown to be highly sensitive to the definition of the diffusion coefficient. There is a discrepancy between the diffusion coefficient relations used in this thesis and those used by Anderson in the previous evaluation of the DLM. Because of this, a thorough investigation of diffusion coefficient modeling was undertaken. The method used in this thesis to evaluate diffusion coefficients was chosen after comparing different methods of prediction with available experimental data for the systems of steam-air, steam-helium, and steam-hydrogen.

5.2.2 Model comparison to experimental data

The discrepancy in the implementation strategy for the DLM between Anderson and the present work raises questions as to the validity of the data comparisons performed by Anderson. Therefore, the DLM (implemented using the baseline definitions of Table 5-1) was again compared to experimental data. Three sets of experimental data were used in this comparison. The first data, from the University of Wisconsin-Madison (UW) [Anderson, 1998], covers a large range of containment conditions. The UW data base comprises the largest, consistent set of experimental values for the range of conditions encountered in advanced containment analysis. The experimental facilities used to gather the data were constructed specifically to mimic the AP600 design, and were painstakingly designed to reduce the errors associated with measurement. As a result the standard deviation of the experimental data is less than 20% in almost all cases. In addition, both atmospheric and pressurized test were completed. The atmospheric tests are unique in that they encompass the conditions which are encountered in a BWR drywell following a LOCA - i.e., most of the noncondensable gases have been ejected from the atmosphere. Also, the UW experiments included tests which were performed with helium present in the atmosphere. It must be noted that the UW facilities use flat plates as condensing surfaces, and the wall temperature was significantly below 100 °C in most cases. The experiments were designed to gather data for significant natural convection driving forces - i.e. high wall subcooling.

A new data set has been developed at MIT in the last year by Liu [Liu, 1999]. The data is for condensation on the outside of a 4 cm O.D., 2.0 meter long vertical smooth tube. The tube assembly is representative of a tube in a condenser system where boiling tube-side water acts as the heat sink for shell-side steam condensation. As a result of this setup, the tube temperature is slightly higher than 100 °C. This results in a significantly lower convection driving force than was present in the UW experiments, and as such, this data represents a completely different set of physical conditions. These data were taken for steam-air and steam-air-helium mixtures at pressures above one atmosphere.

Finally the predictions of the DLM are compared to those of the Dehbi correlation, which is used here to represent comparison to the Dehbi data. Dehbi performed condensation experiments with a similar setup as the Liu data. Steam was condensed on the outside of a vertical tube. In this case, the tube temperature was held significantly below 100 °C by cooling water circulated on the inside of the tube. There are two Dehbi correlations, one for steam-air mixtures, and another for steam-air-helium mixtures at pressures between 1.5 - 4.5 atmospheres. Both are used in this evaluation.
Figure 5-4: Model comparison to UW data for air-steam, \((P = 1.0 \text{ Bar})\)

Figure 5-5: Model comparison to UW and MIT data for steam-air, \((P > 1.0 \text{ Bar})\)
Figure 5-6: Model comparison to UW and MIT data for steam-air-helium, (P > 1.0 Bar)

Figure 5-4 shows the comparison of the DLM, Dehbi, and Uchida relations to the UW steam-air data for one atmosphere. These conditions coincide with those encountered in a BWR drywell following a loss of coolant accident, i.e., most of the noncondensable gases have been ejected from the atmosphere. The figure shows that the DLM predictions agree fairly well with the data. Conversely, the Uchida and Dehbi relations tend to over-predict some of the data at the lower end of the range. This over-prediction is a result of using the relations outside the range of conditions of the original experiments. This over-prediction also highlights that using the Uchida relation for containment analysis does NOT always assure conservative results.

Figure 5-5 shows the comparison of model predictions to data from both UW and MIT for steam-air mixtures at pressurized conditions. The DLM is shown to predict heat transfer coefficients which agree well with the data of both experiments. The DLM also agrees very well with the predictions of the Dehbi relation for the conditions of the UW data which bolsters the confidence in the DLM predictions and the UW database. It is interesting to notice that the Dehbi relation does not consistently agree with the new MIT data. Recall however that the Dehbi data and the new MIT data are gathered under different conditions. In this light, the discrepancy between the Dehbi relation and the MIT data is concluded to be a result of using the Dehbi relation in another situation outside of its range of applicability. As expected, the Uchida relation is shown to consistently under-predict the data from both experiments.

Figure 5-6 shows the comparison of model predictions to data from both UW and MIT for steam-air-helium mixtures at pressurized conditions. The DLM is again shown to predict heat transfer coefficients which agree well with the data of both experiments. In fact, the agreement between
the DLM and the data is better in this case than the case without helium (Figure 5-5). The Dehbi relation for steam-air-helium predicts heat transfer coefficients which agree well with the UW data, but not with the MIT data. The discrepancy between the Dehbi relation and the MIT data is again because of using the Dehbi relations outside its range of applicability. The predictions of the Uchida relation are shown for comparison, and again under-predict the data from both experiments.

5.2.3 Condensation model selection
At the beginning of this project a thorough literature search was performed to identify candidate condensation models for use in advanced containment analyses. The three models identified as the most promising were the diffusion layer model (DLM), the Dehbi correlation, and the Uchida correlation. These three condensation models were subsequently evaluated and compared to a range of experimental data. The conclusion from this analysis was that the DLM is the best model available for predicting condensation in containment analyses.

In addition, the DLM is physically consistent with the assumed phenomena of condensation - that a boundary layer is present at the wall. The DLM is thus considered ideal for use in the GOTHIC computer code with the boundary layer hypothesis, which is discussed next.

5.3 Boundary Layer Hypothesis
The major aspiration of this thesis is to propose and justify a set of modifications for finite-volume containment analysis codes which will increase the ability of the codes to accurately predict the performance of advanced containment system which rely on natural processes for cooling and pressure control. Specifically, there are two goals which must be accomplished to realize this aspiration. These goals are:

- to accurately predict the condensation rate in a given situation,
- to capture the cool steam-depleted boundary layer flow adjacent to a vertical surface.

The first goal, predicting the correct condensation rate, is not achieved by simply choosing a condensation model which is accurate and applicable to the situation under study. The chosen condensation model must also be implemented into the code logic, and utilized by the analyst, in a manner which is consistent with the physical assumptions used to derive the model. The second goal is somewhat more challenging, as most containment analysis codes were not designed to resolve boundary layer flow. Achievement of the second goal is possible if the first goal is attacked in a particular fashion. Specifically, if the condensation model is implemented into the containment analysis code in a way that assures the use of bulk properties to determine the condensation rate while removing the heat and mass from the boundary layer region, then the code will be able to predict both the downward flowing cool boundary layer and the correct condensation rate. This section outlines the methodology employed to achieve this. The methodology developed here follows on the previous work of Gavrila [Gavrila, 1995].
5.3.1 Condensation model implementation and near-wall noding

The condensation model which is used to achieve the above stated goals must meet three criteria. First, it must be accurate for a wide range of conditions. Second, it must be consistent with the physical assumptions employed, i.e. the condensation model must be physically consistent with the assumption of a downward flowing boundary layer. And third, the condensation model must also be readily integrated into the containment analysis code. The Diffusion Layer Model (DLM) is the condensation model of choice because it meets all three criteria. The applicability of the DLM to the conditions under study was established in chapter 2. The derivation of the DLM assumes boundary layer flow, and as such makes a distinction between boundary layer, interface, and bulk properties. And finally, the form of the DLM makes it readily implemented into the GOTHIC containment code.

In order to achieve the second goal, predicting the downward flowing boundary layer, the computational mesh adjacent to the surface must be sufficiently fine to capture this phenomenon. This requires choosing computational volumes which are on the same scale as the boundary layer flow. However, most finite-volume codes calculate heat and mass transfer from the fluid to a solid surface based on the properties of the fluid in the near-wall cell. In the present case, using the properties in the near-wall cell to calculate the condensation rate will result in significant errors. The errors arise because condensation models, including the DLM, are based on bulk properties. Cell which are narrow enough to capture boundary layer flow will not contain bulk properties, but boundary layer properties. Herein lies the reason why containment codes are not well suited for capturing boundary layer flow.

The solution to this problem is straightforward in theory, but extremely complex in practice. The containment code must be modified such that bulk properties are used to calculate condensation rates even with these small near-wall cells, but the heat and mass must still removed from the near-wall cell. This in turn requires an assumption of how many cells will encompass the boundary layer. For the work completed in this thesis, two computational cells were used to resolve the boundary layer, thus the properties in the cell twice removed from the wall are assumed to represent bulk properties. Figure 5-7 shows how this was implemented logically.

![Figure 5-7: Details of the logic of the boundary layer hypothesis](image)
To estimate the total width of the boundary layer, the integral method for turbulent natural convection was employed. Chapter 4 contains details on how to determine the near-wall cell widths, and justification for this specification. The justification draws on the results from the CFD analysis which was carried out and discussed in chapter 3.

5.4 Illustrative Test Case

An idealized test case has been devised and is shown schematically in Figure 5-8. This case is representative of the situation which exists in advanced containment designs. The case consists of a large volume with a cooled wall along one side, which is initially filled with air at one atmosphere. The test case scenario is that steam is injected into the volume in a violent manner, causing a rapid increase in pressure and producing a well-mixed atmosphere. Subsequent to reaching the specified pressure, the steam release is reduced to a plume. The plume is released at 11.5 meters above the floor to establish a situation where stratification should develop.

![Figure 5-8: Test case to illustrate the utility of the boundary layer hypothesis](image)

The test case was simulated using the GOTHIC computer code. Two variations were used. The first run consisted of simply noding the volume with equally spaced nodes. No specialized noding was employed at the cold wall, and the normal heat transfer logic was used. In the second case, the boundary layer hypothesis was employed. A series of narrow near-wall nodes were used along with the modified heat transfer logic in GOTHIC. The results are shown in Figure 5-9. For the “normal” run, the atmosphere is predicted to be relatively uniform and well mixed. There is a slight decrease in steam content at the very bottom of the volume, but the decrease is not significant. The results for the case which employs the boundary layer hypothesis is strikingly different. A very clear stratification layer develops below the plume elevation. The steam content decreases steadily toward the bottom of the volume. As a result of this stratification, the steady-state condensation rate is 25% above that predicted in the run without stratification.
5.5 Conclusions and Future Work

First, many of the condensation models in use today are not well suited for the analysis of advanced containment designs. Most models perform well within the range of conditions that the particular models were derived for, but significantly under-predict or over-predict the condensation rate for situations outside this range. The Diffusion Layer Model (DLM) was determined to be more general and accurate than all of the other models studied, and thus applicable to a much wider range of conditions. This aspect of the DLM was shown in chapter 2 by comparing DLM predictions to experimental data that span a wide range of possible containment conditions.

Second, the derivation of the DLM is physically consistent with the assumption of a downward flowing boundary layer. Because of this, the DLM is well suited for use in the GOTHIC computer code as an integral part of the boundary layer hypothesis. The boundary layer hypothesis was the subject of chapter 4, and is essentially a way of modifying a computer code to improve the ability of the code to:

- correctly predict the condensation rate,
- capture downward flowing cool air adjacent to a vertical surface.

The utility of the boundary layer hypothesis was illustrated in Figure 5-9. Two GOTHIC runs were completed for a scenario that is representative of the situation encountered in advanced containment designs, i.e., a large enclosed volume with a high, cool, vertical surface. The first
run was completed employing the normal noding and heat transfer logic available in GOTHIC. The second run was completed using the boundary layer hypothesis to model condensation at the wall. A well mixed atmosphere was predicted in the first run, whereas a stratified atmosphere was predicted in the second run. This result proves the utility of the hypothesis by showing concretely that the GOTHIC code can be successfully modified to improve the ability of the code to predict this type of phenomenon.

The concepts which are presented and justified in this thesis are:

- the DLM condensation model is accurate and applicable over a range of conditions that may be encountered in the analysis of an advanced containment, the range of conditions for which the DLM was compared to data are listed in Table 5-2,
- the implementation details of the DLM can significantly impact the quality of model predictions,
- the DLM is physically consistent with the assumptions used in the development of the boundary layer hypothesis, and therefore well suited to be used as an integral part of the hypothesis,
- the logic and methodology of the GOTHIC containment analysis code is amenable to modification for incorporation of the boundary layer hypothesis and the DLM
- the utility of the boundary layer hypothesis is clearly demonstrated for a situation which is representative of conditions encountered in an advanced containment.

Table 5-2: Range of conditions for DLM comparison to experimental data

<table>
<thead>
<tr>
<th>Variable</th>
<th>Minimum</th>
<th>Maximum</th>
</tr>
</thead>
<tbody>
<tr>
<td>Pressure (Bar)</td>
<td>1</td>
<td>3.1</td>
</tr>
<tr>
<td>$T_{wall}$ (K)</td>
<td>308</td>
<td>370</td>
</tr>
<tr>
<td>$T_{bulk}$ (K)</td>
<td>358</td>
<td>391</td>
</tr>
<tr>
<td>$X_s$</td>
<td>0.12</td>
<td>0.74</td>
</tr>
<tr>
<td>$X_{He}/X_{nc}$</td>
<td>0.00</td>
<td>0.30</td>
</tr>
</tbody>
</table>

While the concepts listed above are presented and defended in this thesis, there are several practical problems which are encountered during the actual implementation of the boundary layer hypothesis into the GOTHIC code. Before the boundary layer hypothesis is utilized for actual containment analyses, these problems should be addressed. Most of the problems arise from errors which exist in the GOTHIC code or situations where the assumptions of the boundary layer hypothesis are at odds with those used in the GOTHIC code. A list of specific concerns is given below:

- friction along the surfaces of GOTHIC is modeled in an inconsistent manner, i.e., as a wall is covered in liquid, the shear between the wall and the vapor is ramped to zero, but shear between the liquid and the vapor is not ramped up at the same time, this results in “frictionless” flow in the near-wall cell and a significantly higher velocity than is expected in reality,
friction is calculated based on flow inside a smooth tube with a Reynolds number calculated using the hydraulic diameter of the cell - friction on walls should be changed to be consistent with flow along a plate, and also to incorporate the influence of wall roughness which will be encountered in real situations, computer run times are excessively long, the time step is extremely small because of the stability concerns tied to the mass transfer rates at each time step, small near-wall computational cells becomes depleted of steam very quickly which results in this problem, it may be possible to address this concern in the equation solvers of the code.

Finally, to evaluate the utility of the boundary layer hypothesis for use in actual simulations, the GOTHIC code should be used to simulate experimental data where accurate predictions require the code to predict boundary layer flow. A search for available experimental data identified the Westinghouse Large Scale Test (LST) as a candidate. However, there are several problems associated with this data. The test was constructed with large gutters to collect condensate around the perimeter of the test vessel. These gutters introduce significant complications into the development of an adequate noding scheme. Also, most of the data from these tests are proprietary to Westinghouse and have not been released into the free literature.

As an alternative, a simple, small scale test may be carried out at the university level. The best experiment to test the applicability of the boundary layer hypothesis is one which exhibits the same characteristics as the idealized test case shown in Figure 5-8. The experiment should have a relatively large volume-to-surface ratio to assure that the entire volume is not influenced by the condensation process at the wall (i.e., bulk conditions are not directly tied to those at the wall). Second, the test vessel should be sufficiently tall to assure that a turbulent boundary layer develops. A vessel which is 3 to 4 meters in height should be sufficient. Third, the experiment should start with a quiescent atmosphere, followed by a rapid blowdown phase in which the pressure is increased and the atmosphere is thoroughly mixed. This should be followed by a phase in which either a slow cooldown (no steam injection) is allowed to proceed, or a case where a steam plume is injected to maintain a high pressure and allow development of steady-state conditions. At steady-state, the rate of steam injection exactly equals the rate of condensation, and can be used to determine the total heat being removed from the vessel. Several tests should be undertaken where a controlled amount of light gas is injected into the test vessel. The data from runs with light gas addition should then be compared to those for steam-air mixture only in order to determine the influence of the light gas on the stratification layer at the bottom of the vessel. Finally, the test must be adequately instrumented to determine the following properties:

- total pressure,
- bulk temperature as a function of elevation,
- bulk steam fraction as a function of elevation,
- near-wall temperature and steam fraction as a function of elevation,
- near-wall velocity at several elevations.

With data from an experiment similar to that described above, the modified GOTHIC code which employs the boundary layer hypothesis can be adequately benchmarked.
REFERENCES


L. Wolf, University of Maryland College Park, Private communication, January 29, 1999.

Appendix

A. LITERATURE REVIEW OF CONDENSATION MODELS

This appendix gives an overview of selected publications dealing with condensation phenomena, specifically in the presence of a noncondensable gas, that are applicable to the discussions in this thesis. The sequence in which the models are presented follows generally from simplest to most complex. The section is also separated into two sub-sections, dealing with vertical wall and inside tube condensation. The reason for this separation is that the advances in condensation have historically been pursued along one of two separate tracks: internal (inside tube) condensation, and external condensation (flat plates or outside tubes). In the present context, external condensation occurs on large vertical or horizontal containment surfaces while internal condensation occurs inside condenser tubes.

A.1 Condensation on Vertical Surfaces

A.1.1 Nusselt (1916)

The two types of condensation encountered are film-wise and drop-wise. Film-wise condensation results in a condensate film which forms between the vapor and the cooled surface, whereas in drop-wise condensation the condensate coalesces into droplets without forming a complete film over the surface. The first major contribution in the area of film-wise condensation, which is the type most often encountered, was made by Nusselt in 1916. The major advances in pure steam condensation since the original Nusselt paper are reviewed by Rose [Rose, 1988]. Rose discusses condensation on both flat plates and on the outside of tubes, and his work was used as the primary reference for the following discussion.

The Nusselt analysis gives an average heat transfer coefficient for a vertical flat plate of height \( L \) as:

\[
\overline{h} = \frac{k_t}{\delta} = 0.943 \left[ \frac{\rho_t (\rho_t - \rho_v) g h_f k_i^3}{\mu_i L (T_r - T_w)} \right]^{1/4} \tag{A.1}
\]

where the overbar signifies a spatial average. Equation A.1 assumes a parabolic (downward flowing) velocity profile and a linear temperature profile across the condensate film. This theory ignores inertia and vapor shear stress, both of which hinder heat transfer. However, convection and subcooling in the condensate film are also ignored, both of which enhance heat transfer. (The term “Nusselt assumptions” generally refers to neglecting fluid acceleration and heat convection.) These two errors tend to cancel, which allows the equation to predict heat transfer in a natural circulation environment quite well for many conditions [Rose, 1988]. Not using the Nusselt assumptions and including the effects of liquid subcooling can be taken into account by replacing the heat of vaporization \( h_f \) by the term [Mills, 1995]
Several experimental and analytical studies have been carried out which attempt to more accurately predict the pure steam condensation rate. However, for the present application of nuclear containment analysis, this is not important relative to the prediction of condensation degradation due to the presence of a noncondensable gas.

A.1.2 Uchida (1965)

For many years the experimental work of Uchida and Tagami has been used to predict the condensation inside a nuclear reactor containment building following a loss of coolant accident [Uchida, 1965; Tagami, 1965]. These experiments were performed in the same experimental apparatus and studied condensation in the presence of a noncondensable gas onto a vertical cylinder 64 cm in circumference and either 30 cm (Uchida & Tagami) or 90 cm (Tagami) high. The noncondensable gases studied were air, nitrogen, and argon. The experiments took place in a constant volume enclosure (~45 m³), with the initial pressure of noncondensable gas being approximately one atmosphere, and total experimental pressures between 0.1 to 0.5 MPa.

Uchida performed steady state experiments. Steam was supplied at an increasing rate in order to produce a pressure rise, while the plate temperature was held constant at ~49°C. The system was then allowed to come to equilibrium, where the heat addition from the steam balanced the removal by condensation. The inlet and outlet temperatures of the condensing plate cooling water, condensing plate surface temperature, and the bulk gas/vapor mixture temperature were measured to determine the average heat flux, and thus the heat transfer coefficient to the condensing surface. There is no data reported on atmospheric vapor velocity or circulation rate for the experiments. The Uchida steady state data were correlated as a function of steam and gas mass ratio. The average heat transfer coefficient for steam-air mixtures is given by¹:

\[ h' = h_{kr} + \left( 0.683 - \frac{0.228}{Pr_t} \right) \frac{c_p}{(T_{fb}^{sat} - T_w)} \]  

(A.2)

\[ h = 379 \left( \frac{m_g}{m_s} \right)^{-0.707} \text{ (W/m}^2 \text{K)} \]  

(A.3)

for \( m_g / m_s < 20 \).

It had been generally accepted that the Uchida correlation was conservative in most cases because it ignores any contribution from forced convection. However, Peterson has shown that this correlation will over-predict the heat transfer rate when the partial pressure of noncondensable gas is significantly less than one atmosphere, and under-predict the heat transfer rate when the partial pressure of noncondensable gas is significantly greater than one atmosphere [Peterson, 1996]. (See the discussion in section A.1.7). Also, even though the Uchida correlation seems to represent a natural convection state due to its lack of a velocity term, Corradini points out that the experiments may not have been performed in the natural circulation state.

¹ The Uchida and Tagami test description and correlating equations are taken from [Corradini, 1984].
regime due to the steam injection into the volume which must have caused at least minimal mixing\(^2\) [Corradini, 1984].

**A.1.3 Tagami (1965)**

Tagami performed steady state and transient experiments in the same apparatus as Uchida. The steady state experiments followed the same procedure as described for the Uchida tests. The transient experiments were similar to the steady state experiments except that measurements were taken starting when the energy addition to the volume commenced. Measurements were taken of the heat flux on the vertical surface, condensing surface temperature, bulk temperature, total energy addition, and blowdown rate. No measurements of circulation rate or total containment pressure were taken, thus the thermodynamic state of the atmosphere can not be determined. The Tagami steady state data were correlated as:

\[
\bar{h}^{\text{ss}} = 11.4 + 284(m_s/m_g) \quad (\text{W} / \text{m}^2 \text{K})
\]  

for \(0 < (m_s/m_g) < 1.4\)

while the Tagami transient data were correlated as:

\[
\bar{h}^{\text{trans}} = h^{\text{max}} (t / t_A)^{1/2} \quad \text{for} \quad t \leq t_A
\]  

(A.5a)

\[
\bar{h}^{\text{trans}} = \bar{h}^{\text{ss}} + (h^{\text{max}} - \bar{h}^{\text{ss}}) \exp[-0.5(t-t_A)] \quad \text{for} \quad t > t_A
\]  

(A.5b)

where

\[
h^{\text{max}} = 426\left(\frac{E_A}{t_A V_C}\right)^{0.6} \quad (\text{W} / \text{m}^2 \text{K})
\]  

(A.5c)

where \(E_A\) is the total energy added in Btu, \(t_A\) is the total time for the energy addition, and \(V_C\) is the total containment volume in \(\text{ft}^3\). This approach, which attempts to correlate heat transfer using bulk properties is not applicable to a distributed parameter calculation. These experiments can provide some data for comparison to correlations which predict average heat transfer coefficients, but offer little insight into local heat flux calculations.

**A.1.4 Gido and Koestel (1983)**

Gido and Koestel published a paper in 1983 which was critical of using the Uchida and Tagami curve fits for predicting containment condensation [Gido & Koestel, 1983]. Gido and Koestel point out that maximum condensation rates measured in the Carolinas Virginia Tube Reactor (CVTR) containment tests and in the Battelle Frankfurt large scale test setup are appreciably higher than those predicted by the Uchida and Tagami correlations. The relatively small size of the Uchida test assembly is suspected as a primary cause for this discrepancy. Gido and Koestel point out that containment surfaces are often between 10 and 100 meters in height, and have a

\(^2\) Corradini developed a model for forced convection and found that an imposed velocity of 2 m/s gave good predictions of the Uchida and Tagami data [Corradini, 1984].
rough surface. They predict that the condensate film on these surfaces is inherently wavy and will become turbulent within approximately 2 meters of the top of a large wall, thus aiding a transition to turbulence in the gas/vapor boundary layer adjacent to the wall. The argument is then made that heat transfer now becomes a matter of turbulent diffusion of steam through the gas boundary layer. Since the Uchida and Tagami tests were performed on a test section which was less than one meter in height, the transition to turbulence is not observed. Gido and Koestel then derive a heat transfer coefficient based on the triple Reynolds’ analogy of momentum, mass and energy transfer between vapor and liquid at a wavy liquid boundary - both for a turbulent vapor boundary layer (large surfaces) and a laminar vapor boundary layer (small surfaces). The resulting equation for small surfaces is compared to data from the Uchida and Tagami tests, while the large surface equation is compared to data from the CVTR and Battelle tests. In addition, the Gido and Koestel relations are derived for a natural convection case and a forced convection case (the maximum prediction from the two cases is used to determine the heat transfer coefficient in actual scenarios). The average heat transfer coefficients derived for natural convection and forced convection on large surfaces take the form:

\[ \bar{h}_{NC}^{NC} = 5.25 \left[ \left( \frac{u_f}{u_w} \right)^2 \frac{1}{Sc_i} \frac{u_w}{u_b} \frac{(\rho_{s,b} - \rho_{s,i})}{\rho_l} \right]^{12/7} \frac{\rho_l h_{fg}}{T_{b}^{sat} - T_w} \left[ \frac{\rho_l g^4 L^5}{\mu_l} \right]^{11/7} \]  

(A.6)

\[ \bar{h}_{FC}^{FC} = \frac{\left( \frac{u_f}{u_w} \right)^2 \frac{u_b}{u_b} \frac{C^* h_{fg} (\rho_{s,b} - \rho_{s,i})}{1 - \frac{u_w}{u_b} \left( T_{b}^{sat} - T_w \right)} }{Sc_i} \]  

(A.7)

where³

\[ \frac{u_f}{u_w} = \frac{1}{7.0} \quad \text{ratio of the interface friction velocity to the wave crest velocity} \]

\[ \frac{u_w}{u_b} = 1.0 \quad \text{ratio of the wave crest velocity to the mean condensate film velocity} \]

\[ \frac{u_f}{u_b} = 0.05 \quad \text{ratio of the interface friction velocity to the bulk gas velocity} \]

\[ \frac{u_w}{u_b} = 0.425 \quad \text{ratio of the wave crest velocity to the bulk gas velocity} \]

\[ Sc_i = 0.5 \quad \text{turbulent Schmidt number, ratio of momentum to mass diffusivity} \]

The term \( C^* \), called the blowing or suction factor, accounts for the deviation from the heat/mass transfer analogy for high condensation or evaporation rates. (Blowing corresponds to

³ The values listed here for the ratios are those used in the GOTHIC computer code. These values are generally midpoints of the small ranges given in the original reference [Gido & Koestel, 1983].
evaporation, while suction corresponds to condensation.) Blowing factors are often calculated from the following relations:

\[ C^* = \frac{\log(1 + \lambda^*)}{\lambda^*} \quad (A.8) \]

\[ \lambda^* = \frac{X_{s,b} - X_{s,d}}{X_{s,d} - 1} = \frac{P_{s,b} - P_{s,i}}{P_{s,i} - P_T} \quad (A.9) \]

The form of the Gido & Koestel correlation requires velocity ratios which are not always readily available in a computer code simulation. Most of the ratios defined above must be estimated based on prior knowledge about the assumed flow situation. The authors provide arguments in their paper for determining these ratios for the experiments they analyzed. Gido & Koestel report that their model is in good agreement with the Carolinas Virginia Tube Reactor tests and the Battelle Frankfurt large scale tests, which they investigated. The authors did not define a range of applicability for their relations, thus it is assumed that the relations derived are valid for all conditions that could exist in a containment following a loss of coolant accident; namely a saturated atmosphere with a total pressure between 0.1 and 0.5 MPa, and near wall velocities less than 5 m/s. The Gido & Koestel correlation is available in the GOTHIC computer code as one option for modeling condensation heat transfer on surfaces.

### A.1.5 Corradini (1984-1990)

Corradini developed a model to predict heat transfer between steam/air atmospheres and cool walls which considers both sensible and latent heat transfer [Corradini, 1984]. The total heat transfer coefficient is assumed to consist of two resistances in series: that due to energy transfer (diffusion) through the gas/vapor boundary layer, and that due to energy transfer through the condensate film.

\[ \frac{1}{h_T} = \frac{1}{h_{\text{gas}}} + \frac{1}{h_{\text{film}}} \quad (A.10) \]

The heat transfer coefficient through the gas/steam mixture accounts for two energy transfer processes: convection and condensation. Radiation is not considered by Corradini, but in principle it can be easily included. Radiation is only important when modeling hydrogen combustion or when the steam mixture is highly superheated\(^4\).

\[ h_{\text{gas}} = h_{\text{conv}} + h_{\text{cond}} + h_{\text{rad}} \quad (A.11) \]

The original Corradini model for the total heat transfer coefficient was derived for both forced and natural convection, and is based on several key assumptions. The condensation film is represented using a Nusselt (laminar) representation and the film interface is assumed to be

\(^4\) Radiative heat transfer between the fluid in the near wall-cell and the wall is modeled in the standard wall/volume energy interactions within the GOTHIC computer code. See George et al., 1994.
smooth. The argument was made that the film resistance is small when compared to the resistance introduced by the noncondensable gas, thus this simple film representation is justified. The Reynolds and Colburn analogies were then used to derive the condensation and convection heat transfer coefficients.

Kim & Corradini later revised the model to include a turbulent condensate film, a wavy film interface, and replaced the Colburn analogy for mass transfer with a model containing empirical constants [Kim & Corradini, 1990]. The new assumption is that a wavy (or turbulent) condensate film helps to promote turbulence in the vapor boundary layer. Kim & Corradini also argue that the film should be modeled more accurately than a simple Nusselt model since low noncondensable gas concentrations or high vapor velocities could raise the gas heat transfer coefficient $h_{gas}$ sufficiently to be comparable in magnitude to that for the film. The original Corradini model and the revised Kim and Corradini model include terms which account for boundary layer thinning (and higher heat transfer coefficients) due to suction at high mass transfer rates.

The Corradini and Kim & Corradini models were compared to several experiments with very good results for average heat transfer rates$^5$. Corradini found that his natural convection relation under-predicted the Uchida data; however his forced convection model with an imposed velocity of 2 m/s matched the Uchida data well. Corradini also states that if the length of the surfaces is appropriate in scale to those found inside a containment (L > 5 m), the natural convection heat transfer coefficient becomes equal in magnitude to the forced convection coefficient for a velocity of 2 m/s. The major finding which is applicable to the present study is that in the absence of large imposed velocities (which typically occur only during the actual blowdown), the natural convection regime controls the condensation and other heat transfer mechanisms inside the containment. (Low near-wall velocities were seen by Gavrilas who calculated them to be in the range of 2 m/s during her numerical analyses of the AP600 containment system [Gavrilas, 1997]. That the natural convection regime controls the heat transfer in a containment system was also observed during the AP600 Large Scale Test program (see section A.1.9) [Sha, 1997].)

The equations shown below are local heat transfer coefficients for the Kim & Corradini model for a turbulent steam/gas vapor layer and either a smooth or wavy condensate film. The Nusselt and Sherwood numbers are defined differently depending on whether the condensate film is smooth or wavy. The original Corradini model is very similar to the smooth film formulation shown below.

$$h_{conv}^{FC} = C_1 \frac{k_m}{x} \text{Nu}$$
$$\text{Nu}_{conv}^{FC} = \frac{f_{sf} \text{Re}_{x,m} \text{Pr}_m}{2 \text{Pr}_r}$$
$$h_{cond}^{FC} = C_2 \frac{m^* h_{fg}}{(T_b - T_i)}$$
$$\text{Nu}_{cond}^{FC} = \frac{f_{sf} \text{Re}_{x,m} \text{Pr}_m}{2 \text{Pr}_r + \left(\frac{f_{sf}}{2}\right) / St_k}$$

$^5$ Some of these experiments were performed specifically for comparison to this model, see (Kim, 1988).
The heat transfer coefficients can be integrated over the surface length to give the average heat transfer coefficient. In addition, iterations must be performed on the interface temperature in order to equate the condensation and convection heat flux with that through the condensate film. The iteration time required may be prohibitive in a model with hundreds of individual wall condensation sites. The effects of a wavy film interface is included by using an appropriate film tracking model to compute the average film thickness $\delta$, which is used to estimate the film roughness and hence the friction factor between the film and the boundary layer. Finally, suction factors are applied to the friction factor, heat transfer coefficient, and mass transfer coefficient to correct for a high mass transfer rate. The suction factors are defined in equations A.12q,r,s,t.

Since the model is primarily theoretical in nature, the range of applicability is not limited to specific experimental conditions, with the possible exception of equations A.18 and A.19.

While the Corradini models are of the proper form to be used to estimate local heat and mass transfer coefficients, their use in containment analysis computer codes requires more calculations than a simple correlation such as that of Uchida. The major drawbacks of the Corradini models are the complexity and the number of iterations that may be required at each time step in order to predict the correct interface temperature. The Corradini models have been compared to the Peterson model (section A.1.7) and tested against experimental data in recent years. These comparisons are discussed in section A.1.8.

**A.1.6 Dehbi (1991)**

Dehbi performed numerical and experimental studies in an attempt to predict turbulent boundary layer condensation [Dehbi, 1991]. He draws attention to the fact that in general the models based on the heat/mass transfer analogy consistently under-predict the rate of turbulent natural convection condensation. The heat/mass transfer analogy formulation assumes that the boundary layer consists of a thin laminar sublayer and a turbulent core. When mass transfer occurs, the
suction reduces the thickness of the laminar sublayer thereby causing an increase in heat transfer. This enhancement is usually included in the model by the use of a suction factor multiplier on the Sherwood number. Dehbi notes that even with this correction, the historical approach to condensation modeling still produces overly conservative results. In his modeling work, Dehbi assumes that the laminar sublayer disappears completely as a result of mass transfer suction and the turbulent gas/vapor boundary layer interacts directly with the condensate film.

The numerical scheme is derived using the boundary layer mass, momentum, energy, and species conservation equations, a turbulence model for the gas/vapor boundary layer, and the simple Nusselt representation for the condensate film. The Nusselt model is chosen for the condensate film following the belief that a laminar film will prevail in most practical situations. A one-equation turbulence model (TKE model) was used to model the turbulent core. The Prandtl mixing length model was considered but deemed more applicable for forced convection boundary layers. Similarly, the $K-e$ model was considered, but the large number of empirical constants required led to the selection of the TKE model. Dehbi cites a study that states the TKE formulation gives good results for pure natural convection experimental data [Mason & Seban, 1974].

Dehbi performed a set of experiments for external condensation. The apparatus consisted of a 3.8 cm diameter, 3.5 meter vertical cylinder suspended in a pressure vessel. Cooling water flowed on the inside of the cylinder while a steam and noncondensable gas mixture was maintained outside the cylinder. Steam-air mixtures were studied for pressures of 1.5, 3.0 and 4.5 atmospheres with air mass fractions ranging from 0.25 to 0.9. Steam-air-helium mixtures were studied for pressure of 2.7 to 3.5 atmospheres and mass fractions of helium at 0.017, 0.047, and 0.083. Local heat flux data were gathered at six different axial locations, however problems with the cooling water flow rate and flow regime made local data suspect, thus all experimental results were taken on an average basis. The proposed vertical flat plate heat transfer correlation for air-steam mixtures is:

$$\overline{h} = \frac{L^{0.05} \left[ (3.7 + 28.7P) - (2438 + 458.3P) \log_{10}(m_{air,b}) \right]}{(T_b - T_w)^{0.25}}$$

(A.27)

for $0.25 \leq m_a \leq 0.9$

$1.5 \leq P \leq 4.5 \text{atm}$

where $L$ is the length of the condensing section in meters, $P$ is the total pressure in atmospheres, and $m_{e,b}$ is the mass fraction of air in the bulk mixture. Dehbi’s numerical model matched his experimental data quite well. He then used the numerical model to perform several parametric studies to determine the effects of condensing surface length, wall subcooling, total gas pressure, and surface curvature on the heat transfer coefficient. The heat transfer coefficient was shown to decrease with length for a short distance (less than 1 meter), then remain relatively constant or increase slightly over the remaining condensing surface. The effects of length are most notable for a low concentration of noncondensable gases. This is attributed to the resistance of the condensate film which increases as one proceeds down the length of the condensing section.
However, the effect of the condensate film thickness increase is small compared to the resistance of the boundary layer such that the condensate film soon becomes a negligible resistance and the boundary layer becomes dominant. Because the heat transfer coefficient remains relatively constant over most of the condensing section, one can conclude that the height of surface does not play a strong role in natural convection condensation.

For a given bulk temperature, an increase in wall subcooling (decrease in wall temperature) causes a decrease in the heat transfer coefficient. The effect is more pronounced for low concentrations of noncondensable gases, following the correct trend for pure steam condensation. The heat transfer coefficient was shown to increase with increasing pressure for the same air mass fraction. The effect of pressure decreases at higher concentrations of noncondensable gas. The effect of curvature was shown to be more pronounced for higher noncondensable mass fractions, but there was very little effect for a radius of curvature greater than 10 cm. For pure steam, curvature has no effect as long as the radius of curvature is larger than the condensate film thickness. Finally Dehbi compared his numerical condensation model to a curve fit for the Tagami data. The model shows reasonably good agreement with the Tagami data.

A.1.7 Peterson (1993-1996)

Several models have been devised and experimental programs carried out at the University of California Berkeley in an attempt to produce a theoretical basis for describing noncondensable gas effects on condensation. Peterson developed a turbulent diffusion model for natural convection flow which allows the calculation of local heat transfer coefficients for the condensation and convection processes in terms of saturation temperature differences [Peterson, 1993]. These coefficients are then used in conjunction with the condensate film heat transfer coefficient from a relevant film model to predict total heat transfer in a method similar to that described in the Corradini model (A.1.6).

The condensation heat transfer coefficient is based on the definition of a condensation thermal conductivity $k_{\text{cond}}$ which allows smooth integration of the heat/mass transfer analogy into the formulation. The expression for $k_{\text{cond}}$ is

$$
k_{\text{cond}} = \frac{1}{\phi T_{\text{avg}}} \left( \frac{h_f s P M_s D}{R^2 T^2} \right) \tag{A.28}
$$

where

$$
T_{\text{avg}} = \frac{T_{i_{\text{sat}}} + T_{b_{\text{sat}}}}{2}. \tag{A.29}
$$

$k_{\text{cond}}$ reduces to zero when the noncondensable gas concentration is extremely high, which leads to domination by sensible heat transfer, as one would expect. The expression for $k_{\text{cond}}$ also

---

6 As the wall temperature decreases, the saturation pressure at the wall decreases, but at a less-than-linear rate as compared to temperature. The condensation heat flux is controlled by diffusion across the boundary layer, which in turn is governed by the difference in steam saturation pressures. As wall subcooling increases, the condensation heat flux increases, but again at a less-than-linear rate as compared to temperature, thus the heat transfer coefficient must decrease with wall subcooling (for a fixed bulk temperature). See Chapter 2 for a discussion of this process.
approaches infinity when noncondensable gas concentrations are small, thus providing a smooth transition to a pure steam model. In the special case that the bulk steam/gas mixture is saturated, the approach can eliminate iteration on the condensate film interface temperature and instead require iteration on the interface gas concentration. This formulation supposedly requires fewer iterations than a normal mass conductance model (e.g. Corradini model) because the model is formulated in terms of saturation temperatures and the log mean of the steam/air mole fractions in the bulk and at the interface as opposed to simply the difference between them. The log mean mole fraction of a species is defined as:

\[ X_{\text{avg}} = \frac{X_b - X_i}{\ln(X_b / X_i)} \]  
(A.30)

The gas/vapor log mean concentration ratio is then defined as:

\[ \phi = \frac{X_{g,\text{avg}}}{X_{s,\text{avg}}} = \frac{\ln[X_{s,b} / X_{s,i}]}{\ln[X_{g,b} / X_{g,i}]} = \frac{\ln[(1 - X_{g,b})/(1 - X_{g,i})]}{\ln[X_{g,b} / X_{g,i}]} \]  
(A.31)

The heat transfer coefficients for sensible and condensation heat transfer are calculated as shown below. This requires expressions for the Nu and Sh numbers.

\[ q_{\text{conv}}'' = h_{\text{conv}} (T_b - T_i^{\text{sat}}) \]
\[ q_{\text{cond}}'' = h_{\text{cond}} (T_b^{\text{sat}} - T_i^{\text{sat}}) \]
\[ h_{\text{conv}} = \frac{k_m}{x} \text{Nu}_x \]
\[ h_{\text{cond}} = \frac{k_m}{x} \text{Sh}_x \]  
(A.32, A.33, A.34, A.35)

For natural convection on vertical flat surfaces Peterson recommends using the following expressions for the Nusselt and Sherwood numbers.

\[ \text{Nu} = C_{\text{sen}} (Gr_m Pr_m)^{\nu} \]
\[ \text{Sh} = C_{\text{cond}} (Gr_m Sc_m)^{\nu} \]  
(A.36, A.37)

This type of relation eliminates the dependence on surface height for natural convection processes \((Gr \propto x^3)\), a finding which has been shown appropriate for turbulent condensation (Dehbi, 1991). Peterson recommends using \(C_{\text{cond}} = 0.1\) and \(\frac{C_{\text{sen}}}{C_{\text{cond}}} = 7.0\) for the scaling constants.

The McAdams relation calls for using \(C_{\text{sen}} = 0.13\) for vertical surfaces. The increase from 0.13 to 0.7 is to account for the augmentation to heat transfer from mist formation near the condensate interface. This constant was chosen to match the Peterson model to experimental results, where the experiments were carried out in the saturated regime. For superheated mixtures, the value of the two constants will most likely be equal. For conservative design calculations, Peterson recommends using \(\frac{C_{\text{sen}}}{C_{\text{cond}}} = 1.0\).
Peterson applied this model to the conditions of the Uchida (1965) experiments [Peterson, 1996]. He found that the reason the Uchida data is well correlated to the ratio between the steam and gas densities was a consequence of holding the noncondensable gas partial pressure nearly constant at one atmosphere (which in turn holds the gas density essentially constant). According to the Peterson theory, the Uchida correlation will over-predict heat removal for containment conditions where the noncondensable gas partial pressure is significantly less than one atmosphere. This situation occurs in the wetwell of suppression pool containments, and can also exist in sub-atmospheric containments. Also, the Uchida correlation will under-predict the heat removal when the noncondensable gas partial pressure is significantly higher than one atmosphere. These findings show that the Uchida correlation is not always conservative, as has been historically assumed.

A.1.8 Modified Peterson Model (1997)

Recently the two models proposed by Peterson and Corradini have been directly compared to each other and experimental data [Anderson, 1997]. Anderson has proposed a “modified Peterson” model which slightly changes the expression for the condensation conductivity and also adds a term to account for suction effects. This modified model has been compared with atmospheric pressure experimental data gathered at the University of Wisconsin-Madison AP-600 scale test facilities.

Anderson points out that the Peterson expression for $k_{\text{cond}}$ is derived using the Clapeyron equation:

$$\frac{dP}{dT} = \frac{h_{fg}}{Tv_{fg}}$$

(A.38)

to express the mass transfer driving force in terms of saturation temperature differences. In the Peterson approach the Clapeyron relation is approximated as:

$$\frac{\Delta P}{\Delta T} = \frac{h_{fg}}{T_{avg}v_{fg}}.$$

(A.39)

This assumes that both $h_{fg}$ and $v_{fg}$ change little over the temperature range and can be evaluated at a suitable average temperature $T_{avg}$ which characterizes the boundary layer. Anderson argues that while this assumption is valid for $h_{fg}$ which varies approximately 10% for a 25-100 °C temperature change, $v_{fg}$ can change by an order of magnitude over this range. Thus for large temperature jumps across the boundary layer, this approximation can introduce significant error.

Anderson proposes an alternative approximation to the Clapeyron equation by assuming that the steam volume change can be described by the ideal gas law. Using this approach, a slightly different expression is derived for the condensation conductivity which is highly dependent on the interface temperature (this derivation is given in detail in appendix B):
\[ k_{\text{cond}} = \frac{h_f s c M_s^2 D}{R T_{av}^* T_i^2 \phi} \]  
(A.40a)

where \( T_{av}^* \) is a dimensionless correction factor given as equation B.22 in Appendix B.

Anderson shows that expanding the expression for \( T_{av}^* \) in terms of a Taylor series and dropping higher order terms will lead to the simplification of equation A.40a as:

\[ k_{\text{cond}} = \frac{h_f s c M_s^2 D}{R T_b T_i^1 \phi} \]  
(A.40b)

Finally Anderson adds a correction term to account for suction effects at high mass transfer rates. The suction term has been defined in different papers as being one of the following two equations (this author used A.41b):

\[ \Theta = \frac{X_{s,i} - X_{s,b}}{1 - X_{s,i}} \]  
(A.41a)

\[ \Theta = \frac{1 - X_{s,i}}{1 - X_{s,\text{avg}}} \]  
(A.41b)

and is applied to the Sherwood number such that

\[ h_{\text{cond}} = \frac{k_{\text{cond}}}{x} \text{Sh} \Theta. \]  
(A.42)

Anderson then compares the Kim & Corradini model, the original Peterson model, and the modified Peterson model to experimental data taken in the atmospheric pressure AP600 scale test facility at the University of Wisconsin-Madison. The predictions for the two Peterson models are calculated using the McAdams correlation for turbulent natural convection on a vertical surface

\[ Nu = 0.13(Gr_m Pr_m)^{\frac{1}{3}} \quad \text{Sh} = 0.13(Gr_m Sc_m)^{\frac{1}{3}} \]  
(A.43, A.44)

and an average temperature given by

\[ T_{avg} = \frac{T_{b \text{sat}} - T_{i \text{sat}}}{\ln(T_{b \text{sat}} / T_{i \text{sat}})}. \]  
(A.45)

The original Peterson model is stated to significantly under-predict the measured heat transfer coefficient with an average error in the range of 90% [Anderson, 1997]. The modified Peterson model (without suction) and the Kim & Corradini model are both stated to predict nearly identical values, however they are still somewhat conservative with an average error around
The modified Peterson model with suction is stated to show the closest agreement with the experimental data, under-predicting the data by an average error of about 20%. The models were then compared to data from a test with a 30% mole fraction of helium in the noncondensable gas mixture. The modified Peterson model with suction matched the helium mixture data quite well, with an average error in the range of about 13%.

A.1.9 AP600 Small and Large Scale Tests

Westinghouse Electric Corporation performed several experiments in two different scale facilities designed to mimic the operation of the AP600 passive containment cooling system (PCCS). The Small Scale Test (SST) and the Large Scale Test (LST) were both designed to provide experimental data for use in evaluating the AP600 passive containment cooling system design and to furnish benchmark data for computer code validation [van de Venne, 1992].

The COMMIX computer code, which has heat transfer models based on the heat and mass transfer analogy, was used to simulate several of the experiments in both the SST [Sun, 1995] and the LST [Sha, 1997]. The analysis of the SST data revealed that the natural convection heat transfer relation used, equation A.46, for prediction of the Nusselt number resulted in an under-prediction of the condensation rate and subsequent over-prediction of the vessel pressure. Sun then implemented a turbulent-mixed-convection (TMC) relation for the Nusselt number based on a model proposed by Chen [Chen, 1987]. The TMC relation, shown below as equation A.47, predicted a more accurate rate of heat and mass transfer than the natural convection relation. Based on this observation, Sun recommended that a mixed convection relation may be needed in a computer code which is used to simulate the actual AP600 PCCS.

\[
\text{Nu} = 0.14 (\text{Gr} \Pr)^{\frac{1}{3}} \quad (A.46)
\]

\[
\text{Nu} = 1.4 \Re_x^{4/5} F(\Pr) \left[ 1 + a \left( \frac{G(\Pr)}{F(\Pr)} \left( \frac{\Gr_x}{\Re_x^{4.4}} \right)^{1/3} \right)^3 \right]^{1/3} \quad (A.47)
\]

\[
a = \begin{cases} 
0.36 : & (\Gr_x / \Re_x^2) < 1 \\
0.52 : & (\Gr_x / \Re_x^2) \geq 1 
\end{cases} \quad (A.47)
\]

\[
F(\Pr) = 0.0287 \Pr^{0.6} \\
G(\Pr) = 0.150 \Pr^{1/3} \left[ 1 + (0.492 / \Pr)^{9/16} \right]^{16/27}
\]

This author was not able to reproduce the large reported error between the original Peterson model and the modified version when using the Mathcad software to perform analyses on the two models (see Chapter 2). The modification proposed by Anderson, while theoretically correct, does not increase the accuracy of the Peterson method by any discernable amount for the conditions studied. The derivation of the condensation conductivity is given in Appendix B.

COMMIX is a three-dimensional, multiple species, single phase, time-dependent thermal hydraulic computer code. An added liquid film tracking model was added to the original single-phase code formulation to allow the code to model the condensing and evaporating liquid films used in the AP-600 PCCS. [Sun, 1995]
The Large Scale Test (LST), which is approximately a 1/8th scale facility built to mimic the AP600 PCCS, was used to generate experimental data for test conditions more prototypic of those which might exist in the actual AP600 facility than was possible with the SST. The COMMIX analysis of the LST tests showed that while the flow inside the LST experiment may be in the mixed convection regime, it is primarily dominated by free convection. The TMC model (equation A.47) used to simulate the SST experiments failed to adequately describe heat and mass transfer rates in the LST. Further analysis showed that the flow in the LST is primarily dominated by natural convection, while Sha points out that the TMC model under-predicts pure natural convection by 29%. Sha recommends that a more adequate mixed convection formulation be developed in order to have a relation that is valid over all flow regimes.

A.2 Condensation Inside Vertical Tubes

A.2.1 Vierow (1990)

One of the first experimental programs directed specifically at modeling condensation inside vertical tubes was performed at the University of California Berkeley [Vierow, 1990; Vierow, 1991]. The experimental setup consisted of a 2.2 cm inside diameter, 2.1 m length vertical copper tube in a natural convection loop with steam-air mixtures. The experiments were performed for a pressure range of 30 - 452 kPa, vapor temperatures of 72 - 146 °C, coolant temperatures of 9 - 23 °C, and air inlet mass fractions from 0.0 - 0.14. Local heat transfer properties were correlated in the form of correction factors applied to the Nusselt pure steam condensation model (which is valid for laminar flow with zero shear stress between the vapor and the condensate). The correction factor formulation presented in [Vierow, 1991] is given by:

\[
h = f h_{Nu}\quad (A.48)
\]

\[
f = f_1 f_2 = \left(1 + 2.88 \times 10^{-5} \text{Re}^{1.18}_{film}\right) \left(1 - A m_{air}^A\right)\quad (A.49)
\]

where \(\text{Re}_{m}\) is the local steam/gas mixture Reynolds number, and \(m_{air}\) is the local value for the bulk air mass fraction. There is no stated standard deviation for this correlation when compared to the Vierow experimental data. However, when used in the TRAC-G code to analyze the Toshiba tube average data, G.E. Nuclear energy found the correlation underpredicted the data by as much as 30% [Vierow, 1991]. This form is easily implemented into computer codes, and does have the feature of nicely reducing to a pure steam coefficient when the noncondensable gas mass fraction is extremely small. However, the correlation does not represent the physical processes occurring inside the condensing tube.

A.2.2 Siddique (1992)

Siddique performed several sets of experiments at MIT which tested the effects of air and helium on the condensation of steam inside a vertical tube in forced convection [Siddique, 1992]. The
experimental condenser was a 4.6 cm (inside) diameter stainless steel tube through which steam-air and steam-helium mixtures were condensed in a 2.54 m vertical section in concurrent downflow. The tube was cooled on the outside by an upward flowing annulus of cooling water. The Siddique steam-air experiments were performed with inlet temperatures ranging from 100 to 140 °C, air mass fractions from 0.1 to 0.35, and inlet Reynolds numbers from 5000 to 22,700. The major assumption in correlating the data is that the gas boundary layer provides the overriding resistance to heat transfer, thus the condensate film layer is ignored. The proposed local Nusselt number is given by:

$$\text{Nu}(x) = 6.123 \text{Re}_x^{0.223} \left( \frac{m_{\text{air},w} - m_{\text{air},b}}{m_{\text{air},w}} \right)^{1.144} \text{Ja}^{-1.253}$$

where $\text{Re}_x$ is the local mixture Reynolds number, $\text{Ja} = \left( \frac{c_p \left( T_b - T_w \right)}{h_f} \right)$ is the Jacob number (ratio of sensible to latent heat transfer), and $m_{\text{air}}$ is the mass fraction of air. The correlation is nominally valid for the range of variables:

- $0.1 < m_{\text{air}} < 0.95$
- $445 < \text{Re} < 22,700$
- $0.004 < \text{Ja} < 0.07$

The stated standard deviation of the correlation is 40% when compared to the Siddique data, which is quite substantial. There were also large temperature variations along the length of the tube resulting from problems with the cooling water flow and mixing. In order to obtain reliable readings for the coolant bulk temperature, air was bubbled into the cooling water to promote mixing. However this did not solve the problem of large temperature variations along the tube wall. The original intent was to calculate local heat flux data by measuring the temperature difference across the condenser tube. The large temperature fluctuations made this impossible and a given temperature profile was assumed instead. This problem raises questions as to the validity of the local heat flux correlation. Finally, a drawback of this formulation is that it does not allow for a smooth transition to a pure steam solution by virtue of not having terms to account for the resistance of the condensate film. Thus this correlation can not be used for small noncondensible gas concentrations.

**A.2.3 Hasanein (1994)**

Hasanein performed experiments with steam-helium and steam-air-helium mixtures in the same facility as Siddique [Hasanein, 1994]. Hasanein also performed a detailed analytical analysis of condensation in tubes with noncondensible gas. One of his key findings was that the resistance to heat transfer introduced by the condensation film can be significant for large mixture Reynolds numbers and small noncondensible gas concentrations - this finding is contrary to the assumptions made by Siddique in developing his model. Hasanein also pointed out that the MIT facility design often made gathering reliable data difficult, especially for data needed to calculate the local heat flux, which is of primary importance in the development of this type of correlation. Hasanein developed three different correlations for steam-air-helium condensation heat transfer. All three correlations have a standard deviation above 38%, which shows little improvement over
has experienced cooling water problems and temperature variations similar to Siddique. He proposed an improved experimental facility design to address these problems, but was unable to construct the new facility.

**A.2.4 Kuhn (1995)**

Noting the problems with cooling water flows from previous experiments at Berkeley and MIT, Kuhn carefully redesigned the University of California at Berkeley test apparatus. Many embedded thermocouple pairs were placed axially (a pair consisted of two thermocouples placed at an angle of 180 degrees circumferentially) to assure several accurate local measurements of fluid temperature at the tube walls. In addition, a complementary mixture of measurements and calculated results were used to determine the state of the cooling fluid - which eliminated the need to place thermocouples internal to the cooling water flow. These modifications resulted in better experimental values of local heat flux [Kuhn, 1995; Kuhn et. al., 1995]. Kuhn then established a large database for pure steam condensation, steam-air mixture condensation, and steam-helium mixture condensation. From this new data set, three new correlations were developed. The first proposed correlation was a reworking of the Vierow & Schrock correlation which depends on correction factors applied to a pure steam condensation formulation [Vierow, 1991]. The second was a modified version of the Peterson model (presented in section A.1.7). The third is a standard mass transfer theory model which follows closely the theory discussed in section A.1.5. Only the first two will be discussed here since the third formulation is quite complex and adds little to the accuracy of the predictions over the second formulation.

The proposed new correction factors are a function of shear stress and waviness on the condensate film, film Reynolds number, and noncondensable gas mass fraction. The new correction factor correlation appears as:

\[
h = h_{Na} f = h_{Na} f_{1shear} f_{1other} f_2
\]

The interfacial shear stress on the condensate film is accounted for by the factor \( f_{1shear} \), which is the ratio of the film thickness without interfacial shear to the film thickness with interfacial shear. The factor \( f_{1other} \) depends on film Reynolds number and is meant to capture the effects of waves. The factor \( f_2 \) again accounts for the mass fraction of noncondensable gas (only steam-air results are shown here). The steam-air mixture formulation for the correction factors is shown below.

\[
\delta_1 = \left( \frac{3 \mu_{l} \Gamma}{g \rho_{l} (\rho_{l} - \rho_{m})} \right)^{1/3}
\]

\[
\Gamma = \frac{g}{\mu_{l}} \rho_{l} (\rho_{l} - \rho_{m}) \frac{\delta_2^3}{3} + \frac{\rho_{l} \tau_{l} \delta_2^2}{2}
\]

\[
f_{1shear} = \frac{\delta_1}{\delta_2}
\]

\[
f_{1other} = 1 + 7.32 \times 10^{-4} \text{ Re}_f
\]

\[
f_2 = \begin{cases} 
(1 - 2.601 m_{air}^{0.708}) & m_{air} < 0.1 \\
(1 - m_{air}^{0.292}) & m_{air} > 0.1
\end{cases}
\]

\[ (A.51, A.52, A.53) \]

\[ (A.54, A.55) \]

\[ (A.56) \]
The correction factor model has a standard deviation of 17.6% relative to the new data, which is quite impressive given the limited physical description inherent in the model.

Of more interest for the present work however, is the correlation developed based on the Peterson diffusion theory approach (section A.1.7). This model is based on the definition of a condensation thermal conductivity, and employs the analogy between heat and mass transfer. The heat flux from condensation heat transfer and from sensible heat transfer are treated in parallel, then equated to the heat flux through the condensate film. Applying the Peterson model to the present case, the total measured experimental heat transfer can be expressed as:

\[
\dot{q}_T^* = h_T (T_{b,\text{sat}} - T_w) = \frac{(T_{b,\text{sat}} - T_w)}{1 + \frac{h_{\text{cond}}}{h_{\text{conv}}}} \left( \frac{T_b - T_{i,\text{sat}}}{T_{b,\text{sat}} - T_{i,\text{sat}}} \right) h_f \tag{A.57}
\]

In reality, only the total heat transfer coefficient can be measured, thus appropriate models must be applied in order to reduce the data in terms of saturation temperatures in the bulk and at the interface. The Peterson model requires the selection of appropriate correlations for the Nusselt and Sherwood numbers to describe the heat transfer between the gas mixture and the condensate film. Kuhn chose the correlation of Kays and Crawford for turbulent forced convection without suction:

\[
\text{Nu} = 0.021 \text{Re}^{0.8} \text{Pr}^{0.5} \quad \text{Sh} = 0.021 \text{Re}^{0.8} \text{Sc}^{0.5}. \tag{A.58, A.59}
\]

The values for the convection and condensation heat transfer coefficients are then given by:

\[
h_{\text{conv}} = \frac{k_m}{d} \text{Nu} = 0.021 \frac{k_m}{d} \text{Re}^{0.8} \text{Pr}^{0.5} \tag{A.60}
\]

\[
h_{\text{cond}} = \frac{k_{\text{cond}}}{d} \text{Sh} = 0.021 \frac{k_{\text{cond}}}{d} \text{Re}^{0.8} \text{Sc}^{0.5} \tag{A.61}
\]

where the condensation conductivity is defined as:

\[
k_{\text{cond}} = -\frac{\ln[X_{g,b} / X_{g,i}]}{\ln[(1 - X_{g,b})/(1 - X_{g,i})]} \left( \frac{h_{fs}^2 P_T M_i^2 D}{R^2 T_{ave}} \right). \tag{A.62}
\]

The effective Nusselt number for heat transfer to the interface is then:
These quantities are all obtained from experimental data with the exception of \( T_i^{\text{sat}} \) which can be determined from the condensate film heat transfer model. The film model chosen to represent the data was the method of Blangetti [Blangetti, 1982]. This method accounts for the possibility of turbulence in the condensate film. The local film Nusselt number is calculated as:

\[
\text{Nu} = \frac{h \cdot \ell}{k_f} = \left( \text{Nu}_{x, la} + \text{Nu}_{x, t} \right)^{\frac{1}{4}}
\]  

(A.64)

where the laminar regime is described by:

\[
\text{Nu}_{x, la} = \frac{\ell}{\delta_2}
\]

(A.65, A.66)

and \( \delta_2 \) is the film thickness accounting for interfacial shear, presented earlier in this section. The turbulent Nusselt number is given by the relation:

\[
\text{Nu}_{x, t} = a \cdot \text{Re}^b \cdot \text{Pr}^c \left( 1 + e \cdot \delta_{2}^d \right)
\]  

(A.67)

where the constants \( a, b, c, d, \) and \( e \) take on different values dependent on the interfacial shear [Blangetti, 1982].

Kuhn then added a correction factor for suction based on the ratio of the experimentally derived Nusselt number and that predicted by the model. With the suction factors, the convection and condensation heat transfer coefficients are expressed as:

\[
h_{\text{cond}} = 0.021 \left( \frac{k_{\text{cond}}}{d} \right) \text{Re}_m^{0.8} \text{Sc}^{0.5} \left( 1 + 0.046(-\beta_m)^{2.48} \right)
\]  

(A.68)

\[
h_{\text{conv}} = 0.021 \left( \frac{k_m}{d} \right) \text{Re}_m^{0.8} \text{Pr}^{0.5} \left( 1 + 0.046(-\beta_m)^{2.48} \right)
\]  

(A.69)

\[
\beta_m = \frac{m^*}{\rho_m u_{m,b} \text{Pr}_m^{0.2} \text{Sc}^{-0.5}} \quad \text{(suction factor)}
\]  

(A.70)

The total heat transfer coefficient can be calculated using the equation:

---

9 "Blowing factor" is the generic term for a correction factor which is applied to mass transfer equations to account for the effects of a high mass transfer rate. For condensation, the actual process is suction, and thus "suction factor" is the correct terminology, however most relations are still derived using the generic term "blowing factor".
\[ \frac{1}{h_r} = \frac{1}{h_{\text{cond}} + h_{\text{conv}} \left( \frac{T_b - T_{\text{sat}}}{T_{\text{sat}} - T_{\text{sat}}} \right)} + \frac{1}{h_f} \]  

(A.71)

In the special case where the bulk atmosphere is saturated (as usually occurs in reactor containments following a loss of coolant accident), the temperature ratio multiplying \( h_{\text{conv}} \) is equal to unity. When applying the heat transfer model in calculations, an iterative approach is then used to converge on the condensate interface temperature and the interface molar concentration of noncondensable gases. The standard deviation for the total heat transfer coefficient (including the condensate film) compared to the experimental data was 8.41% for steam-air mixtures.

**A.3 Summary and Condensation Model Choices**

Several different models were presented for condensation on external surfaces and inside tubes. The objective of the literature review was to determine the state of knowledge for condensation in the presence of a noncondensable gas (specifically air or nitrogen) and to choose a model which is adequate to describe this phenomenon inside reactor containments, if such a model exists. Several conclusions have been reached. First, modeling the liquid film is important if the condensation model is to be applicable over all ranges of noncondensable gas concentration. Second, it has been shown that most models based on the heat/mass transfer analogy under-predict turbulent natural convection heat transfer. Third, in the past several years a substantial amount of work has been performed on new models for condensation which are directly applicable to the analysis of new passively safe nuclear reactor designs.

For predicting condensation on large vertical containment surfaces, the modified Peterson model is chosen as the best available model (section A.1.7). The Peterson model requires a correlation for the Nusselt number. Based on the findings of Anderson, the McAdams turbulent natural convection heat transfer correlation will be used (equations A.43, A.44). The McAdams correlation is simple and has shown good agreement with available containment data [Anderson, 1997]. A mixed convection heat transfer correlation was investigated based on the initial findings from the AP600 Small Scale Test (SST) [Sun, 1995]. However, recently published findings from the AP600 Large Scale Test (LST) [Sha, 1997] indicate that the mixed convection correlation in question does not describe the heat transfer process adequately in the larger facility. The reason given was that the proposed turbulent mixed convection correlation transitions smoothly to the forced convection regime, but substantially under-predicts heat transfer in the transition to the free convection regime. The SST is dominated by forced convection whereas the LST is dominated by free convection [Sha, 1997]. This finding agrees with previous MIT experience with large containment simulations [Gavrilas, 1997] where near-wall velocities were determined to be in the range of 1 - 3 meters per second; thus the heat transfer is primarily in the natural convection regime.
B. DERIVATION OF CONDENSATION CONDUCTIVITY

This appendix is included to give the reader a complete derivation for the condensation conductivity without reverting to the original reference [Peterson, 1993]. This derivation is slightly different from the original Peterson paper, and is based on the theory of “High Mass Transfer Rate Diffusion” as presented in [Mills, 1995, pp. 922-933]. The equations here closely follow the mass transfer theory equations presented in Chapter 1, section 1.5.2, but several steps have been skipped in this derivation. The reader is referred to Chapter 1 for a more detailed treatment of mass transfer.

The heat of condensation is given by (Mills page 933):

\[ q^*_c = h_{fg} M_s N_s \]  \hspace{1cm} (B.1)

where \( h_{fg} \) is the latent heat of vaporization (J/kg), \( M_s \) is the molecular weight of steam (kg/kmol) and \( N_s \) is the absolute molar flux of the steam (molar flux relative to a stationary coordinate axis). The absolute molar flux is defined as:

\[ N_s = X_s \sum N_i + J^*_s = X_s (N_s + N_g) + J^*_s \]  \hspace{1cm} (B.2)

where \( N_g \) is the absolute molar flux of the noncondensible gas, \( X_s \) is the steam mole fraction, and \( J^*_s \) is the molar diffusion flux relative to the molar-average velocity. \( J^*_s \) is defined as:

\[ J^*_s = c_s (v_s - v^*) \]  \hspace{1cm} (B.3)

The molar-average velocity is defined as:

\[ v^* = \frac{\sum c_i v_i}{\sum c_i} = \frac{\sum c_i v_i}{c} = \sum X_i v_i \]  \hspace{1cm} (B.4)

where \( c_i \) is the molar concentration of species \( i \), and \( v_i \) is the absolute molar velocity of species \( i \) relative to a fixed coordinate axis.

Now the molar diffusion flux (relative to the molar-average velocity) is calculated according to Fick’s Law of diffusion:

\[ J^*_s = -cD_{12} \nabla X_s \]  \hspace{1cm} (B.5)
where $D_{12}$ is the binary diffusion coefficient for steam in the noncondensable mixture. For this diffusion equation it is important to use the total molar concentration of the mixture, $c$, not just of steam, $c_s$, because the steam is diffusing through the mixture, not only through itself.

Substituting equation (B.5) into equation (B.2):

$$N_s = X_s (N_s + N_g) - c D_{12} \frac{dX_s}{dz} \quad (B.6)$$

Since the condensed liquid film is virtually impermeable to the noncondensable gas, at steady state there will be no net movement of gas toward the interface so that the absolute molar velocity of gas will be zero.

$$N_g = X_g (N_s + N_g) + J_g^* = 0 \quad (B.7)$$

Solving equation (B.6) for $N_s$ yields the following relation (same as equation 1.31):

$$N_s = - \frac{c D_{12}}{1 - X_s} \frac{dX_s}{dz} \quad (B.8)$$

At steady state we also expect the molar velocity of vapor to be constant, thus:

$$\frac{d}{dz} N_s = 0 \quad (B.9)$$

Substituting equation (B.8) into (B.9) gives:

$$\frac{d}{dz} \left( - \frac{c D_{12}}{1 - X_s} \frac{dX_s}{dz} \right) = - c D_{12} \frac{d}{dz} \left( \frac{1}{1 - X_s} \frac{dX_s}{dz} \right) = 0 \quad (B.10)$$

where the total concentration and diffusion coefficients are assumed constant. This equation can be applied to the situations shown in Figure B-1 and solved according to the boundary conditions:

$$z = 0 \quad \text{(interface)} \quad X_v = X_{v,i}$$

$$z = \delta \quad \text{(bulk)} \quad X_v = X_{v,b}$$

where $\delta$ is the thickness of the boundary layer. Integrating twice (see equations 1.35-1.38) we get a relation for the mole fraction of steam as a function of position in the boundary layer:

$$\frac{1 - X_s}{1 - X_{s,b}} = \left( \frac{1 - X_{s,i}}{1 - X_{s,b}} \right)^{z/\delta} \quad (B.11)$$
Evaluating the absolute molar flux of steam at the edge of the boundary layer (see equations 1.40 - 1.43):

\[ N_s \bigg|_{z=0} = -\frac{cD_{12}}{1 - X_{s,i}} \frac{dX_s}{dz} \bigg|_{z=0} = \frac{cD_{12}}{\delta} \ln \left( \frac{1 - X_{s,b}}{1 - X_{s,i}} \right) \]  \hspace{1cm} (B.12)

The steam flux can be expressed in terms of the gas mole fraction by using the identity \( X_g = 1 - X_s \): 

\[ N_s = \frac{cD_{12}}{\delta} \ln \left( \frac{X_{g,b}}{X_{g,i}} \right) \]  \hspace{1cm} (B.13)

Now if we define the logarithmic average mole fraction of gas as:

\[ X_{g,ave} = \frac{X_{g,b} - X_{g,i}}{\ln(X_{g,b}) - \ln(X_{g,i})} = \frac{X_{g,b} - X_{g,i}}{\ln \left( \frac{X_{g,b}}{X_{g,i}} \right)} \]  \hspace{1cm} (B.14)

we can rearrange equation (B.13) to be:

\[ N_s = \frac{cD_{12}}{\delta X_{g,ave}} (X_{s,i} - X_{s,b}) \]  \hspace{1cm} (B.15)

Assuming ideal gas behavior, the steam mole fractions can be expressed using partial pressures:
\[ N_s = \frac{cD_{12}}{\delta X_{g,ave}} \left( \frac{P_{s,i} - P_{s,b}}{P_t} \right) = \frac{cD_{12}}{\delta X_{g,ave} P_t} (P_{s,i} - P_{s,b}) \]  

(B.16)

Now the Clapeyron equation is used to express changes in saturation pressure as an equivalent change in saturation temperature:

\[ \frac{\partial P}{\partial T} = \frac{h_{fg}}{T \nu_{fg}} \left[ \left( \frac{T}{T_0} \right) \frac{v_{fg}}{R} \right] = \left[ \left( \frac{T}{T_0} \right) \frac{v_{fg}}{R} \right] \]  

(B.17)

where \( h_{fg} \) is the latent heat of vaporization in units of \([\text{kJ/kg}]\), and \( \nu_{fg} \) is the specific volume change from vapor to liquid in units of \([\text{m}^3/\text{kg}]\). The value of the specific volume change can be calculated assuming that the specific volume for liquid is constant and that for vapor can be represented by the ideal gas law:

\[ \nu_{fg} = \nu_{s} - \nu_{l} = \frac{RT}{M_s P_s} - \nu_{l} = \frac{R_s T}{P_s} - \nu_{l} \]  

(B.18)

where \( P_s \) is the partial pressure of the steam, \( R \) is the universal gas constant, and \( R_s \) is the gas constant for steam. Equation (B.18) is then substituted into equation (B.17) and integrated analytically between \( T_i \) and \( T_b \) to obtain the expression:

\[ \Delta P = \frac{M_s h_{fg} P_s}{R T_{ave} T_i^2} \left( T_{i} - \frac{\nu_{fg}}{R} \right) \]  

(B.19)

According to Anderson [Anderson, 1998] the term \( T_{i} - \frac{\nu_{fg}}{R} \) results in a variance of the interface temperature of less than 0.5 \%, thus equation (B.19) is approximated as:

\[ \frac{\Delta P}{\Delta T} = \frac{M_s h_{fg} P_s}{R T_{ave} T_i^2} \]  

(B.20)

where the steam partial pressure is given by:

\[ P_s = P_t \ X_{s,ave} \]  

(B.21)

The factor \( T'_{ave} \) is a dimensionless factor which relates the corrected and uncorrected temperatures as follows:
The corrected temperature is given by:

\[ T' = T - \frac{v_i P}{R} \]  

(B.23)

Anderson has shown that by expanding equation (B.22) in terms of a Taylor series, one arrives at the following approximation for absolute temperatures over 300K [Anderson, 1998]:

\[ T_{avg} = \frac{T_b}{T_i} \]  

(B.24)

Plugging equations (B.24) and (B.21) into (B.20) gives:

\[ \frac{\Delta P}{\Delta T} = \frac{M_s h_{fg} P_i}{R T_i T_b} X_{s,ave} \]  

(B.25)

which then allows calculation of the absolute molar flux of vapor according to equation (B.16):

\[ N_s = \frac{c M_s D_{12} h_{fg}}{\delta R T_i T_b X_{s,ave}} X_{g,ave} (T_i - T_b) \]  

(B.26)

Thus the condensation heat flux is given by:

\[ q_{cond} = \frac{c M_s^2 D_{12} h_{fg}^2}{\delta R T_i T_b X_{g,ave}} X_{s,ave} (T_i - T_b) \]  

(B.27)

and the condensation conductivity is defined as:

\[ k_c = \frac{c M_s^2 h_{fg}^2 D}{RT_i T_b \phi \left[ \frac{W}{m - K} \right]} \]  

(B.28)

where the ratio of mole fractions has been expressed as:

\[ \phi = \frac{X_{g,ave}}{X_{s,ave}} = \frac{\ln(X_{s,b} / X_{s,i})}{\ln[(1 - X_{s,b})/(1 - X_{s,i})]} \]  

(B.29)
Appendix

C. FLUID MECHANICS AND TURBULENCE MODELING

The field of fluid mechanics is centered around the solution of the conservation equations of mass, momentum, energy, and chemical species. There are also additional equations which must be solved for cases involving turbulent flow. This appendix is intended to serve as a primer on turbulence modeling. Several turbulence models are presented here for easy reference and to familiarize the reader with the different notation standards which are used throughout this thesis. Each of the notation types is widely used in the literature. However, it is often convenient to use different notation types in order to put a particular equation(s) in the form which most clearly highlights the features under discussion. All notation used here are standard in the field.

C.1 Conservation Equations

There are several books on fluid flow which give a derivation and theoretical overview of the conservation equations. Of these, [Schlichting, 1979] is one of the most frequently referenced classical texts. [Tannehill, Anderson, & Pletcher, 1997] and [Wilcox, 1993] are two more recent texts which present the equations and discuss applicable numerical solution schemes for some interesting problems. These three texts provide the basis for the information in this appendix.

The fully compressible, time dependent, conservation equations are presented below. Each is presented first in vector calculus notation, then in three-dimensional Cartesian coordinate notation, and finally in tensor notation. The momentum equations are presented assuming that the Stokes’ hypothesis for viscosity is valid (that the bulk viscosity of the fluid is zero).

C.1.1 Conservation of mass (continuity equation)

Vector calculus
\[ \frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{V}) = 0 \quad \text{or} \quad \frac{D \rho}{Dt} + \rho (\mathbf{V} \cdot \mathbf{V}) = 0 \]  
(C.1a,b)

Cartesian coordinates
\[ \frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x} (\rho u) + \frac{\partial}{\partial y} (\rho v) + \frac{\partial}{\partial z} (\rho w) = 0 \]  
(C.2a)

or
\[ \frac{\partial \rho}{\partial t} + u \frac{\partial \rho}{\partial x} + v \frac{\partial \rho}{\partial y} + w \frac{\partial \rho}{\partial z} = -\rho \left( \frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} + \frac{\partial w}{\partial z} \right) \]  
(C.2b)

Tensor notation
\[ \frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x_i} (\rho \mathbf{V}) = 0 \]  
(C.3)

1 A description of tensor notation (index notation) can be found in [Wilcox, 1993] or [Tannehill, 1997].
C.1.2 Conservation of momentum (Navier-Stokes equations)

**Vector calculus**

$$\rho \frac{DV}{Dt} = \rho g + \nabla \cdot \left( - p \delta_{ij} + \tau_{ij} \right) \quad (C.4)$$

stress tensor: \[ \tau_{ij} = \left[ \mu \left( \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) - \frac{2}{3} \delta_{ij} \mu \frac{\partial u_k}{\partial x_k} \right] \quad (C.5) \]

**Cartesian coordinates**

$$\rho \left( \frac{\partial u_i}{\partial t} + u_j \frac{\partial u_i}{\partial x_j} + v \frac{\partial u_i}{\partial y} + w \frac{\partial u_i}{\partial z} \right) = - \frac{\partial p}{\partial x} + \frac{\partial}{\partial x} \left[ \frac{2}{3} \mu \left( \frac{\partial u_i}{\partial x} \frac{\partial u_i}{\partial x} - \frac{\partial u_i}{\partial y} \frac{\partial u_i}{\partial y} \right) \right]$$

$$+ \frac{\partial}{\partial y} \left[ \mu \left( \frac{\partial u_i}{\partial y} + \frac{\partial u_i}{\partial x} \right) \right] + \frac{\partial}{\partial z} \left[ \mu \left( \frac{\partial u_i}{\partial z} + \frac{\partial u_i}{\partial x} \right) \right] + \rho g_i \quad (C.6a)$$

$$\rho \frac{Dv}{Dt} = - \frac{\partial p}{\partial y} + \frac{\partial}{\partial y} \left[ \mu \left( \frac{2}{3} \frac{\partial v}{\partial y} - \nabla \cdot \mathbf{V} \right) \right] + \frac{\partial}{\partial z} \left[ \mu \left( \frac{\partial v}{\partial z} + \frac{\partial u}{\partial z} \right) \right]$$

$$+ \frac{\partial}{\partial x} \left[ \mu \left( \frac{\partial u}{\partial y} + \frac{\partial v}{\partial x} \right) \right] + \rho g_y \quad (C.6b)$$

$$\rho \frac{Dw}{Dt} = - \frac{\partial p}{\partial z} + \frac{\partial}{\partial z} \left[ \mu \left( \frac{2}{3} \frac{\partial w}{\partial z} - \nabla \cdot \mathbf{V} \right) \right] + \frac{\partial}{\partial x} \left[ \mu \left( \frac{\partial w}{\partial x} + \frac{\partial u}{\partial x} \right) \right]$$

$$+ \frac{\partial}{\partial y} \left[ \mu \left( \frac{\partial u}{\partial z} + \frac{\partial w}{\partial y} \right) \right] + \rho g_z \quad (C.6c)$$

**Tensor notation**

$$\rho \left( \frac{\partial u_i}{\partial t} + u_j \frac{\partial u_i}{\partial x_j} \right) = - \frac{\partial p}{\partial x_i} + \frac{\partial}{\partial x_i} \left[ \mu \left( \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} - \frac{2}{3} \delta_{ij} \frac{\partial u_k}{\partial x_k} \right) \right] + \rho g_i \quad (C.7)$$
C.1.3 Conservation of energy (total enthalpy equation)

**Vector calculus**

\[
\rho \frac{DH}{Dt} = \frac{DP}{Dt} + \nabla \cdot k \nabla T + \Phi + \dot{Q}^* \tag{C.8}
\]

**Cartesian coordinates**

\[
\rho \left( \frac{\partial H}{\partial t} + u \frac{\partial H}{\partial x} + v \frac{\partial H}{\partial y} + w \frac{\partial H}{\partial z} \right) = \left( \frac{\partial p}{\partial t} + u \frac{\partial p}{\partial x} + v \frac{\partial p}{\partial y} + w \frac{\partial p}{\partial z} \right) \\
+ \frac{\partial}{\partial x} \left( k \frac{\partial T}{\partial x} \right) + \frac{\partial}{\partial y} \left( k \frac{\partial T}{\partial y} \right) + \frac{\partial}{\partial z} \left( k \frac{\partial T}{\partial z} \right) + \Phi + \dot{Q}^* \tag{C.9}
\]

**Tensor notation**

\[
\rho \frac{\partial H}{\partial t} + \rho u_i \frac{\partial H}{\partial x_i} = \left( \frac{\partial p}{\partial t} + u_i \frac{\partial p}{\partial x_i} \right) + \frac{\partial}{\partial x_i} \left( k \frac{\partial T}{\partial x_i} \right) + \Phi + \dot{Q}^* \tag{C.10}
\]

Where the dissipation function \( \Phi \) in each type of notation is given by\(^2\):

\[
\Phi = \nabla \cdot (\tau_{ij} \cdot \nabla) - (\nabla \cdot \tau_{ij}) \cdot \nabla \tag{C.11a}
\]

\[
\Phi = \mu \left[ \frac{1}{2} \left( \frac{\partial u_i}{\partial x} \right)^2 + 2 \left( \frac{\partial v}{\partial y} \right)^2 + 2 \left( \frac{\partial w}{\partial z} \right)^2 + \left( \frac{\partial u}{\partial y} + \frac{\partial v}{\partial x} \right)^2 + \left( \frac{\partial u}{\partial z} + \frac{\partial w}{\partial x} \right)^2 + \left( \frac{\partial v}{\partial z} + \frac{\partial w}{\partial y} \right)^2 \\
- \frac{2}{3} \left( \frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} + \frac{\partial w}{\partial z} \right)^2 \right] \tag{C.11b}
\]

\[
\Phi = \tau_{ij} \frac{\partial u_i}{\partial x_j} = \mu \left[ \frac{1}{2} \left( \frac{\partial u_i}{\partial x_j} \right)^2 + \frac{1}{3} \left( \frac{\partial u_i}{\partial x_k} \right)^2 \right] \tag{C.11c}
\]

\(H\) is called the total enthalpy, and is equal to:

\[
H = h + \frac{1}{2} \left( u^2 + v^2 + w^2 \right) = h + \frac{1}{2} u_i u_i \tag{C.12}
\]

For the case of an ideal gas (which is the usual assumption used for steam/air in CFD), the static enthalpy of the fluid can be related to the temperature by the expression:

\[
dh = c_p dT \tag{C.13}
\]

\(^2\) The form of the dissipation function shown here is strictly valid only for problems in a Cartesian coordinate system.
and then equation (C.10) may be written exclusively in terms of temperature, or the conduction term may be written in terms of static enthalpy. One more equation is needed to form a complete set, this is the equation of state for the fluid, which is taken to be the ideal gas law:

\[ \rho = \frac{pM}{RT} \]  

(C.14)

**C.1.4 Conservation of species (mass balance for water vapor)**

**Vector calculus**

\[ \rho \frac{Dm}{Dt} = \nabla \cdot (pD\nabla m) + \dot{m}^* \]  

(C.15)

**Cartesian coordinates**

\[ \rho \left( \frac{\partial m}{\partial t} + u \frac{\partial m}{\partial x} + v \frac{\partial m}{\partial y} + w \frac{\partial m}{\partial z} \right) = \frac{\partial}{\partial x} \left( \rho D \frac{\partial m}{\partial x} \right) + \frac{\partial}{\partial y} \left( \rho D \frac{\partial m}{\partial y} \right) + \frac{\partial}{\partial z} \left( \rho D \frac{\partial m}{\partial z} \right) + \dot{m}^* \]  

(C.16)

**Tensor notation**

\[ \rho \frac{\partial m}{\partial t} + \rho u_i \frac{\partial m}{\partial x_i} = \frac{\partial}{\partial x_i} \left( \rho D \frac{\partial m}{\partial x_i} \right) + \dot{m}^* \]  

(C.17)

**C.1.5 Compressible, weakly compressible, and incompressible flow**

The density of a fluid is a function of the fluid temperature (enthalpy) and pressure. However, there are situations in which the fluid density is independent of changes in temperature, pressure, or both. Table C-1 shows the density dependence for the possible situations along with the auxiliary variables needed to determine the initial density value, and the name given to the type of flow. The auxiliary variables are given in brackets. For instance, density changes in unheated compressible flow depend only on pressure. However, a reference value of enthalpy is needed to determine the absolute value for the density at the beginning of the problem.

The term *compressible* is used to describe a fluid which has a density that is dependent on changes in pressure. Compressible fluids may also be heated or unheated, but there is no distinction made in the name designation. The term *incompressible* is often used to describe a fluid which has a density that is independent of pressure changes, regardless of whether the density changes with temperature. In this thesis, *incompressible* is used exclusively to describe a fluid which has a constant density. That is, the density of an incompressible fluid does not change with either pressure or temperature. In most cases the confusion is alleviated by specifically stating that the fluid is of constant density. A *weakly compressible* fluid (also called thermally expandable) is one in which the density depends on changes in temperature, but is independent of changes in pressure.

The assumption of an incompressible flow is most often associated with modeling liquids where the temperature fluctuation in the problem is small enough to induce only a negligible change in density. (The density of liquids, by their very nature, are only slightly dependent on pressure). Ideal gases are often modeled as constant density when the pressure is low and the velocity of the
gas is low enough that dynamic pressure fluctuations are small. Many researchers have modeled buoyant flow of steam and air mixtures as constant density flow using the Boussinesque approximation in the momentum equation. The constant density assumption allows simplification of the fluid flow equations (see section C.1.6). However, it is usually a better assumption to assume that a low-speed ideal gas is dependent on temperature, and therefore weakly compressible.

<table>
<thead>
<tr>
<th>Table C-1: Fluid designation based on density dependence</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Pressure Dependent</strong></td>
</tr>
<tr>
<td>Unheated</td>
</tr>
<tr>
<td></td>
</tr>
<tr>
<td>Heated</td>
</tr>
<tr>
<td></td>
</tr>
</tbody>
</table>

Note: Variables in brackets [ ] are auxiliary variables needed to determine the initial density value.

C.1.6 Alternate forms of the fluid equations

There are several other forms of the above equations that are encountered in practice. In many cases certain terms in the equations are dropped because they are not important in a particular analysis. For instance, several simplifications can be made for the specific case of constant density (incompressible) flow. If thermal conductivity and viscosity are also constant, the resulting equations are\(^3\): \(^4\):

\[
\nabla \cdot \mathbf{V} = 0
\]

\[
\rho \frac{DV}{Dt} = -\nabla p + \mu \nabla^2 \mathbf{V} + \rho g
\] \hspace{1cm} (C.18)

\[
\rho c_p \frac{DT}{Dt} = \frac{DP}{Dt} + k \nabla^2 T + \mu \Phi + Q^*
\] \hspace{1cm} (C.19)

\[
\Phi = 2 \left[ \left( \frac{\partial u}{\partial x} \right)^2 + \left( \frac{\partial v}{\partial y} \right)^2 + \left( \frac{\partial w}{\partial z} \right)^2 \right] + \left( \frac{\partial u}{\partial y} + \frac{\partial v}{\partial x} \right)^2 + \left( \frac{\partial u}{\partial z} + \frac{\partial w}{\partial x} \right)^2 + \left( \frac{\partial v}{\partial z} + \frac{\partial w}{\partial y} \right)^2
\] \hspace{1cm} (C.20)

\[
\]

\(^3\) The energy equation as written is valid only for an ideal gas, which can be assumed nearly incompressible in the low pressure, low velocity situations studied in this thesis.

\(^4\) Substitution of the mass conservation equation into the expression for the dissipation function results in a simplification for a constant density flow.
C.2 Turbulence Modeling

Turbulence is essentially a vigorous mixing that occurs within a moving fluid; it is a fundamentally unsteady and fully three-dimensional phenomenon. This mixing is most often visualized as eddies which occur within the mean flow field. These eddies cause the flow field to deviate substantially from the behavior of a laminar fluid and molecular properties often have a limited influence on turbulent flows, except near fluid-solid interfaces. The velocity at any distinct point within a turbulent flow is fully three-dimensional, even though the velocity components orthogonal to the direction of mean flow may be small relative to the mean flow velocity. These velocity fluctuations (the eddies) are what cause the significant increase in the transfer of momentum, heat, and mass within the flow itself.

The same characteristics that cause turbulent flows to be efficient transport media also make them difficult to study. Since many flows of engineering interest are turbulent, a great deal of scientific effort has been expended in attempts to describe turbulent behavior. Most turbulence models describe overall flow behavior quite well for the specific situations for which the models were designed. However, no turbulence model to date has been proposed which is sufficiently general to be applicable to all turbulent flows. This section (C.2) provides a brief overview of turbulence modeling starting from the theoretical fluid flow equations and continuing to the details of several specific models which are in wide use.

Most of the turbulence models in this appendix are presented in the context of a constant density, forced convection boundary layer flow even though this thesis is concerned mainly with a natural convection weakly compressible flow. There are several reasons for this. First, the flow equations for constant density two-dimensional boundary layer flow are much simplified from the fully compressible three-dimensional equations presented in section C.1. This allows the primary features of a turbulence model to be clearly presented without the added clutter of complex flow equation terms. Second, to keep the analyses computationally feasible, most early turbulence models were developed for forced flows that could be assumed incompressible. In some cases the extension to natural convection flows or to compressible fluids are given, but the reader should refer to the cited reference for full details.

C.2.1 Direct numerical simulation (DNS)

A time dependent solution of the conservation equations for mass, momentum, and energy will describe all flows, whether they be laminar or turbulent. However, the velocity fluctuations, or eddies, which constitute turbulence occur over a huge range of physical and temporal scales. Large eddies, which can be on the order of pipe diameters in length, play the most important role in the transport of heat and momentum. These large eddies also have a relatively long lifetime within the flow. The large eddies transfer energy to smaller eddies, which again transfer energy to eddies which are smaller still. This cascading process continues until the smallest eddies transfer their kinetic energy to heat via viscous dissipation in the fluid on a very small time scale. The physical scale of the smallest eddies is typically several orders of magnitude less than that of the large eddies. In order for a computer calculation to correctly predict turbulent flow, the size of the flow field which is modeled must be large enough to simulate the large eddies. However,
the discretization of the flow field must be fine enough to capture the smallest dissipating eddies. This fine discretization, along with the need for very small time steps, caused the calculation to be extremely expensive, even by modern computer standards. Direct Numerical Simulation (DNS) is the name given to this type of simulation. DNS offers great potential for providing a fundamental understanding of turbulence phenomena and the data necessary to validate other turbulence models. However, to date the prohibitive expense of this type of calculation has limited the application of the technique to flows with low Reynolds numbers, the highest being about 10,000. Clearly, DNS holds promise for further development, but does not currently offer a practical engineering solution to modeling turbulent fluids [Wilcox, 1993].

C.2.2 Large eddy simulation (LES)

Large eddy simulation follows along the lines of direct numerical simulation, except that the smallest eddies are “modeled” instead of simulated. Below a certain size, the eddies are not deemed important in determining the fluctuations in velocity, momentum, or heat transfer. However, these small eddies are important in that they dissipate into heat, and thus they can not be ignored completely. The large eddies are directly influenced by the flow field and boundary conditions, which leads to them being primary candidates for simulation, while the small eddies are nearly isotropic and more amenable to modeling. This relaxation in the limits of the physical scale of discretization leads to an order of magnitude reduction in the number of grid points necessary to perform a LES versus a DNS. Also, since the smallest eddies occur on the smallest time scale, much larger time steps are allowable in LES simulations.

The prospects for LES to become an important design tool for future use is obvious, however the technique currently has several shortcomings. The first is the amount of computer resources required. Even though LES offers a decrease of an order of magnitude in the required number of grid points and can use much larger time steps than DNS, the amount of computer resources necessary to compute a flow of engineering importance is still prohibitively expensive. Also, LES requires satisfactory modeling of the small eddies to produce closure which sometimes results in a very complex additional set of equations. Advances in LES are very important in helping to verify and improve other methods of turbulence modeling, and the technique continues to advance in the scientific community. [Wilcox, 1993].

C.2.3 Mean flow equations (Reynolds averaging)

The prohibitive nature of simulating turbulent eddies outright has led to the development of turbulence models. These models essentially calculate additional scalar quantities that are transported throughout the flow. These scalar quantities which are assumed to represent key aspects of the turbulent flow, and are used to augment the molecular diffusivities for mass, momentum, and heat transfer. The vast majority of practical turbulent fluid flow problems involve time average quantities such as skin friction coefficient, mean velocity, or heat transfer coefficient. Along these lines, most of the turbulence models start from a “mean flow” formulation. To derive the mean flow formulation, each variable in the conservation equations is separated into an average and a fluctuating component, for example:

\[ \mathbf{u}(x, y, z, t) = \bar{\mathbf{u}}(x, y, z) + \mathbf{u}'(x, y, z, t) \]  

(C.22)
where $\overline{u}(x, y, z)$ indicates the mean value and $u'(x, y, z, t)$ indicates the fluctuating component where the mean value is defined as:

$$
\overline{u} = U = \frac{1}{\Delta t} \int_{t_0}^{t_0+\Delta t} u \, dt
$$

(C.23)

The physical variables are thus decomposed as:

$$
u = \overline{\nu} + \nu' \quad v = \overline{v} + v' \quad w = \overline{w} + w' \quad \rho = \overline{\rho} + \rho'$$

$$h = \overline{h} + h' \quad T = \overline{T} + T' \quad H = \overline{H} + H' \quad p = \overline{p} + p'$$

(C.24)

It follows that the time average of a fluctuating component is equal to zero:

$$
\overline{u'} = \frac{1}{\Delta t} \int_{t_0}^{t_0+\Delta t} u' \, dt = 0
$$

(C.25)

A capital letters indicates a mean value for a single variable, while an overbar can signify the time average of one or multiple variables. This type of averaging is usually referred to as Reynolds-averaging and is valid for constant density flows only. The mean flow formulation for the constant density conservation equations of mass and momentum is derived below by substituting the decomposed variables into the equations and then performing the Reynolds-averaging technique.

Mass conservation in Cartesian coordinates:

$$
\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} + \frac{\partial w}{\partial z} = \frac{\partial (\overline{u} + u')}{\partial x} + \frac{\partial (\overline{v} + v')}{\partial y} + \frac{\partial (\overline{w} + w')}{\partial z}
$$

$$
= \left( \frac{\partial \overline{u}}{\partial x} + \frac{\partial \overline{v}}{\partial y} + \frac{\partial \overline{w}}{\partial z} \right) + \left( \frac{\partial u'}{\partial x} + \frac{\partial v'}{\partial y} + \frac{\partial w'}{\partial z} \right) = 0
$$

(C.26)

Taking the Reynolds-average we have:

$$
\left( \frac{\partial \overline{u}}{\partial x} + \frac{\partial \overline{v}}{\partial y} + \frac{\partial \overline{w}}{\partial z} \right) = 0
$$

(C.27)

In general tensor notation the Reynolds-averaged continuity equation appears as:

$$
\frac{\partial \overline{u}_i}{\partial x_i} = \frac{\partial \overline{U}_i}{\partial x_i} = 0
$$

(C.28)
The constant property instantaneous Navier-Stokes equation ((C.19) ignoring the gravitational body force) in tensor notation is:

\[
\rho \frac{\partial u_i}{\partial t} + \rho u_j \frac{\partial u_i}{\partial x_j} = -\frac{\partial p}{\partial x_i} + \frac{\partial}{\partial x_j} \left[ \mu \left( \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) - \rho u_i u_j' \right]
\]

After performing the Reynolds-averaging technique the equation becomes:

\[
\rho \frac{\partial \bar{u}_i}{\partial t} + \rho \bar{u}_j \frac{\partial \bar{u}_i}{\partial x_j} = -\frac{\partial \bar{p}}{\partial x_i} + \frac{\partial}{\partial x_j} \left[ \mu \left( \frac{\partial \bar{u}_i}{\partial x_j} + \frac{\partial \bar{u}_j}{\partial x_i} \right) - \rho \bar{u}_i \bar{u}_j' \right] \tag{C.30}
\]

Comparing the Reynolds averaged Navier-Stokes equation with the original equation, we see that there is an added term in the viscous component. The term \(-\rho \bar{u}_i \bar{u}_j'\) is called the Reynolds stress tensor, or simply the Reynolds stress. This added term appears to be a viscous term, but it arises from fluctuations of the velocity components in the convective terms. The Reynolds stress tensor adds additional unknowns to the system of equations, and thus the formulation is not mathematically closed. Turbulence modeling centers around ways to predict the values of the terms in the Reynolds stress tensor.

For compressible flows, the time-average is not sufficient and a mass-averaging technique, called Favre-averaging, must be performed for the velocity components and the thermal variables (the pressure and density are time-averaged as before). The mass-average of each of the variables is defined as:

\[
\bar{u} = \frac{\bar{P} \bar{u}_i}{\bar{P}} \quad \bar{v} = \frac{\bar{P} \bar{v}}{\bar{P}} \quad \bar{w} = \frac{\bar{P} \bar{w}}{\bar{P}} \quad \bar{h} = \frac{\bar{P} \bar{h}}{\bar{P}} \quad \bar{T} = \frac{\bar{P} \bar{T}}{\bar{P}} \quad \bar{H} = \frac{\bar{P} \bar{H}}{\bar{P}} \tag{C.31}
\]

The variables are now decomposed into mean and fluctuating parts as:

\[
u = \bar{u} + u' \quad v = \bar{v} + v' \quad w = \bar{w} + w' \quad \rho = \bar{\rho} + \rho' \tag{C.32}
\]

\[
h = \bar{h} + h' \quad T = \bar{T} + T' \quad H = \bar{H} + H' \quad p = \bar{p} + p'
\]

In the case of Favre-averaging, the mean of a double prime quantity is not equal to zero, instead the following relations hold true:

\[
\bar{u}' = -\frac{\bar{\rho}' \bar{u}'}{\bar{\rho}} \quad \bar{\rho} u' \equiv 0 \tag{C.33, C.34}
\]

\[
5 \text{ A complete description of the Reynolds-averaging and Favre-averaging techniques can be found in [Wilcox, 1993], [Schlichting, 1979], or [Tannehill, 1997].}
\]
Performing the Favre-averaging technique results in the following set of equations for fully compressible flow with heat transfer [Tannehill, 1997]:

\[ \frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x_j}(\rho \bar{u}_j) = 0 \]  
\[ \text{(C.35)} \]

\[ \frac{\partial}{\partial t}(\rho \bar{u}_j) + \frac{\partial}{\partial x_j}(\rho \bar{u}_i \bar{u}_j) = -\frac{\partial \rho}{\partial x_i} + \frac{\partial}{\partial x_j} \left[ \bar{T}_j - \rho \bar{u}_i \bar{u}_j \right] \]  
\[ \text{(C.36)} \]

\[ \frac{\partial}{\partial t}(\rho \bar{H}) + \frac{\partial}{\partial x_j}(\rho \bar{u}_j \bar{H} + \rho \bar{u}_i \bar{H} - k \frac{\partial T}{\partial x_j}) = \frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x_j} \left( \bar{u}_i \bar{\tau}_{ij} + \bar{u}_j \bar{\tau}_{ij} \right) \]  
\[ \text{(C.37)} \]

where

\[ \bar{\tau}_{ij} = \mu \left[ \left( \frac{\partial \bar{u}_i}{\partial x_j} + \frac{\partial \bar{u}_j}{\partial x_i} \right) - \frac{2}{3} \delta_{ij} \frac{\partial \bar{u}_k}{\partial x_k} \right] + \mu \left[ \left( \frac{\partial \bar{u}_i^*}{\partial x_j} + \frac{\partial \bar{u}_j^*}{\partial x_i} \right) - \frac{2}{3} \delta_{ij} \frac{\partial \bar{u}_k^*}{\partial x_k} \right] \]  
\[ \text{(C.38)} \]

Strictly speaking, there is no energy transfer in an incompressible flow, thus no energy equation was given when discussing constant density flows earlier in this section. However, it is often convenient to treat engineering flows with heat transfer as nearly-incompressible, thus a useful relationship is the constant density energy equation. This energy equation can be reduced from equation (C.37) and is given below in terms of temperature:

\[ \frac{\partial}{\partial t}(\rho c_p \bar{T}) + \frac{\partial}{\partial x_j}(\rho c_p \bar{T} \bar{u}_j) = \frac{\partial \rho}{\partial t} + \bar{u}_j \frac{\partial \rho}{\partial x_j} + \bar{u}_j^* \frac{\partial \rho^*}{\partial x_j} + \frac{\partial}{\partial x_j} \left( k \frac{\partial T}{\partial x_j} - \rho c_p \bar{T} \bar{u}_j \right) + \Phi \]  
\[ \text{(C.39)} \]

\[ \Phi = \bar{T}_{ij} \frac{\partial u_i}{\partial x_j} = \bar{T}_{ij} \frac{\partial u_i}{\partial x_j} + \bar{T}_{ij} \frac{\partial u_j}{\partial x_i} \]
\[ \bar{T}_{ij} = \mu \left( \frac{\partial \bar{u}_i}{\partial x_j} + \frac{\partial \bar{u}_j}{\partial x_i} \right) \]  
\[ \text{(C.40, C.41)} \]

**C.2.4 Boundary layer equations**

There are two general types of turbulent flows: wall bounded flow and free shear flows. In this thesis we are concerned only with wall bounded flows, and specifically with flow in the boundary layer. The concept of a boundary layer was proposed by Prandtl, and is commonly described as a thin layer near a fluid boundary where viscous effects are as important as inertial effects. The two key assumptions which are most often exploited when studying boundary layer flow are that the viscous sublayer is thin relative to the characteristic dimension of the flow, and that the largest viscous term is on the same order of magnitude as any of the inertial terms. By invoking these assumptions and performing a scale analysis, Prandtl concluded that the second derivatives of velocity components in the direction of main flow are small compared to corresponding derivatives in the transverse direction; thus the momentum equation in the transverse direction can be ignored [Tannehill, 1997] [Schlichting, 1979]. For a nominally two-dimensional boundary layer (which is the kind studied here), these assumptions result in the incompressible boundary layer equations of the form (ignoring the buoyancy term for simplicity):
Performing the Reynolds-averaging technique discussed previously, the mean flow formulation for the turbulent boundary layer flow is:

\[
\frac{\partial U}{\partial x} + \frac{\partial V}{\partial y} = 0 \tag{C.44}
\]

\[
\rho \left( \frac{\partial U}{\partial t} + U \frac{\partial U}{\partial x} + V \frac{\partial U}{\partial y} \right) = -\frac{dP}{dx} + \mu \frac{\partial^2 U}{\partial y^2} - \frac{\partial (\rho u'v')}{\partial y} \tag{C.45}
\]

Based on the boundary layer hypothesis and experimental data, \( \frac{\partial (u'v')}{\partial y} \gg \frac{\partial (u'u')}{\partial x} \), thus the term \( \frac{\partial (u'v')}{\partial x} \) is ignored. Also, for a steady state solution, the first term in the momentum equation drops out. Thus the steady state mean flow formulation for the incompressible turbulent boundary layer equations (ignoring buoyancy) is:

\[
\frac{\partial U}{\partial x} + \frac{\partial V}{\partial y} = 0 \tag{C.46}
\]

\[
\rho \left( U \frac{\partial U}{\partial x} + V \frac{\partial U}{\partial y} \right) = -\frac{dP}{dx} + \mu \frac{\partial^2 U}{\partial y^2} - \frac{\partial (\rho u'v')}{\partial y} \tag{C.47}
\]

Rewriting the momentum equation, it is easy to see the Reynolds stress and the viscous stress.

\[
U \frac{\partial U}{\partial x} + V \frac{\partial U}{\partial y} = -\frac{1}{\rho} \frac{dP}{dx} + \frac{1}{\rho} \frac{\partial}{\partial y} \left( \mu \frac{\partial U}{\partial y} - \rho u'v' \right) \tag{C.48}
\]

Whereas the Reynolds-averaged Navier-Stokes equation resulted in a turbulent stress tensor, the simplified boundary layer equation has only a single turbulent stress term. However, this term is still an unknown quantity and must be modeled. Several of the remaining sections of this appendix discuss different methods to model the Reynolds stress term.

Before a discussion of the turbulent stress models can ensue, a brief overview of the terminology of boundary layer theory is helpful at this point. Conceptually, the boundary layer is the fluid region where the wall effects are important in influencing the flow. Boundary layers are very important for calculating heat transfer between a solid surface and a fluid. In forced convection boundary layers, the fluid velocity is zero at the wall and approaches the free stream velocity at
the edge of the boundary layer. For a natural convection boundary layer, the fluid velocity is zero at the wall, reaches a maximum close to the wall, and then approaches zero (or stagnation) again near the free stream (which is usually considered to be a non-moving fluid). Most turbulence models were developed for forced flow situations, thus the background on the models will naturally center on force flow boundary layers. A few turbulence models were later shown to predict good results for natural convection boundary layers, and this is indicated for the different models where appropriate.

A typical forced flow boundary layer has three distinct regions of interest: the laminar (or viscous) sublayer, the log layer, and the defect layer. The laminar sublayer is that region very close to the wall where the viscous stresses are more important than the turbulent stresses, thus the fluid behaves according to laminar flow equations. The log layer is the region of the boundary layer which is sufficiently close to the wall such that inertial terms can be ignored in the momentum equation but where the turbulent stresses outweigh the viscous stresses. The “law of the wall”, which is generally agreed to be a universal dimensionless velocity profile for turbulent flow near a solid structure, applies in the log layer. The defect layer is between the log layer and the free stream.

Boundary layers are often discussed in terms of dimensionless velocities and distances. An important normalizing quantity is the friction velocity defined as:

$$u_* = \sqrt{\frac{\tau_w}{\rho}} = U_e \sqrt{\frac{C_f}{2}}$$

where $\tau_w$ is the shear stress at the wall. (Recall that the skin friction coefficient is defined as:

$$C_f = \frac{\tau_w}{\frac{1}{2} \rho U_e^2}$$

where $U_e$ is the free stream velocity). The friction velocity is used to normalize the streamwise velocity and distance normal to the wall as follows:

$$u^+ = \frac{u}{u_*} \quad y^+ = \frac{yu_*}{v}.$$  \hspace{1cm} (C.51, C.52)

In the laminar sublayer, it is generally accepted that the velocity profile behaves according to the following relationship:

$$u^+ = y^+ \quad 0 \leq y^+ \leq 7.$$  \hspace{1cm} (C.53, C.54)

The law of the wall, which is used for the region termed the log layer, is the relationship:
\[ u^+ = \frac{1}{\kappa} \ln y^+ + B \] (C.55)

where \( \kappa \) is called the von Karman constant. The constants are usually taken to be close to the following values:

\[ \kappa = 0.41 \quad B \approx 5.0 \] (C.56, C.57)

To describe the defect layer, also called the "wake", an addition term is added to the expression for the law of the wall:

\[ u^+ = \frac{1}{\kappa} \ln y^+ + B + 2 \frac{\Pi}{\kappa} \sin^2 \left( \frac{\pi y}{2 \delta} \right), \] (C.58)

where \( \Pi \approx 0.51 \). This expression is sometimes referred to as the "law of the wake."

In turbulence modeling, these laws are used to derive wall functions. Wall functions allow a turbulent flow simulation to include the effects of a boundary layer without actually having any computational nodes within the layer itself. This technique saves a great deal of computational expense since the gradients in the boundary layer are quite large and would require many nodes to adequately calculate the flow. A more complete discussion of these concepts can be found in [Wilcox, 1993]. A more thorough discussion of boundary layer analysis in general can be found in [Schetz, 1984] or [Schlichting, 1979].

Natural convection boundary layers are quite different from forced convection boundary layers since in natural convection the velocity maximum occurs within the boundary layer. A law-of-the-wall type formulation for natural convection boundary layers is not discussed here. The near-wall effects are very important for natural convection, and thus it is often advantageous to calculate the flow within the boundary layer, and especially the viscous sublayer, to correctly predict the rates of heat and/or mass transfer.

### C.2.5 Algebraic models

The simplest methods proposed for modeling turbulence are based on what is called an eddy viscosity, first proposed by J. Boussinesq\(^6\). The basis for the eddy viscosity model is to assume that turbulent transfer of momentum is analogous to molecular transfer of momentum\(^7\) - in other words that the turbulent shear stress is isotropic and related to the mean strain rate. Thus for the turbulent stress we have:

\[ \tau_{xy} = \tau_r = -\rho u' v' = \mu_r \frac{\partial U}{\partial y} \] (C.59)

---

\(^6\) The eddy viscosity is also sometimes called the Boussinesq approximation, which is different than the well known Boussinesq approximation employed when modeling buoyancy in a virtually incompressible fluid.

\(^7\) Some of the more complex turbulence models are also presented in the form of an eddy viscosity.
where $\mu_e$ is the eddy viscosity. The momentum boundary layer equation then takes the form:

$$
\rho U \frac{\partial U}{\partial x} + \rho V \frac{\partial U}{\partial y} = -\frac{dP}{dx} + \frac{\partial}{\partial y} \left( (\mu + \mu_e) \frac{\partial U}{\partial y} \right).
$$

(C.60)

The best known algebraic model for predicting the turbulent shear stress is called the mixing length model. Prandtl proposed the mixing length model drawing the analogy that the mixing length is similar to the mean free path of molecules. The kinetic theory of gases dictates that the molecular viscosity is given by:

$$
\mu = \frac{1}{3} \rho \text{(mean free path)} \text{(mean molecular speed)}
$$

(C.61)

The eddy viscosity is given by the simple equation:

$$
\mu_e = \rho \ell_m v_t
$$

(C.62)

where $v_t$ is a characteristic turbulent speed. The second part of the mixing length hypothesis approximates this turbulent speed as:

$$
v_t = \ell_m \left| \frac{\partial U}{\partial y} \right|.
$$

(C.63)

The eddy viscosity and the Reynolds stress are then given by:

$$
\mu_e = \rho \ell_m^2 \left| \frac{\partial U}{\partial y} \right| \quad \tau_t = -\rho u' v' = \rho \ell_m^2 \left| \frac{\partial U}{\partial y} \right| \frac{\partial U}{\partial y}.
$$

(C.64, C.65)

The simplest form of the Prandtl mixing length is given by:

$$
\ell_m = K y
$$

(C.66)

which comes directly from the law of the wall (see Schetz, 1984 for the mathematical derivation). However, as one approaches the wall, the turbulence is damped out by the presence of the wall. A well known correction for this effect was proposed by Van Driest. The Van Driest mixing length model for the inner boundary layer region (laminar sublayer and log layer) is:

$$
\ell_m = K y \left[ 1 - \exp \left( -\frac{y^*}{26v} \right) \right]
$$

(C.67)

the eddy viscosity equivalent is:
For the outer region of the boundary layer, where wall effects are not important, the mixing length is proportional to the width of the boundary layer. The following relation has been used by Patankar and Spalding with good results [Schetz, 1984]:

\[ \ell_m = 0.098 \]

where the width of the boundary layer, \( \delta \), is usually assumed to be the point at which the flow reaches 95% of the free stream value.

In a calculation, the inner region mixing length (eddy viscosity) is used starting at the wall and continuing out until it matches the value given by the model for the outer region. The outer region mixing length is then used for the remainder of the boundary layer thickness. (For a complete description of the history of mixing length formulations see [Schlichting, 1979]).

While the simplicity of these models is clear, picking the correct mixing length is a challenge. The mixing length formulation is termed an algebraic, or zero equation, model because the evaluation of the Reynolds stress does not require the solution of a differential equation, as some more complex turbulence models do. The methods described above give generally good performance for forced convection boundary layer calculations since the constants have been tuned for this application. The mixing length and eddy viscosity models do suffer from a major shortfall. They are both of a form called “gradient transport formulations” since the gradient of the mean flow velocity is used in the expression of the turbulent stress. This implies that the Reynolds stress vanishes at local maxima or minima in the velocity profile. This is not the case in reality. However, this limitation is often of little consequence for forced convection boundary layers. In natural convection boundary layers, which is the major concern in this thesis, this limitation is important. The maximum velocity for natural convection is deep in the boundary layer, thus these simple models are probably not suitable for analyses of these cases.

**C.2.6 One-equation models**

The next level of complexity in turbulence modeling is based on solving a differential transport equation for the **turbulent kinetic energy** (TKE). The turbulent kinetic energy is defined to be the kinetic energy of the fluctuating velocity components of the flow:

\[ K = \frac{u'^2 + v'^2 + w'^2}{2} = \frac{1}{2} u'u' \]  

A differential equation for the transport of turbulent kinetic energy is derived by taking a moment of the Navier-Stokes equations and performing the Reynolds-averaging technique described previously. The resulting transport equation for the TKE is (in tensor notation) [Wilcox, 1993]:

\[ \mu_t = \rho \kappa^2 y^2 \left[ 1 - \exp \left( -\frac{y u_*}{26v} \right) \right] \frac{\partial U}{\partial y} . \]  

(C.68)
\[ \rho \frac{\partial K}{\partial t} + \rho \overline{u}_i \frac{\partial K}{\partial x_j} = \tau_y \frac{\partial \overline{u}_i}{\partial x_j} - \rho \varepsilon + \frac{\partial}{\partial x_j} \left[ \left( \mu + \frac{\mu_t}{\sigma_K} \right) \frac{\partial K}{\partial x_j} \right] \]  \hspace{1cm} (C.71)

where the Reynolds stress tensor takes the form\(^8\):

\[ \tau_y = 2\mu_t S_y - \frac{2}{3} \rho K \delta_{ij} \]  \hspace{1cm} (C.72)

and the mean strain-rate tensor is given by:

\[ S_y = \frac{1}{2} \left( \frac{\partial \overline{u}_i}{\partial x_j} + \frac{\partial \overline{u}_j}{\partial x_i} \right). \]  \hspace{1cm} (C.73)

The quantity \( \varepsilon \) is the dissipation per unit mass and it is given by the correlation:

\[ \varepsilon = \mu \frac{\partial \overline{u}_i}{\partial x_k} \frac{\partial \overline{u}_i}{\partial x_k} \]  \hspace{1cm} (C.74)

and \( \sigma_K \) is a Prandtl number for turbulent kinetic energy. This type of formulation is called a one-equation turbulence model because there is a single partial differential equation which is solved for a single variable, namely the turbulent kinetic energy. Each term on the right hand side of the TKE equation must be modeled in terms of the quantities \( \overline{u}, K \), or other auxiliary variables.

A well known form of the TKE model used in boundary layer analysis is called the Prandtl Energy method which takes the form:

\[ \rho \left( \frac{U \partial K}{\partial x} + V \frac{\partial K}{\partial y} \right) = \rho \sqrt{K} \ell \left( \frac{\partial U}{\partial y} \right)^2 - C_D \frac{\rho K}{\ell} - \frac{\partial}{\partial y} \left( \frac{\rho \sqrt{K} \ell}{\sigma_K} \frac{\partial K}{\partial y} \right) \]  \hspace{1cm} (C.75)

where \( \ell \) is a length scale, similar to (but not the same as) the mixing length, \( \sigma_K \) is again the Prandtl number for turbulent kinetic energy (\( \sigma_K = 1.0 \)), and \( C_D \) is an empirical constant (\( 0.07 \leq C_D \leq 0.09 \)). Modeling of the dissipation term \( \varepsilon \) is well accepted, but the diffusion and production terms are modeled differently by different researchers. The Prandtl energy method uses the eddy viscosity approach to model the Reynolds stress and is therefore limited accordingly:

---

\(^8\) \( \delta_{ij} \) is the Kronecker delta, which is equal to unity for \( i = j \), and zero otherwise.
\[ \mu_\tau = \rho \sqrt{K} \ell. \] (C.76)

One advantage of this type of turbulence model for the eddy viscosity, as compared to a zero equation model, is that the eddy viscosity does not vanish when the velocity gradient vanishes thus making this type of model more applicable to natural convection boundary layers.

For the limiting case, close to the wall, the convection and diffusion terms are negligible. Setting the production and dissipation equal we get

\[ \rho \sqrt{K} \ell \left( \frac{\partial U}{\partial y} \right)^2 = C_D \rho \frac{K^{\frac{\nu}{\ell}}}{\ell}. \] (C.77)

Comparing this with the Prandtl mixing length model it can be shown that

\[ \ell = \ell_m C_D \frac{\nu}{\ell}. \] (C.78)

which means that the previously defined mixing length models can be used to model the quantity \( \ell \). Further scrutiny shows that this TKE method collapses to the familiar mixing length method near the wall. Thus the differences in prediction of turbulence parameters between the TKE method and the mixing length methods discussed previously must occur in the outer boundary layer region. The one equation turbulence models suffer from limitations most often associated with the way in which the characteristic length scale is evaluated. Since the characteristic length must be “modeled”, the one equation turbulence formulations are not complete. In order to model the length scale, the state of the flow must be known in advance. Much effort has been invested in two equation turbulence models to overcome this limitation for describing more general flow situations.

### C.2.7 Two-equation models

The two equation turbulence models are based on one differential equation for the turbulent kinetic energy and a second differential equation for the characteristic length scale (or the dissipation rate). The most popular two equation model is called the \( K-\epsilon \) model. The \( K-\epsilon \) model is based on the turbulent kinetic energy equation already given as eq. (C.71) and an equation for the dissipation rate \( \epsilon \). The dissipation has already been defined in eq. (C.74). A transport equation for \( \epsilon \) is derived by taking the appropriate moment of the Navier-Stokes equation and performing the correct averaging. The resulting equation is extremely complex, and there is little chance of solving the exact equation for any case of interest. The exact equation for \( \epsilon \) is thus transformed by modeling of several terms. The general form of the “standard” \( K-\epsilon \) model (based on the papers [Jones, 1972] [Launder, 1974]) is given by [Wilcox, 1993]:

\[ \rho \frac{\partial K}{\partial t} + \rho \left[ \bar{u}_i \frac{\partial K}{\partial x_i} - \rho \epsilon + \frac{\partial}{\partial x_j} \left( \mu + \frac{\mu_\tau}{\sigma_\epsilon} \frac{\partial K}{\partial x_j} \right) \right]. \] (C.79)
where the eddy viscosity is defined as:

\[ \mu_t = \rho C_\mu \frac{K^2}{\varepsilon} \]  
(C.81)

and the closure coefficients for most cases are defined as:

\[ C_{e_1} = 1.44 \quad C_{e_2} = 1.92 \quad C_\mu = 0.09 \quad \sigma_K = 1.0 \quad \sigma_\varepsilon = 1.3 \]  
(C.82)

The steady state, incompressible boundary layer equations for the standard K-\( \varepsilon \) model are easily arrived at by applying the boundary layer assumptions:

\[
\frac{\partial K}{\partial x} + \frac{\partial K}{\partial y} = \mu_t \left( \frac{\partial U}{\partial y} \right)^2 - \rho \frac{\partial}{\partial y} \left[ \mu_t + \frac{\mu_t}{\sigma_K} \right] \frac{\partial K}{\partial y} + G
\]  
(C.83)

\[
\frac{\partial \varepsilon}{\partial x} + \frac{\partial \varepsilon}{\partial y} = C_{e_1} \frac{\varepsilon}{K} \mu_t \left( \frac{\partial U}{\partial y} \right)^2 - C_{e_2} \frac{\varepsilon^2}{K} \frac{\partial}{\partial y} \left[ \mu_t + \frac{\mu_t}{\sigma_\varepsilon} \right] \frac{\partial \varepsilon}{\partial y}
\]  
(C.84)

where \( G \) is an extension to the standard model to account for production due to buoyancy:

\[
G = \frac{\mu_t}{Pr_t \varepsilon} \left( \frac{\rho - \rho\infty}{\rho} \right)
\]  
(C.85)

The standard K-\( \varepsilon \) model, although very popular, suffers from one major shortfall which is of primary concern here. It is impossible to predict the correct behavior in the viscous sublayer using the “standard” model - because no terms are present which will account for the turbulence damping which occurs near a solid boundary. There are numerous modifications to the K-\( \varepsilon \) model to account for the damping of \( K \) at the wall, these are called low-Reynolds-number modifications. The main aim is to achieve an asymptotic prediction of the velocity profile near the wall (ie. reproduce the law-of-the-wall). The landmark papers of Jones & Launder [Jones, 1972] and Launder & Sharma [Launder, 1974], where the “standard” model comes from, were actually concerned with the low-Reynolds-number effects. The low-Reynolds-number K-\( \varepsilon \) model of Jones & Launder with coefficients from Launder & Sharma is given by the following equations:

\[ \rho \frac{\partial \varepsilon}{\partial t} + \rho \bar{u}_j \frac{\partial \varepsilon}{\partial x_j} = C_{e_1} \frac{\varepsilon}{K} \tau_j \frac{\partial \bar{u}_i}{\partial x_j} - C_{e_2} \frac{\varepsilon^2}{K} \frac{\partial}{\partial x_j} \left[ \left( \mu_t + \frac{\mu_t}{\sigma_\varepsilon} \right) \frac{\partial \varepsilon}{\partial x_j} \right] \]  
(C.80)

9 It has been shown that buoyant production for gases with Pr–0.7 is negligible [Lin, 1978; Kasagi, 1997].

10 The “low” in low Reynolds number turbulence models refers to the Reynolds number of turbulence, eq. (C.89f), which decreases as one approaches the wall.
\[ \mu_t = C_{t} \mu_{t} \rho \frac{K^2}{\varepsilon} \]  

\[ \rho U \frac{\partial K}{\partial x} + \rho V \frac{\partial K}{\partial y} = \mu_t \left( \frac{\partial U}{\partial y} \right)^2 - \rho \varepsilon + \frac{\partial}{\partial y} \left[ \mu + \frac{\mu_t}{\sigma_k} \frac{\partial K}{\partial y} \right] - \varepsilon_0 \]  

\[ \rho U \frac{\partial \varepsilon}{\partial x} + \rho V \frac{\partial \varepsilon}{\partial y} = C_{t1} f_1 \frac{\varepsilon}{K} \left( \frac{\partial U}{\partial y} \right)^2 - C_{t2} f_2 \frac{\rho \varepsilon^2}{K} + E + \frac{\partial}{\partial y} \left[ \mu + \frac{\mu_t}{\sigma_\varepsilon} \frac{\partial \varepsilon}{\partial y} \right] \]  

where \( \varepsilon_0 \) is the value of \( \varepsilon \) at the wall. The damping functions and closure coefficients for the Launder-Sharma model are shown below (the remaining constants are given in eq. (C.82)):

\[ f_\mu = \exp \left( -3.4 \left( 1 + \frac{Re_t}{50} \right)^2 \right) \]  

\[ f_1 = 1 \]  

\[ f_2 = 1 - 0.3 \exp(-Re_t^2) \]  

\[ \varepsilon_0 = 2 \mu \left( \frac{\partial \sqrt{K}}{\partial y} \right)^2 \]  

\[ E = 2 \frac{\mu \mu_t}{\rho} \left( \frac{\partial^2 U}{\partial y^2} \right)^2 \]  

\[ \text{Re}_t = \frac{\rho K^2}{\mu \varepsilon} \]  

A second, less well known, two equation model is the \( K-\omega \) model. The second parameter in this model, \( \omega \), is the rate of dissipation per unit turbulent kinetic energy \( \left( \omega \propto \varepsilon/K \right) \). The \( K-\omega \) model again uses equation (C.71) for the turbulent kinetic energy, and then prescribes a similar equation for \( \omega \). The dissipation rate and eddy viscosity are given by the following relations:

\[ \varepsilon = \beta^* \omega K \]  

\[ \mu_t = \rho \frac{K}{\omega} \]  

The two-dimensional, incompressible boundary layer equations for the Wilcox \( K-\omega \) model are [Wilcox, 1993]:

\[ \rho U \frac{\partial K}{\partial x} + \rho V \frac{\partial K}{\partial y} = \mu_t \left( \frac{\partial U}{\partial y} \right)^2 - \beta^* \rho \omega K + \frac{\partial}{\partial y} \left[ \mu + \sigma^* \mu_t \frac{\partial K}{\partial y} \right] \]  

\[ \rho U \frac{\partial \omega}{\partial x} + \rho V \frac{\partial \omega}{\partial y} = \alpha \frac{\omega}{K} \mu_t \left( \frac{\partial U}{\partial y} \right)^2 - \beta \rho \omega^2 + \frac{\partial}{\partial y} \left[ \mu + \sigma \mu_t \frac{\partial \omega}{\partial y} \right] \]  

\[ \alpha = 5/9 \quad \beta = 3/40 \quad \beta^* = 9/100 \quad \sigma = 1/2 \]  

Wilcox compared several low-Reynolds-number \( K-\varepsilon \) models with the \( K-\omega \) model and concludes the following. The low-Reynolds-number corrections, which help to reproduce the correct velocity profiles near the wall, do not help in producing the correct value of skin friction
[Wilcox, 1993]. All low-Reynolds number $K$-$\varepsilon$ models compared showed large errors for $C_f$. In contrast, the $K$-$\omega$ model can be integrated through the viscous sublayer without any modifications and produces reasonably accurate results. Both the $K$-$\varepsilon$ and $K$-$\omega$ models predict transition from laminar to turbulent flow at Reynolds numbers which are an order of magnitude too small.

The $K$-$\varepsilon$ model is also not accurate for describing boundary layers with adverse pressure gradients (i.e., where the pressure field is causing the flow to decelerate - this usually leads to boundary layer separation), while the $K$-$\omega$ model does produce reasonably accurate results. The main advantage of the $K$-$\varepsilon$ model is that it is not sensitive to values of freestream boundary conditions for free shear flows, while the $K$-$\omega$ is. However, for wall boundary conditions, the standard $K$-$\varepsilon$ model requires accurate wall functions to be specified, which often cause instabilities in the numerical scheme. According to Wilcox, the $K$-$\omega$ model is better than the low-Reynolds-number $K$-$\varepsilon$ model for boundary layer calculations [Wilcox, 1993]. The $K$-$\varepsilon$ model also is reportedly not capable of predicting accurate results for surface injection [Schetz, 1984], which implies that mass transfer calculations using the $K$-$\varepsilon$ model may prove problematic.

### C.2.8 Algebraic stress model (ASM)

The primary assumption for all of the models discussed so far has been the use of the Boussinesq eddy viscosity concept. There are many cases where the eddy viscosity approach fails, most related to unequal normal Reynolds stresses or sudden changes in mean strain rate. Examples of where the eddy viscosity concept is inaccurate are flow over a curved surface, flow in a duct with secondary motion, three-dimensional flow, and boundary layer separation. In order to obtain realistic calculations for these flows, the Reynolds stresses must be computed directly. There are several approaches to this, but one of the simplest is called an Algebraic Stress Model (ASM). In this type of model, the components of the Reynolds stress tensor are computed without introducing any additional differential equations to be solved. Instead, a nonlinear algebraic constitutive relations is defined as [Wilcox, 1993; Tannehill, 1997]:

$$\frac{\tau_{ij}}{\rho K} \left[ \frac{\partial \bar{u}_m}{\partial x_n} - \rho \varepsilon \right] = \tau_{ik} \frac{\partial \bar{u}_j}{\partial x_k} + \tau_{jk} \frac{\partial \bar{u}_i}{\partial x_k} + \varepsilon_{ij} - \Pi_{ij} \quad (C.95)$$

where $\tau_{ij} = -\rho \bar{u}_i \bar{u}_j$

For a vanishing mean strain rate, this can be simplified to:

$$-\rho \bar{u}_i \bar{u}_j = \frac{K}{\varepsilon} \left( \Pi_{ij} - \varepsilon_{ij} \right) \quad (C.96)$$

where the closure approximations are given by:

$$\Pi_{ij} = C_1 \frac{\varepsilon}{K} \left( -\rho \bar{u}_i \bar{u}_j + \frac{2}{3} \rho K \delta_{ij} \right) \quad \varepsilon_{ij} = \frac{2}{3} \rho \varepsilon \delta_{ij} \quad (C.97, C.98)$$

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\( C_i \) is a closure coefficient which is dependent on the particular ASM being used, and \( \varepsilon \) is the dissipation appearing in the \( K-\varepsilon \) model equations. The ASM is only a nonlinear relation for the Reynolds stress tensor and it must be used in conjunction with a \( K-\varepsilon \) or \( K-\omega \) model to completely describe the turbulent flow. The main advantages of using an ASM along with a two equation model is that it is much better at describing flow in ducts with secondary motion and flow along curved surfaces. The ASM still does not account correctly for sudden changes in mean strain rate, and therefore is not recommended for use with the \( K-\varepsilon \) model for separated or reattaching boundary layers. (Wilcox claims that the standard the \( K-\omega \) model accurately predicts boundary layer reattachment [Wilcox, 1993]).

### C.2.9 Differential stress model

The next jump in sophistication in turbulence modeling is to the so called second order closure models (also referred to as Differential Stress Models (DSM)). Most second order closure models use the differential equation for the behavior of the Reynolds stress tensor as the starting point of the formulation. This equations is derived from a moment of the Navier-Stokes equations:

\[
\frac{D(u_j'u_i')}{Dt} = -\rho u_j'u_i' \frac{\partial u_j'}{\partial x_i} - \rho u_j'u_i' \frac{\partial u_i}{\partial x_j} + \varepsilon_{ij} - \Pi_{ij} + \frac{\partial}{\partial x_k} \left[ \mu \frac{\partial (u_j'u_i')}{\partial x_i} + C_{ij} \right]
\]

(C.99)

\[
\Pi_{ij} = \rho \left( \frac{\partial u_j'}{\partial x_i} + \frac{\partial u_i'}{\partial x_j} \right)
\]

\[
\varepsilon_{ij} = 2\mu \frac{\partial u_i'}{\partial x_k} \frac{\partial u_j'}{\partial x_k}
\]

(C.100, C.101)

\[
C_{ij} = \rho u_i'u_j'u_k' + \rho u_i'u_k' \delta_{jk} + \rho u_j'u_k' \delta_{ik}
\]

(C.102)

where \( \Pi_{ij} \) is the pressure-strain correlation tensor, \( \varepsilon_{ij} \) is the dissipation tensor, and \( C_{ij} \) is the turbulent-transport tensor. It is now obvious that equation (C.95) for the ASM is a simplification of equation (C.99). Equation (C.99) automatically accounts for the effects of flow history via the presence of the convection and diffusion of \( (pu_j'u_i') \). The convection and production terms should naturally account for the effects of flow curvature. Also, because the formulation does not require the normal stresses to be equal, this type of model should account correctly for sudden changes in strain rate. These advantages are realized only with the trade-off of significantly more complex closure approximations and increased difficulty in computation.

The dissipation tensor has been modeled in a low-Reynolds-number scheme (model by [Hanjalic, 1976]) as [Wilcox, 1993]:

\[
\varepsilon_{ij} = \frac{2}{3} \rho \varepsilon \delta_{ij} + 2f_\rho \varepsilon b_{ij}
\]

(C.103)
The second term on the right hand side of equation (C.103) is an anisotropic term. Many models which make the assumption of isotropic dissipation use equation (C.103) without this added term. However, anisotropy plays an important role near solid boundaries. The dissipation rate $\varepsilon$ must be calculated using the differential equation from the $K$-$\varepsilon$ or the $K$-$\omega$ models.

**C.2.10 Turbulent heat and mass transfer**

The discussion up to this point has generally been about the incompressible turbulent boundary layer equations, which were chosen because the equations are simple and it is easy to highlight important terms. The subject of compressible flow and heat transfer is more complex due to the momentum and energy equations being coupled for the general case. To simplify the following discussion, there are several assumptions that will be made. The first is that the fluid will be considered weakly compressible (also called thermally expandable) - which means that the density of the fluid will be treated as a function of temperature only. This is generally only applied in the buoyancy term in the momentum equation. Second, the energy equation is simplified for a low speed ideal gas, meaning that the viscous term will be ignored - this assumption is valid for low velocity, low pressure, gas flows where heat transfer from boundary conditions far outweighs that produced from viscous dissipation. For weakly compressible flow, the Reynolds averaged boundary layer equations are (simplified from equations C.35 - C.37) [Tannehill, 1997]:

\[
\frac{\partial \overline{u}}{\partial t} + \frac{\partial \overline{u}}{\partial x} = 0
\]

\[
\rho \left( \frac{\partial \overline{u}}{\partial t} + \frac{\partial \overline{u}}{\partial x} + \frac{\partial \overline{u}}{\partial y} \right) = -\frac{dP}{dx} + \frac{\partial}{\partial y} \left( \mu \frac{\partial \overline{u}}{\partial y} - \rho \overline{u} \overline{v} \right) + g_x (\rho - \rho_w)
\]

\[
\rho \left( \frac{\partial \overline{H}}{\partial t} + \overline{u} \frac{\partial \overline{H}}{\partial x} + \overline{v} \frac{\partial \overline{H}}{\partial y} \right) = \overline{u} \frac{dP}{dx} + \frac{\partial}{\partial y} \left( k \frac{\partial \overline{T}}{\partial y} - \rho c_p \overline{v} \overline{T} \right) + Q''
\]

Further simplification is added by ignoring the contribution to total enthalpy from kinetic energy and turbulent kinetic energy, which means the energy equation is solved for static enthalpy only. The temperature gradient in the conduction term is expressed in terms of the static enthalpy by using the relation (C.13). Finally, treating heat transfer analogously to momentum transfer, the molecular Prandtl number is used, which is defined as:

\[
Pr = \frac{\mu c_p}{k}.
\]

Thus, using an eddy viscosity type approach, the weakly compressible turbulent boundary layer equations can be transformed to:
\[ \frac{\partial U}{\partial x} + \frac{\partial V}{\partial y} = 0 \]  
\[ \rho \left( \frac{\partial U}{\partial t} + U \frac{\partial U}{\partial x} + V \frac{\partial U}{\partial y} \right) = -\frac{\partial}{\partial x} + \frac{\partial}{\partial y} \left[ (\mu + \mu_t) \frac{\partial U}{\partial y} \right] + g_x (\rho - \rho_w) \]  
\[ \rho \left( \frac{\partial h}{\partial t} + U \frac{\partial h}{\partial x} + V \frac{\partial h}{\partial y} \right) = \frac{\partial}{\partial y} \left[ \left( \frac{\mu}{\text{Pr}} + \frac{\mu_t}{\text{Pr}_t} \right) \frac{\partial h}{\partial y} \right] + \frac{\partial P}{\partial t} + Q^* \]

where \( \text{Pr}_t \) is the turbulent Prandtl number, most often taken to be in the range 0.9 - 1.0.

A similar equation is derived for the mass transfer process:

\[ \rho \left( \frac{\partial m}{\partial t} + U \frac{\partial m}{\partial x} + V \frac{\partial m}{\partial y} \right) = \frac{\partial}{\partial y} \left[ \left( \frac{\mu}{\text{Sc}} + \frac{\mu_t}{\text{Sc}_t} \right) \frac{\partial m}{\partial y} \right] + m'' \]

where \( \text{Sc} \) is the Schmidt number (\( \mu/\text{Sc} = \rho D \)) and \( \text{Sc}_t \) is the turbulent Schmidt number which is generally taken to be equal to the turbulent Prandtl number.

### C.2.11 Summary and conclusions about turbulence models

Turbulent natural convection boundary layer heat and mass transfer are modeled in this thesis for vertical walls. This appendix was compiled after the author thoroughly researched the theoretical and practical aspects of the available turbulence models. The second order closure models (Differential Stress Models) are the most accurate. However, the added accuracy comes at the expense of computational time and convergence difficulties. The added difficulty of these models is considered to be greater than the benefits, and a two equation \( K-E \) model will be used.

Henkes showed that the low-Reynolds-number \( K-E \) model of Jones and Launder (and Launder and Sharma) will predict high Grashof number natural convection turbulent boundary layer flows quite accurately [Henkes, 1989]. Earlier work by Lin showed similar results [Lin, 1978]. Peeters compared the \( K-E \) model to a fully differential Reynolds stress model (RSM) and to an algebraic stress model (ASM) for natural convection boundary layers [Peeters, 1992]. He found that the RSM predicts better results than the \( K-E \) model, but at a substantially higher computation cost. The ASM did not perform as well as the \( K-E \) model.

There are a few studies in the literature of turbulence models used for mass transfer. An early study looked at allowing the turbulent Prandtl and Schmidt numbers to change across the thickness of the boundary layer [Jischa, 1979], but concluded that constants \( \text{Pr}_t = \text{Sc}_t = 0.9 \) seemed to be adequate for many situations. Another study performed for natural convection heat and mass transfer found that a \( K-E \) model is adequate to describe an evaporating liquid film boundary layer [Yan, 1989]. More recently, researchers at Purdue have looked at the evaporation of water from a falling film into a column of rising air using a compressible two-dimensional
representation and a low-Reynolds-number $K\epsilon$ turbulence model. The results agree fairly well with experiment and seem to confirm that 0.9 is appropriate for the turbulent Prandtl and Schmidt numbers [Fedorov, 1997]. No data has been discovered which looks at the $K\epsilon$ model being used in the prediction of high mass transfer rate condensation, which is the subject of the present thesis. From the studies cited above, it seems that a low-Reynolds-number $K\epsilon$ turbulence model along with a two-dimensional flow field should give a fairly good solution for this type of situation. Since this thesis is concerned with predicting the general trends encountered in turbulent boundary layers, and only an initial approximation of boundary layer size for different situations, a great deal of physical accuracy is not required. Thus the low-Reynolds number turbulence models are deemed adequate.
Appendix

D. MATHCAD WORKSHEET FOR CONDENSATION MODEL COMPARISON

This appendix contains the Mathcad worksheet that was used to evaluate the Diffusion Layer Model and compare the DLM to other condensation models. The DLM sensitivity analysis was performed using a variant of this worksheet. This appendix has been included to give the reader more detail about the evaluation of physical properties used in the implementation of the DLM.

File = c:\files\mathcad\condensation\Thesis2.mcd

This MATHCAD file is set up to calculate the value of heat transfer coefficients for several models based on properties that are read into the DATA array.

Option := 1
Setting of option determines settings for the following:
1: Spec=1, Visc=1, Cond=1, Diff=1
2: Spec=2, Visc=1, Cond=1, Diff=1
3: Spec=1, Visc=2, Cond=1, Diff=1
4: Spec=1, Visc=1, Cond=2, Diff=1
5: Spec=2, Visc=2, Cond=2, Diff=1
6: Spec=1, Visc=1, Cond=1, Diff=2
7: Spec=2, Visc=2, Cond=2, Diff=2

Spec :=
2 if Option=2
2 if Option=5
2 if Option=7
1 otherwise

Spec=1 normal, Spec=2 use simple mole weight mixture rule

Visc :=
2 if Option=3
2 if Option=5
2 if Option=7
1 otherwise

Visc=1 normal, Visc=2 use simple mole weight mixture rule

Cond :=
2 if Option=4
2 if Option=5
2 if Option=7
1 otherwise

Cond=1 normal, Cond=2 use simple mole weight mixture rule

Diff :=
2 if Option=6
2 if Option=7
1 otherwise

Diff=1 normal, Diff=2 use Wilke-Lee method, Viscosity constants
Read in steam and water properties from prepared comma delimited files.

Matrix A holds the following saturation properties tabulated by Temperature in°C (20°C - 181°C)
Pressure (MPa), liquid density (kg/m³), vapor density (kg/m³), liquid enthalpy (kJ/kg),
vapor enthalpy (kJ/kg), liquid conductivity (W/m°C), vapor conductivity (W/m°C),
liquid viscosity (u kg/s m), vapor viscosity (u kg/s m), liquid specific heat (kJ/kg C),
vapor specific heat (kJ/kg C), vapor coefficient of expansion (1/C)

Matrix B holds saturation temperatures tabulated by Pressure (0.01 MPa - 0.6 MPa,
T = °C)
If saturation properties are needed as a function of pressure, the saturation temperature
will be found, then the properties evaluated as a function of the saturation temperature
This was done to reduce the amount of data needed to be loaded for the worksheet.

A := READPRN"T_SAT.csv"
B := READPRN"P_SAT.csv"
cols(A) = 13  rows(A) = 324

Section 1: Calculation of saturated properties as a function of temperature (T=K).
Properties are tabulated with Temp in degrees C, but changed to degrees K in function.

1.1 Pressure
\[ P_{ST}(T) := \text{linterp}(A_{<0>}, A_{<1>}, T - 273.15) \]  (P = MPa)

1.2 Density
\[ \rho_{fT}(T) := \text{linterp}(A_{<0>}, A_{<2>}, T - 273.15) \]  (\( \rho = \text{kg} / \text{m}^3 \))
\[ \rho_{gT}(T) := \text{linterp}(A_{<0>}, A_{<3>}, T - 273.15) \]

1.3 Enthalpy
\[ h_{fT}(T) := \text{linterp}(A_{<0>}, A_{<4>}, T - 273.15) \cdot 10^3 \]  (h = J/kg)
\[ h_{gT}(T) := \text{linterp}(A_{<0>}, A_{<5>}, T - 273.15) \cdot 10^3 \]

1.4 Conductivity
\[ k_{fT}(T) := \text{linterp}(A_{<0>}, A_{<6>}, T - 273.15) \]  (k = W/m-K)
\[ k_{gT}(T) := \text{linterp}(A_{<0>}, A_{<7>}, T - 273.15) \]

1.5 Viscosity
\[ \mu_{fT}(T) := \text{linterp}(A_{<0>}, A_{<8>}, T - 273.15) \cdot 10^{-6} \]  (visc = kg/m-sec)
\[ \mu_{gT}(T) := \text{linterp}(A_{<0>}, A_{<9>}, T - 273.15) \cdot 10^{-6} \]

1.6 Specific heat
\[ C_{p fT}(T) := \text{linterp}(A_{<0>}, A_{<10>}, T - 273.15) \cdot 10^3 \]  (Cp = J/kg-K)
\[ C_{p gT}(T) := \text{linterp}(A_{<0>}, A_{<11>}, T - 273.15) \cdot 10^3 \]

1.7 Expansion coeff
\[ \beta_{gT}(T) := \text{linterp}(A_{<0>}, A_{<12>}, T - 273.15) \]  (Beta = 1/K)

Section 2: Calculation of saturated properties as a function of pressure (P=MPa)

2.1 Temperature
\[ T_{sp}(P) := \left( \text{linterp}(B_{<0>}, B_{<1>}, P) + 273.15 \right) \]  (T = C, changed to K)

2.2 Density
\[ \rho_{fP}(P) := \rho_{fT}(T_{sp}(P)) \]  (\( \rho = \text{kg} / \text{m}^3 \))
\[ \rho_{gP}(P) := \rho_{gT}(T_{sp}(P)) \]
2.3 Enthalpy
\[
h_{gP}(P) := h_{gT}(T_{sp}(P)) \quad (h = J/kg) \]
\[
h_{pP}(P) := h_{gT}(T_{sp}(P)) \]

2.4 Conductivity
\[
k_{gP}(P) := k_{gT}(T_{sp}(P)) \quad (k = W/m-K) \]
\[
k_{pP}(P) := k_{gT}(T_{sp}(P)) \]

2.5 Viscosity
\[
\mu_{gP}(P) := \mu_{gT}(T_{sp}(P)) \quad (\text{visc} = \text{kg} / \text{m-sec}) \]
\[
\mu_{pP}(P) := \mu_{gT}(T_{sp}(P)) \]

2.6 Specific Heat
\[
C_{pP}(P) := C_{pT}(T_{sp}(P)) \quad (C_{p} = J/kg-K) \]
\[
C_{pP}(P) := C_{pT}(T_{sp}(P)) \]

Lennard-Jones Potential Force Constants for Viscosity

<table>
<thead>
<tr>
<th>(\sigma_0)</th>
<th>(\varepsilon_0)</th>
<th>(\sigma_1)</th>
<th>(\varepsilon_1)</th>
<th>(\sigma_2)</th>
<th>(\varepsilon_2)</th>
<th>(\sigma_3)</th>
<th>(\varepsilon_3)</th>
</tr>
</thead>
<tbody>
<tr>
<td>2.641</td>
<td>809.1</td>
<td>3.711</td>
<td>78.6</td>
<td>2.551</td>
<td>10.22</td>
<td>2.827</td>
<td>59.7</td>
</tr>
</tbody>
</table>

Molecular weight of gas species

<table>
<thead>
<tr>
<th>(M_0)</th>
<th>(M_1)</th>
<th>(M_2)</th>
<th>(M_3)</th>
</tr>
</thead>
<tbody>
<tr>
<td>18.016</td>
<td>28.96</td>
<td>4.003</td>
<td>2.016</td>
</tr>
</tbody>
</table>

\(T_{sp}(.325) = 273.15 = 1\)

Set \(N\) to index for last gas in mixture

\(N = \text{rows}(M) - 1\)

\(N = 3\)

Steam-Air (Leinhard for steam, viscosity for air)

\[
\sigma_{dd\ ab\ 1} := \frac{(\sigma_0 + \sigma_1)}{2} \quad \varepsilon_{dd\ ab\ 1} := \sqrt{\varepsilon_0 \cdot \varepsilon_1} \]

Steam-Helium (viscosity for steam, viscosity for Helium)

\[
\sigma_{dd\ ab\ 2} := \frac{(\sigma_0 + \sigma_2)}{2} \quad \varepsilon_{dd\ ab\ 2} := \sqrt{\varepsilon_0 \cdot \varepsilon_2} \]

Steam-Hydrogen (Leinhard for steam, viscosity for Hydrogen)

\[
\sigma_{dd\ ab\ 3} := \frac{(\sigma_0 + \sigma_3)}{2} \quad \varepsilon_{dd\ ab\ 3} := \sqrt{\varepsilon_0 \cdot \varepsilon_3} \]

Universal Gas Constant

\(R_u = 8314.3\) (J/kgmol-K) or (Pa-m^3/kgmol-K)
Relations for gas property calculations

\[ \sigma_{ab(i,j)} := \frac{\sigma_i + \sigma_j}{2} \quad \epsilon_{ab(i,j)} := \sqrt{\epsilon_i \epsilon_j} \quad M_{ab(i,j)} := \frac{2}{\frac{1}{M_i} + \frac{1}{M_j}} \]

\[ \sigma_{\text{dab}(i,j)} := \begin{cases} \sigma_{\text{dab}} & \text{if } i \neq 0 \\ \sigma_{ab(i,j)} & \text{otherwise} \end{cases} \quad \epsilon_{\text{dab}(i,j)} := \begin{cases} \epsilon_{\text{dab}} & \text{if } i \neq 0 \\ \epsilon_{ab(i,j)} & \text{otherwise} \end{cases} \]

Collision Integrals for Diffusion Coefficients

Neufield, from Reid p. 583

\[ C_1 = 1.06036 \quad C_2 = 0.15610 \quad C_3 = 0.19300 \quad C_4 = 0.47635 \quad C_5 = 1.03587 \quad C_6 = 1.52996 \quad C_7 = 1.76474 \quad C_8 = 3.89411 \]

\[ \Omega_D(T_s) := \frac{C_1}{T_s^2} + \frac{C_3}{\exp(C_4 \cdot T_s)} + \frac{C_5}{\exp(C_6 \cdot T_s)} + \frac{C_7}{\exp(C_8 \cdot T_s)} \]

Collision Integrals for Viscosity and Conductivity

Neufield (Reid, p. 393) (valid for 0.3 <= Ts <= 100)

\[ B_1 = 1.16145 \quad B_2 = 0.14874 \quad B_3 = 0.52487 \quad B_4 = 0.77320 \quad B_5 = 2.16178 \quad B_6 = 2.43787 \]

\[ \Omega_\mu(T_s) := B_1 \cdot T_s^{-B_2} + B_3 \cdot \exp(-B_4 \cdot T_s) + B_5 \cdot \exp(-B_6 \cdot T_s) \]

Calculate absolute mole fractions of gases from relative mole fractions of the gases after a change in the mole fraction of steam

\[ Y(X) := \frac{X_{nc}}{\sum_{n=1}^{N} X_n} \quad \text{for } i \in 1..N \]

\[ Y_i := \frac{X_i}{X_{nc}} \cdot (1 - X_0) \]

\[ Y_0 := X_0 \]

Calculate mass fractions from mole fractions

\[ W(X) := \frac{M_{\text{eff}}}{\sum_{n=0}^{N} X_n \cdot M_n} \quad \text{for } i \in 0..N \]

\[ W_i := \frac{M_i}{M_{\text{eff}}} \]

\[ W(x) = \begin{bmatrix} 0.487 \\ 0.4697 \\ 0.0433 \\ 0 \end{bmatrix} \]
Calculate molar densities and mixture mass density

Molar density of noncondensable gas for a given temperature, and nc gas partial pressure (using the ideal gas law) \((P=\text{MPa}, T=\text{K}, C=\text{kmol/m}^3)\)

\[
C_{nc}(T, Pnc) := \frac{Pnc \cdot 10^6}{R_u(T)}
\]

\(R_u = 8314.3\)

Molar density of saturated steam at a given temperature \((T=\text{K}, C_s = \text{kmol/m}^3)\)

\[
C_s(T) := \frac{\rho gT(T)}{M_0}
\]

Molar density of mixture including saturated steam

\[
C_{\text{mix}}(T, P, Xs) := \begin{cases} 
C_{nc}(T, P) & \text{if } Xs=0 \\
C_{nc}(T, P \cdot (1 - Xs)) + C_s(T) & \text{otherwise}
\end{cases}
\]

Average mass density of the noncondensable gas mixture \((T=\text{K}, P=\text{MPa}, \rho=\text{kg/m}^3)\)

\[
\rho_{nc}(T, P, X) := X_{nc} \sum_{n=1}^{N} X_n \\
M_{nc} := \sum_{n=1}^{N} \frac{X_n \cdot M_n}{X_{nc}} \\
C_{nc}(T, P \cdot (1 - X_0)) \cdot M_{nc}
\]

Average mass density of the noncondensable gas mixture at the wall \((T=\text{K}, P=\text{MPa}, \rho=\text{kg/m}^3)\)

\[
\rho_{ncw}(T, P, X) := X_{nc} \sum_{n=1}^{N} X_n \\
M_{nc} := \sum_{n=1}^{N} \frac{X_n \cdot M_n}{X_{nc}} \\
C_{nc}(T, P - P_sT(T)) \cdot M_{nc}
\]

Mass density of the gas mixture including steam \((T=\text{K}, P=\text{MPa}, \rho=\text{kg/m}^3)\)

\[
\rho_{mix}(T, P, X) := \begin{cases} 
\rho_{nc}(T, P, X) & \text{if } X_0=0 \\
\rho gT(T) + \rho_{nc}(T, P, X) & \text{otherwise}
\end{cases}
\]
Calculation of gas viscosity for all gases and mixtures

Chapman-Enskog (Reid p 392) \((T=K, i = \text{species index}, u=\text{kg/m-s})\)
(also used in GOTHIC 4.1 - uses Nuefeld collision integral)

\[
\mu_g(T, i) := \begin{cases} 
\mu_g(T) & \text{if } i=0 \\
2.669 \times 10^{-6} \frac{\sqrt{M_i(T)}}{\left(\sigma_i \cdot \Omega \frac{T}{\varepsilon_i}\right)} & \text{otherwise}
\end{cases}
\]

Average viscosity of the mixture (Wilke method)

\[
\phi(T, i, j) := \sqrt{8\left(1 + \frac{M_i}{M_j}\right)^{0.5}}
\]

\[
\mu_{\text{mixf}}(T, X) := \sum_{m=0}^{N} \frac{X_m \mu_g(T, m)}{\sum_{n=0}^{N} X_n \phi(T, m, n)}
\]

\[
\mu_{\text{mix2}}(T, X) := \sum_{m=0}^{N} X_m \mu_g(T, m)
\]

Anderson relation

\[
\mu_{\text{mix}}(T, X) := \begin{cases} 
\mu_{\text{mixf}}(T, X) & \text{if } \text{Visc}=1 \\
\mu_{\text{mix2}}(T, X) & \text{if } \text{Visc}=2
\end{cases}
\]

Calculate the specific heat of pure gases and mixtures

Air (from GOTHIC 4.1) \((T=K, C_p \text{ originally in Btu/lbm-R, but changed to J/kg-K})\)

\[
C_{p_a}(T) := \begin{bmatrix} 
0.244388 \\
4.20419 \times 10^{-5} \\
9.61128 \times 10^{-8} \\
1.116383 \times 10^{-11}
\end{bmatrix}
\]

\[
\left[ \sum_{n=0}^{3} \left( \frac{F_n \cdot T^n}{3}\right) \right] \times 4186.8
\]

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Helium (from GOTHIC 4.1) \((T=K, C_p=J/kg-K)\)

\[
C_{p_{he}} := 1.24044186.8
\]

Hydrogen (from GOTHIC 4.1) \((T=K, C_p\text{ originally in Btu/lbm-R, but changed to } J/kg-K)\)

\[
C_{p_h}(T) := \begin{cases} 
F_0 \leftarrow 1.46910 \\
F_1 \leftarrow 1.60057 \times 10^{-2} \\
F_2 \leftarrow -4.44048 \times 10^{-5} \\
F_3 \leftarrow 4.21220 \times 10^{-8} \\
\sum_{n=0}^{3} \left(F_n \cdot T^n\right) \text{ if } T<400 \\
\sum_{n=0}^{3} \left(F_n \cdot T^n\right) \text{ otherwise}
\end{cases}
\]

\[
F_0 \leftarrow 3.56903 \\
F_1 \leftarrow -4.89591 \times 10^{-4} \\
F_2 \leftarrow 6.22549 \times 10^{-7} \\
F_3 \leftarrow -1.19686 \times 10^{-10}
\]

Make \(C_p\) a general function of the index \(i\) so it can be used in conductivity calculations

\[
C_{p_g}(T, i) := \begin{cases} 
C_p g(T) \text{ if } i = 0 \\
C_{p_a}(T) \text{ if } i = 1 \\
C_{p_{he}} \text{ if } i = 2 \\
C_{p_h}(T) \text{ if } i = 3
\end{cases}
\]

Calculate \(C_p\) of the noncondensable gas mixture (mass fraction basis) \((T=K, C_p=J/kg-K)\)

\[
C_{p_{nc}}(T, X) := \begin{cases} 
m \leftarrow W(X) \\
m_{nc} \leftarrow \sum_{n=1}^{N} m_n \\
\sum_{n=1}^{N} \frac{m_n}{m_{nc}} \cdot C_{p_g}(T, n)
\end{cases}
\]
Calculate $C_p$ of the mixture including steam (T=K, Cp=J/kg-K)

$$C_{p_{\text{mix}}}(T, P, X) := \begin{cases} 
C_{p_{\text{nc}}}(T, X) & \text{if } X_0 = 0 \\
\frac{\rho_{\text{nc}}(T, P, X) C_{p_{\text{nc}}}(T, X) + \rho_{gT}(T) C_{p_{gT}}(T)}{\rho_{\text{nc}}(T, P, X) + \rho_{gT}(T)} & \text{otherwise}
\end{cases}$$

$$C_{p_{\text{mix}}}(T, P, X) := \sum_{m=0}^{N} X_m C_{p_{gT}}(T, m)$$

$$C_{p_{\text{mix}}}(T, P, X) := \begin{cases} 
C_{p_{\text{mix}}}(T, P, X) & \text{if Spec = 1} \\
C_{p_{\text{mix}}}(T, P, X) & \text{if Spec = 2}
\end{cases}$$

******************************************** Calculate the conductivity of pure gases ********************************************

Conductivity (from GOTHIC 4.1) (T=K, k=W/m-K)

Conductivity of a pure monatomic gas at low pressure ($P < 1.0 \text{ MPa}$)

$$k_1(T, i) := \begin{cases} 
\frac{15 R_u}{4 \mu g(T, i)} & \text{if } i = 0 \\
\frac{15 R_u}{4 \mu g(T, i)} & \text{otherwise}
\end{cases}$$

Polyatomic gas conductivity component at low pressure ($P < 1.0 \text{ MPa}$)

$$k_2(T, i) := \begin{cases} 
0 & \text{if } i = 0 \\
0 & \text{if } i = 2 \\
\frac{2 - C_{p_{gT}}(T, i) M_i}{5 R_u} & \text{otherwise}
\end{cases}$$

Conductivity for a pure gas at low pressure (T=K, k=W/m-K)

$$k_g(T, i) := k_1(T, i) + k_2(T, i)$$

Conductivity of a gas mixture (Wilke-Method) (T=K, k=W/m-K)

$$k_{\text{mix}}(T, X) := \sum_{m=0}^{N} \frac{X_m k_g(T, m)}{\sum_{n=0}^{N} X_n \phi(T, m, n)}$$

$$k_{\text{mix}}(T, X) := \sum_{m=0}^{N} X_m k_g(T, m)$$

$$k_{\text{mix}}(T, X) := \begin{cases} 
k_{\text{mix}}(T, X) & \text{if Cond = 1} \\
k_{\text{mix}}(T, X) & \text{if Cond = 2}
\end{cases}$$
Chapman-Enskog Kinetic Theory equation for Binary Diffusion Coefficient for
(T=K, was originally for P=atm but is converted to P=MPa, D=m²/sec)

\[
D_{ab}(T, P, i, j) := \frac{1.86 \times 10^{-7} \sqrt[3]{T} \left(\frac{1}{M_i} + \frac{1}{M_j}\right)}{(P - 9.86923) \sigma_{ab(i, j)}^2 \Omega D \frac{T}{\epsilon_{ab(i, j)}}}
\]

Wilke-Lee Binary Diffusion Coefficient
(T=K, was originally for P=bar but is converted to P=MPa, D=m²/sec)

\[
D_{ab2}(T, P, i, j) := \frac{\left[3.03 - \left(\frac{0.98}{\sqrt{M_{ab(i, j)}}}\right)\right] \times 10^{-7} \cdot T^{1.5}}{(P - 10) \sqrt{M_{ab(i, j)}} \sigma_{ab(i, j)}^2 \Omega D \frac{T}{\epsilon_{ab(i, j)}}}
\]

********** Calculate Steam Diffusion Coefficient through gas mixture **************

\[
D_{mix}(T, P, X) := X_{nc} \left\{ \begin{array}{ll}
N \sum_{n=1}^{N} X_n & \text{if Diff=1} \\
\frac{X_{nc}}{N} \sum_{n=1}^{N} \frac{X_n}{D_{ab}(T, P, 0, n)} & \text{if Diff=2} \\
\frac{X_{nc}}{N} \sum_{n=1}^{N} \frac{X_n}{D_{ab2}(T, P, 0, n)} & \text{if Diff=2}
\end{array} \right.
\]

\[
D_{mix2}(T, P, X) := X_{nc} \left\{ \begin{array}{ll}
N \sum_{n=1}^{N} X_n & \\
\frac{X_{nc}}{N} \sum_{n=1}^{N} \frac{X_n}{D_{ab}(T, P, 0, n)} & \\
\end{array} \right.
\]
Schmidt number for the gas/steam mixture (defined for debugging purposes only)

\[
\text{Sc}_{\text{mix}}(T, P, X) := \frac{\mu_{\text{mix}}(T, X)}{\rho_{\text{mix}}(T, P, X) \cdot D_{\text{mix}}(T, P, X)}
\]

Prandtl number for liquid, steam and the steam gas mixture (defined for debugging purposes only)

\[
\begin{align*}
\text{Pr}_{\text{f}}(T) & := \frac{\mu_{\text{f}}(T) \cdot C_p}{k_{\text{f}}(T)} \\
\text{Pr}_{\text{g}}(T) & := \frac{\mu_{\text{g}}(T) \cdot C_p}{k_{\text{g}}(T)} \\
\text{Pr}_{\text{mix}}(T, P, X) & := \frac{\mu_{\text{mix}}(T, X) \cdot C_p}{k_{\text{mix}}(T, X)}
\end{align*}
\]

Calculate Average Temperature and mole fractions in Boundary layer

\[
\begin{align*}
T_{\text{ave}}(T_b, T_i) & := \frac{T_b - T_i}{\ln \left( \frac{T_b}{T_i} \right)} \\
T_{\text{ave}}(T_b, T_i) & := T_b \\
T_{\text{ave}}(T_b, T_i) & := \frac{T_b + T_i}{2}
\end{align*}
\]

\[
\begin{align*}
X_{\text{ave}}(T_b, T_i, P, X) & := \begin{cases} 
X_{\text{ave}}(T_b, T_i) & \text{if } T_{\text{ave}}(T_b, T_i) \\
X_{\text{ave}} & \text{otherwise}
\end{cases} \\
X_{\text{ave}} & := X
\end{align*}
\]

\[
\begin{align*}
X_{\text{ave}}(T_b, T_i, P, X) & := \begin{cases} 
\frac{P_{sT}(T_i)}{P} & \text{if } x_i \\
\frac{P_{sT}(T_b)}{P} & \text{if } x_b \\
\frac{x_b - x_i}{\ln \left( \frac{x_b}{x_i} \right)} & \text{otherwise}
\end{cases} \\
X_{\text{ave}} & := \frac{x_b + x_i}{2}
\end{align*}
\]

\[
\begin{align*}
X_{\text{ave}}(T_b, T_i, P, X) & := \begin{cases} 
X_{\text{ave}} & \text{if } T_{\text{ave}}(T_b, T_i) \\
\frac{P_{sT}(T_i)}{P} & \text{if } x_i \\
\frac{P_{sT}(T_b)}{P} & \text{if } x_b \\
\frac{x_b - x_i}{\ln \left( \frac{x_b}{x_i} \right)} & \text{otherwise}
\end{cases} \\
X_{\text{ave}} & := \frac{x_b + x_i}{2}
\end{align*}
\]
Calculate Grashof and Schmidt numbers for the mixture in boundary layer

$$\text{Gr}(T_b, T_i, P, X, L) :=$$

\[
\begin{align*}
G &\leftarrow 9.81 \\
T_{av} &\leftarrow T_{ave}(T_b, T_i) \\
X_{av} &\leftarrow X_{ave}(T_b, T_i, P, X) \\
\rho_b &\leftarrow \rho_{nc}(T_b, P, X) + \rho g(T_b) \\
\rho_i &\leftarrow \rho_{ncw}(T_i, P, X) + \rho g(T_i) \\
\rho &\leftarrow \frac{\rho_b + \rho_i}{2} \\
\mu &\leftarrow \mu_{mix}(T_{av}, X_{av}) \\
D &\leftarrow D_{mix}(T_{av}, P, X) \\
g \cdot \rho \left( \frac{\rho_i - \rho_b}{2} \right) &\leftarrow \frac{1}{\mu^2} L^3
\end{align*}
\]

$$\text{Sc}(T_b, T_i, P, X, L) :=$$

\[
\begin{align*}
T_{av} &\leftarrow T_{ave}(T_b, T_i) \\
X_{av} &\leftarrow X_{ave}(T_b, T_i, P, X) \\
\rho_b &\leftarrow \rho_{nc}(T_b, P, X) + \rho g(T_b) \\
\rho_i &\leftarrow \rho_{ncw}(T_i, P, X) + \rho g(T_i) \\
\rho &\leftarrow \frac{\rho_b + \rho_i}{2} \\
\mu &\leftarrow \mu_{mix}(T_{av}, X_{av}) \\
D &\leftarrow D_{mix}(T_{av}, P, X) \\
\mu &\leftarrow \frac{\mu}{\rho D}
\end{align*}
\]

Calculate Prandtl product for mixture in the boundary layer

$$\text{Pr}(T_b, T_i, P, X, L) :=$$

\[
\begin{align*}
T_{av} &\leftarrow T_{ave}(T_b, T_i) \\
X_{av} &\leftarrow X_{ave}(T_b, T_i, P, X) \\
\mu &\leftarrow \mu_{mix}(T_{av}, X_{av}) \\
C_p &\leftarrow C_{p, mix}(T_{av}, P, X_{av}) \\
k &\leftarrow k_{mix}(T_{av}, X_{av}) \\
\frac{C_p \mu}{k}
\end{align*}
\]

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Calculate Sherwood number based on the McAdams correlation

\[ Sh_{\text{mix}}(T_b, Ti, P, X, L) := 0.13 \left( \frac{G(T_b, Ti, P, X, L)}{Sc(T_b, Ti, P, X, L)} \right)^{\frac{1}{3}} \]

Calculate Nusselt number based on the McAdams correlation

\[ Nu_{\text{mix}}(T_b, Ti, P, X, L) := 0.13 \left( \frac{G(T_b, Ti, P, X, L)}{Pr(T, Ti, P, X, L)} \right)^{\frac{1}{3}} \]

************************************************************************************

Begin calculating the pieces of the Condensation heat transfer model

Inputs:
- \( T_b \) (K) - bulk temp,
- \( T_w \) (K) - wall temp,
- \( z \) = position down wall,
- \( L \) = length of wall

Outputs:
- \( h_{\text{film}} \), \( h_{\text{cond}} \), \( h_{\text{conv}} \), \( q_{\text{cond}} \)

************************************************************************************

Calculate local film heat transfer coefficient for distance \( z \) down the wall \((T_w=T_i=K, z=\text{meters})\)

\[ h_{\text{film}}(T_i, T_w, z) := \frac{T_f - T_w + 0.25(T_i - T_w)}{\rho_i + \frac{\rho_v}{\rho_g(T_i)} + \frac{k_i}{k_g(T)} + \frac{\mu_i}{\mu_g(T)}} \]

\[ \text{Liquid Reynolds number from Anderson's code} \]

\[ Re(T_i, T_w, z) := \frac{T_f - T_w + 0.25(T_i - T_w)}{\rho_i + \frac{\rho_v}{\rho_g(T_i)} + \frac{k_i}{k_g(T)} + \frac{\mu_i}{\mu_g(T)}} \]
Film heat transfer coefficient corrected for waviness effects

\[ h_{\text{film}}(T_i, T_w, z) := h_{\text{film}}(T_i, T_w, z) \cdot Re(T_i, T_w, z)^{0.04} \]

Heat flux through liquid film

\[ q_{\text{film}}(T_i, T_w, z) := h_{\text{film}}(T_i, T_w, z) \cdot (T_i - T_w) \]

Log mean concentration gradient as defined by Peterson

\[ \Phi(X_s, X_{si}) := -\ln \left( \frac{X_s}{X_{si}} \right) \ln \left( \frac{1 - X_s}{1 - X_{si}} \right) \]

\[ \Phi_2(X_s, X_{si}) := \] 
\[ \begin{align*} 
X_g &\rightarrow 1 - X_s \\
X_{gi} &\rightarrow 1 - X_{si} \\
X_s_{\text{avg}} &\rightarrow \frac{(X_s - X_{si})}{\ln \left( \frac{X_s}{X_{si}} \right)} \\
X_{gi}_{\text{avg}} &\rightarrow \frac{(X_g - X_{gi})}{\ln \left( \frac{X_g}{X_{gi}} \right)} \\
X_s_{\text{avg}} &\rightarrow X_g_{\text{avg}} \\
X_{gi}_{\text{avg}} &\rightarrow X_g_{\text{avg}} 
\end{align*} \]

\[ \Phi_3(X_s, X_{si}) := \] 
\[ \begin{align*} 
X_g &\rightarrow 1 - X_s \\
X_{gi} &\rightarrow 1 - X_{si} \\
\ln \left( \frac{X_g}{X_{gi}} \right) &\rightarrow \ln \left( \frac{1 - X_g}{1 - X_{gi}} \right) \\
\ln \left( \frac{X_s}{X_{si}} \right) &\rightarrow \ln \left( \frac{1 - X_s}{1 - X_{si}} \right) 
\end{align*} \]

\[ \Phi(0.5, 0.2)^{-1} = 0.5129 \]
\[ \Phi_2(0.5, 0.2) = 0.5129 \]
\[ \Phi_3(0.5, 0.2) = -0.5129 \]

Condensation Conductivity as Defined by Peterson

\[ k_{cp}(T_b, T_i, P, X) := T_{av} \rightarrow T_{ave}(T_b, T_i) \]
\[ X_{av} \rightarrow X_{ave}(T_b, T_i, P, X) \]
\[ M_v \rightarrow M_0 \]
\[ X_s \rightarrow X_0 \]
\[ X_{si} \rightarrow \frac{P_s(T_i)}{P} \]
\[ h_{fg} \rightarrow h_{gT(T_{av})} - h_{fT(T_{av})} \]
\[ D \rightarrow D_{mix}(T_{av}, P, X) \]
\[ P \cdot 10^6 \cdot M_v^2 \cdot h_{fg}^2 \cdot D \]
\[ R_u^2 \cdot T_{av}^3 \cdot \Phi(X_s, X_{si}) \]

\[ R_u = 8314.3 \]
Condensation Conductivity as modified by Anderson (Tb=Ti=K, P=MPa)

\[ k_{CC}(T_b, T_i, P, X) := T_{av} - T_{ave}(T_b, T_i) \]

\[ X_{av} - X_{ave}(T_b, T_i, P, X) \]

\[ C_g - C_{mix}(T_{av}, P, X_{av}) \]

\[ M_v - M_0 \]

\[ X_s - X_0 \]

\[ \frac{P_{st}(T_i)}{P} \]

\[ h_{fg} - h_{gt}\left(T_{av}\right) - h_{gt}\left(T_{av}\right) \]

\[ D - D_{mix}(T_{av}, P, X) \]

\[ \frac{C_g M_v^2 h_{fg}^2 D}{R u T_i T_b \Phi (X_s, X_{si})} \]

Calculate the suction terms for the Sherwood numbers

\[ \Theta 1(T_b, T_i, P) := \frac{P_{st}(T_b)}{P} \]

\[ \Theta 2(T_b, T_i, P) := \frac{P_{st}(T_i)}{P} \]

\[ \Theta 3(T_b, T_i, P) := \frac{P_{st}(T_b)}{P} \]

\[ \Theta 1(320, 310, .3) = 1.0149 \]

\[ \Theta 2(320, 310, .3) = 1.0074 \]

\[ \Theta 3(320, 310, .3) = 1.0074 \]

\[ \Theta 1(340, 310, .3) = 1.0768 \]

\[ \Theta 2(340, 310, .3) = 1.0374 \]

\[ \Theta 3(340, 310, .3) = 1.0361 \]

\[ \Theta 1(360, 310, .3) = 1.2351 \]

\[ \Theta 2(360, 310, .3) = 1.1093 \]

\[ \Theta 3(360, 310, .3) = 1.0982 \]

\[ \Theta 1(400, 350, .3) = 4.744 \]

\[ \Theta 2(400, 350, .3) = 1.9727 \]

\[ \Theta 3(400, 350, .3) = 1.446 \]

\[ \Theta (T_b, T_i, P) := \begin{cases} 
\Theta 1(T_b, T_i, P) & \text{if } \text{Suc}=1 \\
\Theta 2(T_b, T_i, P) & \text{if } \text{Suc}=2 \\
\Theta 3(T_b, T_i, P) & \text{if } \text{Suc}=3 
\end{cases} \]

Choose difference suction parameters
***** Calculate the CONVECTION Heat Transfer Coefficient ***************

\[ h_{\text{conv}}(T_b, T_i, P, X, L) := \frac{T_{\text{av}} - T_{\text{ave}}(T_b, T_i)}{X_{\text{av}} - X_{\text{ave}}(T_b, T_i, P, X)} \]

\[ \frac{\text{Nu} \times k_{\text{mix}}(T_{\text{av}}, X_{\text{av}})}{L} \]

***** Calculate the condensation Heat Transfer Coefficients **************

Standard (no suction)

\[ h_{cS}(T_b, T_i, P, X, L) := \frac{T_{\text{av}} - T_{\text{ave}}(T_b, T_i)}{C_{\text{vb}} - C_{\text{vi}} + X_{\text{av}} - X_{\text{ave}}(T_b, T_i, P, X)} \]

\[ D = D_{\text{mix}}(T_{\text{av}}, P, X) \]

\[ Sh = Sh_{\text{mix}}(T_b, T_i, P, X, L) \]

\[ \frac{Sh \times D_{\text{mix}} h_{\text{bi}}}{(T_b - T_i) \times L \times (C_{\text{vb}} - C_{\text{vi}})} \]

Mills based on density (heat and mass transfer, with suction)

Condensation mass flow

\[ m_{\text{Ms}}(T_b, T_i, P, X, L) := \frac{T_{\text{av}} - T_{\text{ave}}(T_b, T_i)}{X_{\text{av}} - X_{\text{ave}}(T_b, T_i, P, X)} \]

\[ \rho \times \rho_{\text{mix}}(T_{\text{av}}, P, X_{\text{av}}) \]

\[ D = D_{\text{mix}}(T_{\text{av}}, P, X) \]

\[ Sh = Sh_{\text{mix}}(T_b, T_i, P, X, L) \]

\[ \frac{g \times \rho \times Sh \times D}{L} \]

\[ X = X \]

\[ X = \frac{P_{\text{st}}(T_i)}{P} \]

\[ W_{\text{sb}} = W(X)_0 \]

\[ W_{\text{si}} = W(Y(X))_0 \]

\[ B_m = \frac{W_{\text{sb}} - W_{\text{si}}}{W_{\text{si}} - 1} \]

\[ \text{Blow} = \frac{\ln(1 + B_m)}{B_m} \]

\[ m''_m = g_m B_m \text{Blow} \]

\[ m''_m = g_m (W_{\text{sb}} - W_{\text{si}}) \]

\[ m''_m \]
\[
h_{cM}(T_b, T_i, P, X, L) := \frac{-m'_{M}(T_b, T_i, P, X, L) \cdot \left( h_g T(T_b) - h_f T(T_i) \right)}{(T_b - T_i)}
\]

**Suction factor for Mills convection relation**

\[
\Theta_M(T_b, T_i, P, X, L) := \left| \frac{T_{av} - T_{ave}(T_b, T_i)}{B_h} \right|
\]

\[
h_{M}(T_b, T_i, P, X, L) = \frac{m'_{M}(T_b, T_i, P, X, L) \cdot C_p \cdot g T(T_{av}) \cdot h_{conv}(T_b, T_i, P, X, L)}{B_h \cdot \exp(B_h) - 1}
\]

**Peterson (no suction)**

\[
h_{cp}(T_b, T_i, P, X, L) := \frac{S_{mix}(T_b, T_i, P, X, L) \cdot k_{cP}(T_b, T_i, P, X)}{L}
\]

**DLM (no suction)**

\[
h_{CC}(T_b, T_i, P, X, L) := \frac{S_{mix}(T_b, T_i, P, X, L) \cdot k_{cC}(T_b, T_i, P, X)}{L}
\]

**DLM (with suction)**

\[
h_{css}(T_b, T_i, P, X, L) := \frac{S_{mix}(T_b, T_i, P, X, L) \cdot \Theta(T_b, T_i, P) \cdot k_{cC}(T_b, T_i, P, X)}{L}
\]

**** Calculate condensation and convection heat transfer coefficient ****

**Standard (no suction)**

\[
h_g(T_b, T_i, P, X, L) := h_{cs}(T_b, T_i, P, X, L) + h_{conv}(T_b, T_i, P, X, L)
\]

**Mills (with suction)**

\[
h_{Ms}(T_b, T_i, P, X, L) := h_{cMs}(T_b, T_i, P, X, L) + h_{conv}(T_b, T_i, P, X, L) \cdot \Theta_M(T_b, T_i, P, X, L)
\]

**Peterson (no suction)**

\[
h_p(T_b, T_i, P, X, L) := h_{cp}(T_b, T_i, P, X, L) + h_{conv}(T_b, T_i, P, X, L)
\]

**DLM (no suction)**

\[
h_{CC}(T_b, T_i, P, X, L) := h_{cC}(T_b, T_i, P, X, L) + h_{conv}(T_b, T_i, P, X, L)
\]

**DLM (with suction)**

\[
h_{css}(T_b, T_i, P, X, L) := h_{cCs}(T_b, T_i, P, X, L) + h_{conv}(T_b, T_i, P, X, L)
\]
***** Calculate total heat transfer coefficient *****

Standard (no suction)
\[ h_{TS}(T_b, T_i, T_w, P, X, L, z) := \frac{h_{film}(T_i, T_w, z) \cdot \delta(T_b, T_i, P, X, L)}{h_{film}(T_i, T_w, z) + \delta(T_b, T_i, P, X, L)} \]

Mills (with suction)
\[ h_{TM_s}(T_b, T_i, T_w, P, X, L, z) := \frac{h_{film}(T_i, T_w, z) \cdot h_{Ms}(T_b, T_i, P, X, L)}{h_{film}(T_i, T_w, z) + h_{Ms}(T_b, T_i, P, X, L)} \]

Peterson (no suction)
\[ h_{TP}(T_b, T_i, T_w, P, X, L, z) := \frac{h_{film}(T_i, T_w, z) \cdot h_p(T_b, T_i, P, X, L)}{h_{film}(T_i, T_w, z) + h_p(T_b, T_i, P, X, L)} \]

DLM (no suction)
\[ h_{TC}(T_b, T_i, T_w, P, X, L, z) := \frac{h_{film}(T_i, T_w, z) \cdot h_C(T_b, T_i, P, X, L)}{h_{film}(T_i, T_w, z) + h_C(T_b, T_i, P, X, L)} \]

DLM (with suction)
\[ h_{TC_s}(T_b, T_i, T_w, P, X, L, z) := \frac{h_{film}(T_i, T_w, z) \cdot h_{Cs}(T_b, T_i, P, X, L)}{h_{film}(T_i, T_w, z) + h_{Cs}(T_b, T_i, P, X, L)} \]

***** Calculate the heat flux through the boundary layer *****

Standard (no suction)
\[ q'(T_b, T_i, P, X, L) := h \cdot \delta(T_b, T_i, P, X, L) \cdot (T_b - T_i) \]

Mills (with suction)
\[ q'_{Ms}(T_b, T_i, P, X, L) := h_{Ms}(T_b, T_i, P, X, L) \cdot (T_b - T_i) \]

Peterson (no suction)
\[ q'_{p}(T_b, T_i, P, X, L) := h_p(T_b, T_i, P, X, L) \cdot (T_b - T_i) \]

DLM (no suction)
\[ q'_{C}(T_b, T_i, P, X, L) := h_C(T_b, T_i, P, X, L) \cdot (T_b - T_i) \]

DLM (with suction)
\[ q'_{Cs}(T_b, T_i, P, X, L) := h_{Cs}(T_b, T_i, P, X, L) \cdot (T_b - T_i) \]
Dehbi HTC for Steam-Air \((T_b - T_w = K, P = MPa, L = m, h = W / m^2-K)\)

\[
h_{D1}(T_b, T_w, P, X, L) := \begin{align*}
&W_a <- W(X)_1 \\
&P_1 <- 9.86923P \\
&L^{0.05} \cdot \frac{(3.7 + 28.7P_1) - (2438 + 458.3P_1) \cdot \log(W_a)}{(T_b - T_w)^{0.25}}
\end{align*}
\]

Dehbi HTC for Steam-Air-Helium \((T_b - T_w = K, P = MPa, L = m, h = W/m^2-K)\)

\[
h_{D2}(T_b, T_w, P, X, L) := \begin{align*}
&W_a <- W(X)_1 \\
&W_{he} <- W(X)_2 \\
&P_1 <- 9.86923P \\
&Part1 <- \frac{L^{0.05} \cdot ((3.7 + 28.7P_1) - (2438 + 458.3P_1) \cdot \log(W_a + W_{he}))}{(T_b - T_w)^{0.25}} \\
&Part2 <- 0.948 - 8.67W_{he} + 7.36W_{he} \cdot (W_{he} + W_a) \\
&Part1 + Part2
\end{align*}
\]

\[
h_{D}(T_b, T_w, P, X, L) := \begin{align*}
&h_{D1}(T_b, T_w, P, X, L) \text{ if } X_2 = 0 \\
&h_{D2}(T_b, T_w, P, X, L) \text{ otherwise}
\end{align*}
\]

Calculate Uchida heat transfer coefficient \((h = W / m^2-K)\)

\[
h_{U}(X) := \begin{align*}
&m_s <- W(X)_0 \\
&m_{nc} <- 1 - m_s \\
&379. \left( \frac{m_{nc}}{m_s} \right)^{-0.707}
\end{align*}
\]

******* Calculate Kataoka heat transfer coefficient \((h = W / m^2-K)\) **************
Calculate the Gido & Koestel natural convection heat transfer coefficient \( (h = \frac{W}{m^2 \cdot K}) \)

\[
h_{GK}(T_b, T_w, P, L) := \frac{\rho v - \rho g T(T_b)}{\rho v \mu g T(T_w)} \frac{\rho v h f g}{T_b - T_w} \left( \frac{\rho v^4 \cdot L}{\mu_l} \right) \]

Solve for heat transfer parameters for different temperatures

\[
\begin{align*}
    DATA & := \text{READPRN "Input.txt" } \\
    P_t & := 0.1 \times \text{DATA}^0 \\
    P_{\text{steam}} & := 0.1 \times \text{DATA}^1 \\
    X_{\text{air}} & := 0.1 \times \text{DATA}^2 \\
    X_{\text{he}} & := 0.1 \times \text{DATA}^3 \\
    T_w & := 273.15 + \text{DATA}^1 \\
    T_{\text{bulk}} & := 273.15 + \text{DATA}^2 \\
    RH & := \text{DATA}^4 \\
    L & := 2.0 \\
    z & := 1 \\
    i & := 0..I - 1
\end{align*}
\]
I := rows(DATA)

Relative mole fraction of noncondensable gases

\[ X_{sT_b} := \frac{P_{sT} T_{bulk}}{P_t} \]

\[ X_{s2} := \frac{P_{air}}{P_t} \]

\[ X_{a} := \frac{P_{steam}}{P_t} \]

\[ X_{he} := \frac{P_{he}}{P_t} \]

Calculate the mole fraction matrix based on bulk saturation temperature and total pressure

\[ X_{X <i,j>} := \begin{bmatrix} X_i \\ 1 - XP_{he_i} \\ XP_{he_i} \\ 0 \end{bmatrix} \]

\[ XX_{1,2} = 0.2896 \]

PRESS \(_{00} := P_t \cdot 10^0\]

\[ PRESS_{1,0} := PRESS_{0,0} \cdot XX_{0,i} \]

\[ PRESS_{1,1} := PRESS_{0,1} \cdot XX_{1,i} \]

\[ PRESS_{1,2} := PRESS_{0,2} \cdot XX_{2,i} \]

WRITEPRN("PRES.TXT") := PRESS

****** Solve for HTC -- Standard Conductance (no suction) ***********

** i := 0.. I - 1

j := 0

Given

\[ q^\text{film}(T_{guess}, T_w, z) - q^S(T_b, T_{guess}, P, X, L) = 0 \]

\[ T_{ii}(T_b, T_w, P, X, L, z, T_{guess}) := \text{Find}(T_{guess}) \]

Store the interface temperature

\[ T_{\text{int},i,j} := T_{ii}(T_{bulk}, T_w, P, XX_{<i,j>}, L, z, T_{w} + 1) \]

Store the total heat transfer coefficient (Standard - no suction model)

\[ THTC_{i,j} := h TS(T_{bulk}, T_{\text{int},i,j}, T_w, P, XX_{<i,j>}, L, z) \]
******* Solve for HTC -- Mills Heat/Mass Transfer Model (with suction) ****************************

j := j + 1

Given

\[ q''_{\text{film}}(T_{\text{guess}}, T_w, z) - q''_M(T_b, T_{\text{guess}}, P, X, L) = 0 \]

\[ T_{ii}(T_b, T_w, P, X, L, z, T_{\text{guess}}) := \text{Find}(T_{\text{guess}}) \]

Store the interface temperature

\[ T_{\text{int}_{i,j}} := T_{ii}(T_{\text{bulk}_{i}}, T_{w_{i}}, P_{t_{i}}, XX^{<i>}, L, z, T_{w_{i}} + 1) \]

Store the total heat transfer coefficient (Mills model)

\[ \text{TH}_{	ext{HC},i,j} := h_{\text{TM}_{s}}(T_{\text{bulk}_{i}}, T_{\text{int}_{i,j}}, T_{w_{i}}, P_{t_{i}}, XX^{<i>}, L, z) \]

******* Solve for HTC -- Peterson Model (no suction) ****************************

j := j + 1

Given

\[ q''_{\text{film}}(T_{\text{guess}}, T_w, z) - q''_P(T_b, T_{\text{guess}}, P, X, L) = 0 \]

\[ T_{ii}(T_b, T_w, P, X, L, z, T_{\text{guess}}) := \text{Find}(T_{\text{guess}}) \]

Store the interface temperature

\[ T_{\text{int}_{i,j}} := T_{ii}(T_{\text{bulk}_{i}}, T_{w_{i}}, P_{t_{i}}, XX^{<i>}, L, z, T_{w_{i}} + 1) \]

Store the total heat transfer coefficient (Peterson model)

\[ \text{TH}_{	ext{HC},i,j} := h_{\text{TP}}(T_{\text{bulk}_{i}}, T_{\text{int}_{i,j}}, T_{w_{i}}, P_{t_{i}}, XX^{<i>}, L, z) \]

******* Solve for HTC -- DLM Model (no suction) ****************************

j := j + 1

Given

\[ q''_{\text{film}}(T_{\text{guess}}, T_w, z) - q''_C(T_b, T_{\text{guess}}, P, X, L) = 0 \]

\[ T_{ii}(T_b, T_w, P, X, L, z, T_{\text{guess}}) := \text{Find}(T_{\text{guess}}) \]

Store the interface temperature

\[ T_{\text{int}_{i,j}} := T_{ii}(T_{\text{bulk}_{i}}, T_{w_{i}}, P_{t_{i}}, XX^{<i>}, L, z, T_{w_{i}} + 1) \]

Store the total heat transfer coefficient (DLM suction model)

\[ \text{TH}_{	ext{HC},i,j} := h_{\text{TC}}(T_{\text{bulk}_{i}}, T_{\text{int}_{i,j}}, T_{w_{i}}, P_{t_{i}}, XX^{<i>}, L, z) \]
**** Solve for HTC -- DLM Model (with suction) ****************

Given

\[ q''_{film}(T_{guess}, Tw, z) - q''_{Cs}(Tb, T_{guess}, P, X, L) = 0 \]

\[ T_{ii}(Tb, Tw, P, X, L, z, T_{guess}) := \text{Find}(T_{guess}) \]

Store the interface temperature

\[ T_{int,j} := T_{ii}(T_{bulk}, T_{w}, P, X, L, z, T_{w} + 1) \]

Store the total heat transfer coefficient (DLM suction model)

\[ THTC_{j} := h_{TCs}(T_{bulk}, T_{int,j}, T_{w}, P, X, L, z) \]

**** Solve for HTC -- Dehbi Model ****************

\[ j := j + 1 \]
\[ THTC_{j} := h D(T_{bulk}, T_{w}, P, X, L) \]

**** Solve for HTC -- Uchida Model ****************

\[ j := j + 1 \]
\[ THTC_{j} := h U(X<\{<\}) \]

**** Solve for HTC -- Kataoka Model ****************

\[ j := j + 1 \]
\[ THTC_{j} := h K(X<\{<\}) \]

**** Solve for HTC -- Gido-Koestel model, natural convection only ******

\[ j := j + 1 \]
\[ THTC_{j} := h_{GK}(T_{bulk}, T_{w}, P, L) \]

\[ j = 8 \]

\[ \frac{1 - W(X<\{<\})}{W(X<\{<\})} \]

Store mass fraction ratio NC/steam

** Option = 1
Spec = 1
Visc = 1
Cond = 1
Diff = 1
Suc = 3
**

PRNPRECISION=5
PRNCOLWIDTH:= 10

WRITEPRN "Tbulk.txt" := T_{bulk}

WRITEPRN "Tint.txt" := T_{int}

WRITEPRN "MM.txt" := MM

WRITEPRN "aaTHTC.txt" := THTC

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Appendix

E. GOTHIC 4.1c INPUT DECK FOR ILLUSTRATIVE TEST CASE

This appendix contains the tables of input parameters for the test case in chapter 4 which illustrates the utility of the boundary layer hypothesis.
### Control Volumes

<table>
<thead>
<tr>
<th>#</th>
<th>Description</th>
<th>Vol (m³)</th>
<th>Elev (m)</th>
<th>Ht (m)</th>
<th>Hyd. D. Pl (m)</th>
<th>Area (m²)</th>
<th>Burn Opt</th>
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### 3D Volumes - Volume 1s

#### Nominal Values - Vertical

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<th>Chan. #</th>
<th>Area (m²)</th>
<th>Ver. Flow (m²)</th>
<th>Hyd. D. Loss (m)</th>
<th>Coeff.</th>
<th>De-ent. Vari.</th>
<th>Factor</th>
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### 3D Volumes - Volume 1s
#### Vertical Noding

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<th>Height (m)</th>
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### 3D Volumes - Volume 1s
#### Vertical Variation - Channel 1

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<th>Hyd. D. (m)</th>
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Vertical Variation - Channel 8

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Vertical Variation - Channel 9

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### 3D Volumes - Volume 1s

**Horizontal Variation - Channel 10**

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### Fluid Boundary Conditions - Table 1

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**Gas Pressure Ratios**

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### Flow Paths - Table 1

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#### Heat Transfer Coefficient Types - Table 1

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### Thermal Conductor Types

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<th>O.D. (cm)</th>
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### Thermal Conductor Type 1
#### Steel Wall

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<td>Density (kg/m³)</td>
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Material Type

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2 Aluminum

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3 Carbo Zinc

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## Material Type

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## Valves & Doors

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**Function 1**
Flow fraction

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**Function 2**
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**Fast Temp**

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**Flow Ramp**

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**Slow Flow Ramp**

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### Function 7
**On Switch**

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Valve Loss

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### Function 9
Sump

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### Volume Initial Conditions

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<th>Pressure (kPa)</th>
<th>Vapor Temp (C)</th>
<th>Liquid Temp (C)</th>
<th>Humidity (%)</th>
<th>Volume (m^3)</th>
<th>Ice Volume (m^3)</th>
<th>Ice Surf. A. (m^2)</th>
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### Initial Gas Pressure Ratios

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<th>He</th>
<th>H</th>
<th>Kr</th>
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### Run Parameters Menu

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### Ice Condenser Parameters

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