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INVESTIGATION OF HEAT AND MASS TRANSFER CHARACTERISTICS IN
AN ABSORBER WITH PERFORATED PLATES

DISSertation

Presented in Partial Fulfillment of the Requirement for
the Degree Doctor of Philosophy in the Graduate School of
The Ohio State University

By

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1998

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ABSTRACT

With increased environmental restrictions and concerns for the rational consumption of primary energy, absorption chillers and heat pumps are emerging as the most viable alternative to standard vapor compression system for residential and commercial air-conditioning. The GAX absorber is one of the most critical components in a GAX absorption system and also one of the most difficult to model. In this work, a mathematical model for simultaneous heat and mass transfer in an ammonia-water, falling film type of absorber was developed. The governing equations for the momentum, heat and mass transfer, along with their corresponding boundary conditions were formulated. Their nondimensional forms were then simplified based on the relative order of magnitude of each term in the equations. The simplified equations showed that the overall absorption process can be decomposed into two basic processes: absorption owing to subcooling of the liquid solution, and absorption owing to the cooling from the wall. These two processes can be directly superimposed. An order of magnitude analysis showed that the ratio of the vapor diffusion term to the liquid diffusion term is less than 5%. Thus, its influence in the mass flux boundary condition for the liquid flow can be neglected in the analysis of general film flows. With this approximation, the effect of the vapor flow can be directly taken into account by the mass flux boundary condition for the liquid flow. Therefore, the mass transfer problem in the vapor flow need not be explicitly investigated. The nondimensional equations were then solved numerically for a wide
range of the key parameters $eRePr$ and $eReSc$. The effects of $eRePr$ and $eReSc$ on the mass absorption flux, the species boundary layer thickness and other important parameters were investigated. Empirical correlations for the nondimensional absorption flux, the wall temperature and the interface temperature were successfully developed. Heat and mass transfer coefficients were then developed for film flows with short mixing distances. Numerical results showed that both the heat and mass coefficients are affected by the subcooling of the inlet solution as well as the transport properties of the liquid and the film thickness. At the end of this work, a component design model using the numerical results obtained in this work was developed to design a “W” fin absorber. In this design model, the Colburn-Drew equation was used on the vapor side to determine the composition of the absorption flux. Design results showed that the amount of diffusion flux in the vapor flow could be greater than 10% of the amount ammonia flux into the liquid flow. Geometric parameters for this “W” absorber were parametrically varied, and optimal trends in related key parameters were identified for the “W” fin absorber. An optimized ‘W” fin absorber was proposed for a 5 RT ammonia-water absorption chiller.
Dedicated to my parents
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NOMENCLATURE

A : area
B : breadth of the perforated plate
c : concentration
cp : heat capacity
D : diameter, diffusion diffusivity
E : thermodynamic relation at equilibrium state
F : mass transfer coefficient in vapor flow
Fr : Froude Number $gh_0^* \sin \alpha U_o^2$
g : gravitational acceleration
$h_0^*$ : film thickness at the inlet
h: film thickness
$h_q$ : heat transfer coefficient
i : incremental number, 1,2,3 ...
j : superficial velocity
$j^*$ : dimensionless parameter defined in Eqn (3)
k: conductivity
L: reference length
Le: Lewis number
LMTD: logarithmic mean temperature difference (K)

\( \dot{M} \) : molar flow rate (kg mole/s)

\( \dot{m} \) : mass flow rate [kg/s]

\( n \) : normal direction of the wall

\( n_1, n_2 \) : tangential direction of the upper and lower plate

\( N \) : molar flux (kg mole/m\(^2\)-s)

\( N_f \) : number of flutes

\( \text{Nu} \) : Nusselt number

\( \text{Pr} \) : Prandtl number

\( Q \) : heat transfer (W)

\( \text{Re} \) : Reynolds number

\( R_w \) : wall resistance (m\(^2\)-K/W)

\( \text{Sc} \) : Schmidt number, v/D\(_{12}\)

\( \text{Sh} \) : Sherwood number, \( k_d/D_{12}\)

\( T \) : temperature (K)

\( t_w \) : wall thickness (m)

\( U \) : overall heat transfer coefficient (W/m\(^2\)-K); reference velocity.

\( u, v, w \) : velocity component in x, y, z direction

\( x \) : mass fraction of ammonia (percentage)

\( y \) : vapor quality, normal direction of the interface

\( z \) : film flow direction
Greek symbols

\( \alpha \) : inclined angle of the wall
\( \lambda \) : absorption/desorption heat
\( \Gamma \) : Mass flow rate per wetted perimeter in the film flow
\( \delta \) : film thickness or \( \varepsilon Re Pr \)
\( \varepsilon \) : nondimensional parameter \( h^*_i/L \)
\( \phi \) : composition of ammonia in absorbing/desorbing vapor
\( \mu \) : dynamics viscosity
\( \omega \) : nondimensional concentration defined by Equation (19)
\( \rho \) : density
\( \theta \) : nondimensional temperature defined by Equation (19)
\( \sigma \) : surface tension

Subscripts

0: at the inlet
\( a \) : assumed, absorber
\( \text{abs} \) : absorption/desorption
\( \text{c} \) : coolant, condenser
\( \text{d} \) : desorber
\( \text{g} \) : vapor
\( \text{h} \) : hydraulic
\( \text{i} \) : inside
in : inlet
int: interface
l : liquid
lb: bulk liquid
m: molar based, mass transfer
o : outside
r : rectifier
sat : saturation
senl : sensible liquid
senv : sensible vapor
vb : bulk vapor
vi : vapor at interface
w : wall

Superscripts

~: nondimensional parameters
*: dimensional parameters
CHAPTER 1

INTRODUCTION

1.1 Background

The energy used for cooling and heating residential and commercial buildings comprises one third of the total energy consumed in the United States (Devault, 1988). With increased environmental restrictions and concerns for the rational consumption of primary energy, as well as the ban of the ozone-depleting CFC-based refrigerants, absorption chillers and heat pumps are emerging as viable alternatives for residential and commercial air-conditioning.

In an absorption cycle, the working fluid is a binary mixture; not a single component fluid as used in a conventional vapor-compression refrigerant cycle. Figure 1 shows a schematic of a basic absorption heat pump system. For comparison purposes, a schematic of vapor compression cycle is plotted below the absorption cycle. From these two schematic diagrams, one sees that the fundamental difference between the vapor-compression refrigerant cycle and the absorption cycle is the mechanism which increases
the refrigerant vapor pressure. In a vapor-compression cycle, the pressure of the vapor leaving the evaporator is increased a compressor. In an absorption system, the vapor is pressurized using an absorption-desorption process. The term "absorption" describes the transfer of a binary vapor into the liquid absorbent, and the term "desorption" describes
the generation of vapor from the condensed phase of a mixture (Herold [1996]). The vapor refrigerant is first absorbed into a liquid solution in the absorber. A pump is then used to bring this solution to a higher pressure. At this high pressure, the refrigerant vapor is then driven from the liquid solution by heating it in a desorber. Because the pumping of a liquid consumes much less energy than directly compressing a vapor, the electrical demand in an absorption cycle is much lower than for a vapor-compression cycle. This feature can be used to reduce the impact of electric power demand associated with air conditioning, especially in highly-populated areas. Since the major energy input is from thermal energy, absorption chillers and heat pumps are also attractive because of their potential to be driven by low grade energy, such as solar energy or waste heat. Use of absorption chillers and heat pumps will reduce global warming through the reduction of fossil fuel consumption.

1.2 Generator/Absorber Heat Exchanger (GAX) Absorption Cycle

For a binary mixture, the saturated temperature of the solution changes with its composition. As a result, there are substantial temperature glides between the inlet and the outlet of the generator. Therefore, the outlet weak solution from the generator can be used to preheat the inlet solution to the generator before the weak solution goes into the absorber. Similarly, the strong solution exiting the absorber can be used to pickup the heat released at the top of the absorber before it returns to the top of the generator. To use this energy recovery technique, two additional components are added to the basic absorption cycle. These two components are the solution heated desorber (SHD) and the
absorption cycle. These two components are the solution heated desorber (SHD) and the solution cooled absorber (SCA), as shown in Figure 2. The cycle resulted from this improvement is the single effect absorption cycle. In the cooling mode, the typical value of coefficient of performance (COP) for the single effect absorption cycle is about 0.5.

![Diagram of GAX Absorption Cycle](image)

*Figure 2 Diagram of GAX Absorption Cycle*

To further improve the performance of the single effect absorption cycle, the pressures and concentrations of the solutions in the absorber and generator are selected in such a way that temperatures in the generator are partially overlapped with those in the absorber. Thus, the heat energy which is released during the exothermal absorption of the ammonia refrigerant into the water can be recovered to heat the top portion of the generator. This
this modification is the Generator/Absorber Heat Exchanger (GAX) absorption cycle. Figure 2 shows a schematic diagram of a GAX cycle. In the cooling mode, the typical value of coefficient of performance (COP) for the GAX absorption cycle is about 0.7. The first cost of the GAX cycle is comparable to that of a single effect system, but the COP of a GAX cycle is much higher than that of the single effect system. Beside that, ammonia-water is non-toxic and innocuous to the ozone layer. Thus, the ammonia-water GAX absorption heat pump is more suitable for residential heating and cooling than other absorption cycles (Phillips [1990]).

In a GAX absorption cycle, ammonia is the refrigerant, and water serves as the absorbent. The concentrations of saturated liquid and vapor ammonia-water mixture at different temperatures are shown in Figure 3 and Figure 4. Figure 3 shows the concentrations at 70 psi, a typical pressure in the absorber and evaporator for a chiller. Figure 4 shows that at 300 psi, a typical pressure in the generator and condenser. In an absorption chiller, the liquid concentration ranges from 2% to 50% while corresponding vapor concentration ranges from 30% to 99.9%.
Figure 3 Concentration of Saturated Liquid and Vapor Ammonia-Water Mixture at 70 psi

Figure 4 Concentration of Saturated Liquid and Vapor Ammonia-Water at 300 psi
1.3 Current Status in the Component Design

From the previous system description for the GAX cycle, one sees that the number of components in a GAX absorption system is greater than that in a conventional vapor compression system, and the components are more complex. As a result, existing absorption systems are more expensive than convention air-conditioners. This drawback is the primary hurdle in commercializing the existing technology. In order to be economically competitive, it is vitally important to have manufacturable and cost effective compact heat and mass exchangers that form the components of the absorption systems.

The first stage of developing an absorption system is the cycle modeling. The objectives of the cycle modeling are to determine the steady-state operating conditions of each component in the system and optimize the system by adjusting certain parameters. To determine the operating conditions, the mass conservation and energy conservation equations for all the components, as well as the assumptions about the thermodynamic state at various points of the cycle are solved simultaneously. Even though the working solution is a binary mixture, none of the current available cycle modeling tool for absorption system is capable of considering the mass transfer between the vapor and the liquid. In all current cycle modelings, it is assumed that the vapor and the liquid are in thermodynamic equilibrium.
The next stage is the component design. The objective of the component design is to select a proper geometry for each component and optimize the geometric parameters of each component. In selecting the geometries, the primary concerns include flow distribution, flooding condition and wettability of the surface. Flow distribution is a common problem for heat exchangers with multi-channels. In absorption systems, fluid flows inside the components usually are two-phase flows. This makes it more challenging to evenly distribute the flows because of the random nature of two-phase flows.

From a thermodynamic point of view, it is important that the flow arrangement of the liquid and vapor is in counter-current; this decreases the production of entropy. In counter-current flow, as the gas velocity is gradually increased, a point would eventually be reached at which large waves are formed on the interface, resulting in a chaotic flow pattern with the liquid droplets being entrained by the upward gas flow. This phenomenon is referred as “flooding”. If flooding occurs in a component, the liquid flow rate will decrease substantially and the component will not function properly.

In a typical falling film counter-current absorber, a thinner film usually is preferred in order to increase the heat transfer and decrease the flow rate of the circulating solution. However, owing to the low surface tension of ammonia-water solution on carbon steel, a rupture of a very thin film may occur. This will leave a dry patch on the surface and
significantly decrease the heat and mass transfer area. Wettability is, therefore, one of the primary concerns in choosing the geometry of the component.

After selecting the geometry for each component, the heat and mass transfer processes in each component are investigated and the sizes of the components are determined based on the requirement on the heat transfer or mass transfer. Theories of absorption and desorption are still in the development stage. Many of the associated phenomena are still not well understood. The key controlling parameters in these processes are unclear. As a result, there are no systematical methods to correlate experimental results for heat and mass transfer. Thus, there are no empirical correlations for these processes in open literature. Absorption and desorption processes are simultaneous heat and mass transfer processes. Because of the difficulty of solving the heat and mass transfer equations simultaneously, neither any analytical heat and mass correlations are available in the open literature, even for very simple geometries. In the meantime, in order to solve the problem with wettability, many complicated surfaces have been used to improve the wettability. The complexity of the geometries precludes the prediction of the heat and mass transfer coefficients in the liquid and vapor regions. As a result, sizing of components and prediction of their performance are a significant challenge. Optimization is practically impossible.

In most current component design models, it is assumed that the liquid and vapor are in equilibrium state and heat transfer correlations for single component fluid are directly
used to estimate the heat transfer coefficients in the fluid flows. Experimental results have showed that the heat exchangers designed by this manner are undersized. In some cases, it is found that the amount of heat transfer, or the amount of vapor absorbed in the absorber, is significantly less than what is required by the cycle modeling.

As discussed in the development of the GAX cycle, the GAX absorber/desorber is the most critical component in the GAX cycle. If this component does not function properly, a GAX cycle would degrade to a single effect absorption cycle. As a result, the COP of the cycle will decrease substantially. Thus, develop a very effective GAX absorber/desorber is vitally important for commercializing the GAX heat pump or chiller. In most existing systems, experimental results showed the performance level of the GAX absorber/desorber must be improved. Experimental results also suggested that the problems in the GAX absorber/desorber were on the absorption side. Thus, in this work, the investigation will focus on the absorption process.

1.4 Scope of Work

The objective of this work is to develop a very effective GAX absorber/desorber. For this purpose, a fundamental study of the absorption process in a thin film over a flat plate was first carry out. The absorption is a complicated physical process involving three fundamental transport phenomena; momentum, heat and mass transfer. In general, these three processes affect each other and must be studied simultaneously. Solving the complete form of the governing equations simultaneously would be quite a challenge,
whether by analytical or numerical methods. Reasonable simplifications and approximations must be made. A nondimensionlization process is needed for these simplifications and approximations. The governing equations and their corresponding boundary conditions can then be simplified based on the relative order of magnitude of each equation.

The simplified equations with their boundary conditions can be potentially solved either numerically or analytically. Conlisk [1992] has shown that an analytical solution can be obtained when $\frac{eRePr}{eReSc}$ are in certain ranges. Even when these two parameters are in these ranges, quantitative results still need to be obtained by numerical techniques. In practical situations, both of these two parameters can be much greater or much smaller than unity. Furthermore, since the results of these analyses will be applied to the component design, explicit expressions for absorption flux, wall temperature and other important physical parameters must be obtained for the component modeling and later be calibrated by experimental data. For these reasons, it is preferable to employ a numerical technique to directly solve the equations. By correlating the numerical results for these parameters under different operating conditions, one can obtain general empirical correlations for important parameters. The correlations developed in this stage can be applied to a component design model and can be verified by comparing the results from the design models for particular experiments with experimental data.
For these reasons, the following work has been carried out to investigate the characteristics of heat and mass transfer in the absorption process in a thin liquid film.

1. A mathematical model for falling film absorption problems on a flat plate was developed. The governing equations for momentum, heat and mass transfer, along with their corresponding boundary conditions, were nondimensionalized. The equations based on the relative order of magnitude of each term in the equations were simplified. The critical variables on which absorption flux and other important parameters depend were identified.

2. The simplified equations were numerically solved using the commercial fluid dynamics package FIDAP. Numerical results for the nondimensional absorption flux, wall temperature and interface liquid concentrations were correlated for the parameter \( eRePr \) and Lewis number.

3. A one-dimensional GAX-SCA absorber design model, based on the correlations developed at stage (2), was then created.

4. The one-dimensional design model was applied to the design of a "W-fin" absorber. Geometric parameters for this "W" absorber were parametrically varied, and optimal trends in related key parameters were identified for the "W" fin absorber. An optimized "W" fin absorber was proposed for a 5 RT ammonia-water absorption chiller. Other currently available engineering design models were compared with this model.
CHAPTER 2

LITERATURE REVIEW

2.1 Challenges in Component Design

Designing components for an ammonia-water system includes the problems associated with common heat exchanger design, as well as other considerable challenges. These include (1) scarce experimental data and correlation for heat transfer and mass transfer coefficients, (2) difficulty in predicting the occurrence of flooding in counter-flow arrangement, and (3) unavailability of transport properties for an ammonia-water mixture. Extensive research has been carried out in this field in recent years involving both theoretical studying and experimental testing. Several types of heat exchangers have been proposed specifically for an ammonia-water heat pump system.

Like most components in other refrigerant systems, the flow arrangement between the solution liquid and the vapor in these proposed components includes parallel-flow and counter-flow. From the thermodynamic point of view, vapor flow should be counter to the flow of the liquid solution in order to minimize the entropy production caused by the differences in temperature and equilibrium mass fraction between the vapor and the
liquid streams. This arrangement is especially important for the absorber and the desorber to achieve the desired outlet concentration and temperature gradient. For the condenser and evaporator, however, this thermodynamic advantage is not significant, and the selection of a flow arrangement should be based on other requirements such as heat transfer, simplicity and cost. The parallel flow arrangement is usually selected. Some commonly used industrial two-phase heat exchangers, such as those with tubes in a shell, a coiled smooth tube, a tube coil with plate fins, etc., have been employed for condensers and evaporators with this arrangement.

Compared with the counter-flow component design that will be discussed in the following section, there is more literature available for the design of parallel-flow components. Heat transfer and pressure drop correlations for flow with a vapor quality from 20% to 90% are relatively well developed for both evaporation and condensation in different geometries. The main challenge in the heat transfer estimation is associated with the refrigerant, ammonia-water pair, being a binary mixture. The mechanism for nucleate boiling of a binary mixture is not understood well enough, and experiment data are scarce. Few heat transfer correlations have been developed for binary mixtures. For the parallel-flow component, the heat enhancement is mainly limited by the pressure drop requirement.

There are problems associated with the counter-counter arrangement, such as flooding, which would not be encountered in co-current arrangement. Thus, from the component
For the absorber and desorber with the counter-flow arrangement, several different types of heat exchangers have been proposed for the components in ammonia-water absorption heat pumps. Based on the flow pattern, all of these heat exchangers could fall into two categories: falling-film type heat exchangers and bubble type heat exchangers. The main interest of this project is the falling-film type of heat exchangers. Therefore, only a brief review for bubble type heat exchangers will be given here.

2.2 Heat and Mass Transfer in Bubble Columns

Bubble columns are extensively used in the chemical industry. In a typical counter-current bubble absorber, vapor is injected from the bottom of the column and bubbles are trapped in the solution pool. Liquid is introduced from the top of the column and extracted from the bottom of the pool. Coolant flows in an outside jacket counter-current to the liquid flow. This type of heat exchanger minimizes the adverse effects of phase separation and mass transfer resistance because mixed better. In order to promote mass transfer between the liquid and the vapor, enhance the heat transfer between the liquid
and the coolant, and minimize the axial liquid backmixing, different perforated fins are inserted across the liquid flow direction inside the column.

Many papers have been published on different aspects of bubble columns. These include studies of flow regimes, coalescence and breakup of bubbles in liquids, bubble diameter, gas holdup, interfacial area, axial liquid phase dispersion coefficient, mass transfer coefficient and heat transfer coefficient between the liquid and the vapor phase. A unified review on the bubble column reactor design was given by Shah et al. [1982]. However, little work has been done on the heat transfer between the liquid and the heat transfer surface. Kast [1963] pointed out that the radial component of the liquid velocity, which is induced by the rising bubbles, is pertinent to the heat transfer coefficients in the bubble column. Deckwer [1980] presented a theoretical heat transfer model for a homogeneous bubble column by combining a surface renewal model of mass transfer with isotropic turbulent theory. For a bubble column with an insert device, there is no general correlation to predict the heat transfer coefficient between the heat transfer surface and the liquid.

2.3 Heat and Mass Transfer in Falling-Film Type Heat Exchangers

In this type of heat exchanger, the liquid solution flows though a dripper at the top of the exchanger and falls along the heat transfer area owing to gravity, forming a thin film. Meanwhile, the vapor flows upward through the space surrounded by the heat transfer area. With coolant flow on the other side of the heat transfer surface, heat is transferred
from (or to) the liquid solution and vapor is condensed (or evaporated) on the liquid surface. Several types of falling-film absorbers have been studied. These absorbers may have; (1) horizontal smooth tube banks, (2) vertical smooth tubes, (3) tubes in a shell, (4) coiled smooth tubes, (5) vertical fluted tubes, (6) confined cross flow with fluted tubes, or (7) perforated fin and other designs with a thin liquid film on the heat transfer surface. This type of heat exchanger offers several advantages, including relatively high heat transfer coefficient on the solution side, low mass transfer resistance on the liquid solution side and little backmixing.

Since the pioneering work by Nusselt [1916] on film condensation on a vertical wall, many theoretical studies in the field of heat transfer have been performed and a considerable number of papers have been published. McAdams [1954] observed that heat transfer rates often vary between 80 to 170 percent of Nusselt's predicted values for normal fluids. This suggests a need for a more exact, analytical description of the process. Rohsenow [1956] included energy convection in the heat balance, while continuing to neglect the inertial force. His results showed that a term needs to be added to the latent heat of evaporation to account for the degree of liquid subcooling. In these papers, however, many authors neglected the effect of liquid-vapor interfacial shear on the heat transfer in the liquid film. Koh et al. [1961] considered the problem of the condensation of a pure stationary vapor on a vertical wall. They reformulated the problem in terms of two-phase boundary layer theory, including liquid film and vapor flow boundary induced by the liquid flow. Both convection and the interfacial shear stress
were taken into account, and the equations were solved numerically. Their results indicated that the effects of the interfacial shear on the heat transfer are negligible for fluids with Prandtl numbers ten or greater and are quite small even for Prandtl number of one. Chen [1961] investigated the similar problem. Integral equations were used to describe the thermal boundary layer. These equations were simplified for the case of 
\[ \mu_r \rho_v < \mu_i \rho_i \], and they were solved by a perturbation method. By analyzing the similarity in the solutions, an explicit expression for Nusselt number was obtained. Owing to condensation on the surface, the flow rates of the film flow change along the plate. Experimental observations of the condensate flow indicate that the laminar film can be described as wavy in the segment where the local film Reynolds number is in the range of 30 to 1800. Farther down stream, the film appears turbulent. Chen et al. [1987] reviewed the sizable experimental studies and correlations that have been carried out in the past. They developed a correlation for the average heat transfer coefficient for a long film that may have wavy and turbulent regions. In more recent years, modeling efforts have been devoted to the prediction of heat transfer in a turbulent liquid film. Yih and Liu [1983] summarized important turbulence models for predicting heat transfer. There are at least 14 different turbulence models, including their own, in their summary.

Since the classic work of Colburn and Drew [1937], much mass transfer work has been done on the falling-film absorption and condensation of a binary component vapor mixture. Many articles on liquid film absorption have been published. In most of these published works, the controlling mass transfer resistance was assumed to occur in the
liquid film. This assumption may be due to the fact that the dominant solution pair in commercial absorption machines is the lithium-bromide water solution. In a lithium-bromide system, there is only steam in the vapor region, so there is no mass transfer resistance in the vapor. In order to investigate the influence of the mass transfer resistance in the liquid film, Nakoryakov and Grigoreva [1977] established a theoretical model for the absorption of vapor into liquid films and drops. In their model, the authors considered the influence of temperature variations in the direction of the flow. This paper suggested the existence of subcooling in the bulk liquid region. Instead of assuming a uniform velocity profile across the film, which was adopted by Nalotyakov and Grigoreva, Grossman [1983] used the general diffusion and energy equations simultaneously to analyze the heat and mass transfer phenomena in the process of the absorption of vapor into the laminar liquid film. By using the method of separation of variables, the author obtained an analytical expression for the film concentration in the form of an infinite series of eigenfunctions. This expression explicitly indicated that the concentration not only depends upon mass transfer, but also strongly relies on heat transfer. When the Lewis number is less than one, the development of the concentration boundary layer falls behind that of the thermal boundary. Conlisk [1992] used Laplace transforms to obtain a temperature distribution in a very thin film. Numerical techniques were employed to obtain quantitative results. Mass flux, temperature distribution and film thickness were obtained and compared with experimental results. It was shown in his paper that mass transfer took place in a thin layer of fluid near the liquid-vapor interface, which indicated a very high level of mass transfer resistance in the liquid film.
Most of these analytical methods cannot be applied to the absorption process for ammonia-water vapor which is a binary mixture and for which mass transfer resistance exists. Before the work of Conlisk and Mao [1996], it was widely accepted that the mass transfer resistance in the vapor region for the ammonia-water mixture cannot be neglected. In order to consider the effect of mass resistance in the vapor region, while neglecting the mass transfer resistance in the liquid film, Price and Bell [1973] developed a computational framework to apply the Colburn-Drew equations to the design of a binary vapor condenser. Based on their benchmark, Kang et al. [1996] investigated the absorption and desorption processes in all of the components found in ammonia-water absorption heat pumps. The authors analyzed the effects of heat and mass transfer on the composition of the mass flux across the interface. The ranges of composition values of the flux were given for all types of components. In order to investigate the dominant factors controlling the absorption process, Perez-Blanco [1993] developed a one-dimensional model including the mass transfer resistant effect in the liquid film and the vapor region. It was concluded from his model and experimental results that the mass transfer process in the falling-film controls the absorption rate. Arman and Panchal [1993] carried out an analysis to determine the effects of the mass transfer resistance on the rate of the absorption of ammonia. The results in this paper showed that the mass transfer resistance is equally important for the vapor and liquid phases. The two-phase boundary layer theory was adopted to develop the mass and energy balance in the boundary layers. Takuma et al. [1993] performed a theoretical and experimental investigation on the condensation heat transfer of an ammonia-water vapor mixture on a
vertical flat surface. Their analysis revealed that the diffusion process in the liquid film is only important for the limited region near the leading part of the vertical plate. Experiments were carried out to measure the concentration profile in the vapor layer by using the CARS (Coherent Anti-Stokes Raman Spectroscopy Technique). Conlisk and Mao [1996] developed a mathematical model for the absorption process of ammonia-water into the liquid film on a horizontal tube. The boundary condition for mass fraction in the film at the interface is modified to account for the effect of the vapor. The resulting partial differential equations were then solved by using a Fourier cosine transform. In their paper, it was found that the diffusion effect in the vapor has no effect on the absorption in the liquid film.

2.4 Conclusions from the Literature

The conclusions drawn from the few available studies in the literature seem inconsistent. The reasons for this could be associated with the differences in solution concentration used in experiments and analytical models as well as the limited knowledge of transport properties and transport correlations. From these papers, no conclusive results can be drawn regarding the role of mass transfer resistance on the liquid film side in the absorption/desorption process. This is a critical issue in the component design. If the mass resistance in the liquid film is significant in the absorption process, then the bulk liquid will be substantially subcooled. The subcooling in the solution will decrease the temperature difference between the film and the coolant, and, thus, reduce the heat
transfer. To achieve the same amount of heat transfer for the case of a saturated solution, a much bigger heat exchanger will be needed.

From all of the published works and experiments at The Ohio State University, it is believed that an increase in the vapor mass transfer coefficient and a decrease in the film thickness are critical to the enhancement of the absorption process. One of possible ways to achieve these enhancements is to increase the vapor velocity and decrease the liquid flow rate, which would result in a decrease in the film thickness and heat and the associated mass transfer resistance. However, flooding conditions would pose an upper limit to this vapor velocity, and the uniform wetting problem imposes a lower limit on the flow rate. Other ways to enhance the absorption/desorption process are:

1. Periodic disruption to the film flow. This will enhance the mixing of the liquid film and result in an increase in the heat transfer rate along with a decrease in the level of subcooling in the liquid film. Heat exchangers which employ this idea are those with house fins, offset strip fins and horizontal tube banks.

2. Increasing the interfacial area. This will directly increase the mass and heat transfer area. Heat exchangers with fin tubes and packing materials, as well as plate type heat exchangers with plate fins, are inspired by this idea.

3. Increasing the length of vapor flow pass. This would increase the time of vapor contact with the liquid phase, resulting in thermodynamic equilibrium between the
liquid and vapor phases. Heat exchangers with baffles or insertion devices use this technique.
CHAPTER 3

MODEL AND GOVERNING EQUATIONS

3.1 Introduction

In this chapter, the problem of absorption of ammonia-water vapor into a liquid film falling over a flat wall is formulated and analyzed. In a counter flow absorber, the low concentration hot liquid solution flows from the top of the absorber in a thin film flow. The high concentration cold vapor mixture flows up from the bottom of the absorber. This vapor is absorbed into the low concentration liquid film. Latent heat is released at the interface in this exothermal process. A hot saturated ammonia-water solution contains less ammonia than a cold solution. In order to continue the absorption of ammonia vapor, the liquid film must be cooled by the coolant on the other side of the wall. From heat and mass transfer point of view, it is desirable to frequently break the thermal and concentration boundaries. This can be accomplished by mixing the liquid flow at every certain distance L. The frequent mixing will decrease the subcooling in the solution and increase the heat transfer coefficient of the film flow. The mixing distance L is usually on the order of an inch. In the following discussion, only the film between the mixing points is analyzed, not the entire film in the absorber. It is also assumed that at each inlet, the
solution is well mixed, and the temperature and concentration of the liquid are uniform across the film.

Figure 5 Typical temperature and concentration profiles during a countercurrent absorption process
Figure 5 shows the typical temperature and concentration profiles in the liquid and vapor across the flow direction. In the absorption process, absorption heat is released at the interface, and the liquid film is cooled down at the wall, thus the temperature at the interface is the highest for liquid flow along the width of the film. Meanwhile, since the temperature of the inlet vapor from the bottom of the absorber is much lower than that of the inlet liquid from the top of the absorber, the interface is also the highest temperature for the vapor flow. Because ammonia is absorbed into the liquid through the interface, the liquid concentration is highest at interface. The interface vapor concentration is highest at the bottom of the absorber along the liquid flow direction. This concentration is lower than the inlet vapor concentration. Thus, the bulk vapor concentration, \( x_{vb} \), is higher than the interface vapor, \( x_{v,i} \), at any cross section. This means ammonia will diffuse from bulk vapor flow to the interface in addition to being convected to the interface with the condensation flux.

Since the liquid and vapor flows are separated, it is through the interface that they affect each other. The continuity, momentum, energy and mass transfer equations for single-phase flow can be directly applied to both the liquid and vapor flow. Their effects on each other can be reflected on the boundary conditions at the interface. It is obvious that the liquid flow can be treated as a thin-film flow. In most cases, the ratio of film length to the film thickness is much larger than 100, so the entrance and exit effects for velocity can be neglected without significantly sacrificing the accuracy of the analysis. The vapor flow, however, is much more complicated than the liquid flow. Nevertheless, what is of most concern in an absorption process is the absorption rate into the liquid flow. If the
effect of vapor flow can be taken into account by modifying the boundary conditions at
the interface, then the vapor flow can be ignored in the analysis of liquid flow (Conlisk
and Mao [1996]). For this purpose, the boundary conditions at vapor–liquid interface
must be analyzed first.

3.2 General Boundary Conditions at the Interface

At the interface, the momentum, heat and mass transfer must be matched in both the
liquid and vapor phases in such a way that the physical laws are satisfied. The general
boundary conditions at the interface can be summarized as the following:

(i) Interface velocity. Along the liquid-vapor interface, the vapor and liquid velocities
tangent to the interface must be equal if there is no slip. Within the accuracy of the
boundary layer, the no slip condition at the interface is fulfilled if velocity components in
the flow direction in the liquid and vapor are equal;

\[ w_l = w_v \]  \hspace{1cm} (1)

(ii) Mass flow across the interface. According to the law of mass conservation, the total
mass transfer from the vapor to the interface must equal the total mass transfer from the
interface to the liquid:

\[ \rho_i v_l - \rho_l w_l \frac{d\delta}{dz} = \rho_v v_v - \rho_v w_v \frac{d\delta}{dz} \]  \hspace{1cm} (2)
Since the liquid and vapor flows are binary mixtures, the mass flow for each species across the interface should also be conserved. The continuity equation for ammonia is:

\[
D_t \frac{\partial c_t}{\partial y} + c_{i,i} \left(-v_i + w_i \frac{d\delta}{dz}\right) = D_v \frac{\partial c_v}{\partial y} + c_{v,i} \left(-v_v + w_v \frac{d\delta}{dz}\right)
\]  

(iii) Interface shear stress. By Newton's Third Law, the force exerted on the liquid by the vapor must be equal to the force exerted on the vapor by the liquid.

\[
\mu_t \frac{\partial w_t}{\partial y} = \mu_v \frac{\partial w_v}{\partial y}
\]

(iv) Interface temperature. At the interface, vapor and liquid are in thermodynamic equilibrium, so the temperatures must be equal. Therefore,

\[
T_{i,i} = T_{i,v}
\]

(v) Interface heat flow. According to energy conservation, the heat transfer from the interface to the bulk liquid should be equal to the sum of sensible heat transfer from the vapor to the interface and the absorption heat released in the phase change process.

\[
-k_i \frac{\partial T_i}{\partial y} = -k_v \frac{\partial T_v}{\partial y} + \lambda \rho_v (-v_v + w_v \frac{d\delta}{dz})
\]

(vi) Thermodynamic equilibrium at the interface. The temperature, pressure and concentration at the interface can be related by their thermodynamic relations at the equilibrium state:

\[
x_{u} = c_{i,i} / \rho_i = E_i(T_{i,i}, P)
\]

\[
x_{v,i} = c_{v,i} / \rho_v = E_v(T_{v,i}, P)
\]
Functions $E_t$ and $E_v$ are empirical functions developed from the database for ammonia-water solution at the equilibrium state.

(vii) The normal stress at the interface. The pressure of liquid and vapor at the interface must be equal if surface tension is neglected. Therefore,

$$P_{t,i} = P_{v,i} \quad (9)$$

The foregoing boundary conditions generally are valid for any separated two-phase flow. For the falling-film absorption problem, however, it is possible to further simplify these boundary conditions by using certain features of thin film flow.

The shear stress in the film flow and the vapor flow are on the order of $\mu_t U_t / \delta$ and $\mu_t U_v / L_v$, respectively. An order of magnitude analysis can show that the shear stress in the liquid phase at the wall is much larger than that at the interface. Therefore, the shear stress at the interface can be neglected. Koh et al. [1961] and Chen [1961] showed that the effects of the interfacial shear on the heat transfer are also negligible for fluids with Prandtl numbers of ten or greater and are quite small even for liquids with a Prandtl number of one. The Prandtl number of ammonia-water solution is on the order of one. Thus, the zero shear stress assumption is valid from the heat transfer point of view.

In most cases, the absorption rate is much less than the liquid film flow rate. Therefore, in a short region, one can assume that the film thickness is constant. This assumption, as well as the zero shear stress assumption will enable the complete separation of the motion of liquid flow from vapor flow. Furthermore, the latent heat associated with the phase
change in the absorption process is much larger than the change in the sensible heat of the vapor flow, and the heat transfer from the liquid to the vapor can be ignored in the present model.

3.3 Mathematical Model

The previous simplifications and other additional assumptions made in this work are summarized in the following:

1. The liquid is Newtonian and has constant physical properties;
2. Momentum effects and shear stress at the free surface are negligible;
3. The film is a laminar film with no wave at the interface;
4. Absorption rate is small compared to the film mass flow rate;
5. Thermodynamic equilibrium exists between the vapor and liquid at the interface;
6. All absorption heat is released at the interface;
7. Temperature and concentration at the inlet are uniform;
8. There is no heat transfer from liquid to vapor;
9. There is no Soret effect.
3.3.1 Momentum Equations

As mentioned before, because of the low absorption rate and small shear stress at the interface, the motion of liquid flow can be treated as independent of the motion of vapor flow. The dimensionless continuity equation and the momentum equations are given by:

\[
\frac{\partial \bar{v}_l}{\partial \bar{y}} + \varepsilon \frac{\partial \bar{w}_l}{\partial \bar{z}} = 0 \tag{10}
\]

\[
\bar{v}_l \frac{\partial \bar{w}_l}{\partial \bar{y}} + \bar{w}_l \frac{\partial \bar{v}_l}{\partial \bar{y}} = -\frac{\partial \bar{p}}{\partial \bar{z}} + \frac{1}{Re_l} \left( \frac{\partial^2 \bar{w}_l}{\partial \bar{y}^2} + \varepsilon^2 \frac{\partial^2 \bar{v}_l}{\partial \bar{z}^2} \right) - Fr \tag{11}
\]

\[
\bar{v}_l \frac{\partial \bar{v}_l}{\partial \bar{y}} + \bar{w}_l \frac{\partial \bar{v}_l}{\partial \bar{z}} = -\frac{\partial \bar{p}}{\partial \bar{y}} + \frac{1}{Re_l} \left( \frac{\partial^2 \bar{v}_l}{\partial \bar{y}^2} + \varepsilon^2 \frac{\partial^2 \bar{v}_l}{\partial \bar{z}^2} \right) \tag{12}
\]

where \( \varepsilon = \frac{h_0}{L} \). The distance normal to the wall \( y \) was normalized by the inlet film thickness \( h_0^* \) and the axial coordinate \( z \) was normalized by the mixing distance \( L \). Other nondimensional parameters are given by Conlisk [1992] and Conlisk and Mao [1996]:

\[
\begin{align*}
  h &= h^* / h_0^*, \\
  \bar{y} &= y / h_0^*, \\
  \bar{z} &= z / L \\
  U_0^* &= g \sin \alpha h_0^2 / \nu, \\
  \bar{v} &= v / U_0^*, \\
  \bar{w} &= w / U_0^* \\
  \bar{p} &= p h_0^* / \mu U_0^* \\
  Re_l &= U_0^* h_0^* / \nu, \\
  Fr &= g \sin \alpha h_0^* / U_0^{*2} \tag{13}
\end{align*}
\]

The boundary conditions for the momentum Equation (11) are given by the no-slip condition at the wall and no shear stress at the interface:

\[ \bar{w} = 0 \text{ at } \bar{y} = 0 \]
Because of the low absorption rate, the liquid velocity component in the z direction is constant in the flow direction \( \partial \tilde{w} / \partial z = 0 \). Neglecting terms with \( \varepsilon \) and \( \varepsilon^2 \) in Equation (11), the axial direction velocity component \( w \) can be expressed by the Nusselt type velocity (Conlisk and Mao [1996]):

\[
\tilde{w} = \text{Re}F_r(\tilde{y}h - \tilde{y}^2/2)
\]

(15)

By substituting this solution into the continuity equation, the velocity component \( v \) can be found as (Conlisk and Mao [1996]):

\[
\tilde{v} = -\varepsilon\text{Re}F_r\tilde{y}^3h/2
\]

(16)

It should be noticed that these approximated solutions for the velocity field are valid even for \( \varepsilon\text{Re} \gg 1 \), as long as the absorption rate is low. The y-direction momentum Equation (12) can be simply reduced to \( \partial \tilde{p} / \partial \tilde{y} = 0 \), which will be not needed in the following discussion.

### 3.3.2 Heat and Mass Transfer Equations

The nondimensional heat and mass transfer equations for a thin film flow can be written as (Conlisk and Mao [1996]):

\[
\tilde{v}_l \frac{\partial \theta_l}{\partial \tilde{y}} + \varepsilon \tilde{w}_l \frac{\partial \theta_l}{\partial \tilde{x}} = \frac{1}{\text{Re}_l\text{Pr}_l} \left( \frac{\partial^2 \theta_l}{\partial \tilde{y}^2} + \varepsilon^2 \frac{\partial^2 \theta_l}{\partial \tilde{x}^2} \right)
\]

(17)

\[
\tilde{v}_l \frac{\partial \omega_l}{\partial \tilde{y}} + \varepsilon \tilde{w}_l \frac{\partial \omega_l}{\partial \tilde{x}} = \frac{1}{\text{Re}_l\text{Sc}_l} \left( \frac{\partial^2 \omega_l}{\partial \tilde{y}^2} + \varepsilon^2 \frac{\partial^2 \omega_l}{\partial \tilde{x}^2} \right)
\]

(18)
The nondimensional parameters are defined by:

\[
\theta = \frac{T - T_{sat, in}}{h_f/c_p}, \quad \omega = \frac{x - x_{i, in}}{x_{v, i, in} - x_{l, i, in}}
\]

\[
\Delta T = \frac{h_f}{c_p}, \quad \bar{q}_w = \frac{q_w h^* c_p}{eRe_i Pr_i kh_f}
\]

(19)

It should be noted that the reference temperature is \( T_{sat, in} \), which is the saturated solution temperature corresponding to the inlet liquid concentration, \( c_{l, in} \), not the inlet solution temperature, \( T_{i, in} \). By this definition, the nondimensional inlet temperature, \( \theta_{i, in} \), is a measure of the subcooling of the inlet solution. The temperature scale is taken to be \( \Delta T = h_f/c_p \) and in this scale the nondimensional latent heat is unity. Thus the magnitude of heat flux at the interface is identical to the magnitude of mass flux.

It is assumed that the heat flux through the wall, \( q_w^* \), is uniform, and the heat flux across the interface is proportional to the absorption flux \( m_c^* \). These dimensional boundary conditions for the heat transfer equation can be expressed as:

\[
T = T_{i, in} \quad \text{at} \quad z = 0
\]

\[
-k_i \frac{\partial T}{\partial y} = q_w^* \quad \text{at} \quad y = 0
\]

\[
-k_i \frac{\partial T}{\partial y} = h_f m_c^*(z) \quad \text{at} \quad y = h^*(z)
\]

(20)
Similarly, a uniform inlet concentration throughout the liquid film is assumed. The physical condition at the wall does not allow ammonia diffusion through the wall. The total ammonia flux across the interface is the sum of the diffusion flux by molecular diffusion and the convection flux accompanied by the condensation flow (net flow). These physical boundary conditions for the mass transfer equation can be expressed as:

\[ c_I = c_{i,in} \quad \text{at} \quad z = 0 \]

\[ D_I \frac{\partial c_I}{\partial y} = 0 \quad \text{at} \quad y = 0 \]

\[ -D_I \frac{\partial c_I}{\partial y} + m_c'(z)x_I = -D_v \frac{\partial c_v}{\partial y} + m_c'(z)x_v \quad \text{at} \quad y = h'(z) \quad (21) \]

The last boundary condition shows that mass transfer in the liquid film is strongly affected by the conditions in the vapor phase. On the RHS of equation (21), the interface vapor concentration can be directly related to the interface temperature by the thermodynamic relation. The diffusion term in the vapor flow, however, is not known yet. In order to compare the order of magnitude of this term with others in equation (21), this equation is nondimensionalized as:

\[ -\frac{L}{\varepsilon Re_iSc_i} \frac{\partial c_I}{\partial y} = -\frac{\rho_v D_v}{\varepsilon \rho_i U L_v} \frac{\partial c_v}{\partial y} + \tilde{m}_c + O \left( \frac{x_v - x_{i,in}}{x_{v,in} - x_{i,in}} - 1 \right) \quad (22) \]

where \( \tilde{m}_c = m_c' / \varepsilon \rho_i U \) and \( L_v \) is the characteristic width of the vapor flow. Since the value of \( x_v - x_{i,in} \) changes vary little along a short film, say 1 inch long, in the GAX absorber, the last term on the LHS is negligible. In most cases, the inlet vapor flow in an absorber is a turbulent flow. When it flows from the bottom to the top of the absorber, vapor is
absorbed into the liquid and the vapor flow rate decreases. Therefore, at some point of the absorber, the vapor flow will transit from turbulent to laminar flow. In a counter flow absorber, the maximum nondimensional vapor concentration gradient is at the bottom of the absorber. The concentration gradient on the vapor side can be approximated by:

\[ \frac{\partial \omega_v}{\partial \gamma_v} = Sh_v (\omega_v - \omega_{vb}) \]  

(23)

where \( Sh_v \) is the Sherwood number on the vapor side. For most internal turbulent flows, this Sherwood number can be approximated by \( Sh = 0.023 \, Re^{0.83} \, Sc^{0.3} \). Thus the boundary Equation (22) can be rewritten as:

\[ -\frac{l}{\varepsilon Re_i Sc_l} \frac{\partial \omega_v}{\partial \eta} = -0.023 \, Re_v^{0.83} \, Sc_v^{0.3} \frac{\rho \, D_v}{\varepsilon \rho U L_v} (\omega_v - \omega_{vb}) + \bar{m}_c \]  

(24)

Table 1 lists the typical values of the parameters and properties for vapor flow in a GAX absorber. Substituting the numerical values from Table 1 into Equation (24), one can estimate the magnitude of the first term on the RHS. This term can be rewritten as:

\[ 0.023 Re_v^{0.83} Sc_v^{0.3} \frac{\rho \, D_v}{\varepsilon \rho U L_v} (\omega_v - \omega_{vb}) \]

\[ = 0.023 Re_v^{0.83} Sc_v^{0.3} \frac{\rho \, D_v \, L_v}{3 \Gamma L_v} (\omega_v - \omega_{vb}) \]  

(25)

\[ \approx 8.6 \times 10^{-7} \frac{L}{L_v} Re_v^{0.83} (\omega_v - \omega_{vb}) \]
Meanwhile, the vapor diffusion term on the LHS of Equation (22) can be approximated by:

$$-\frac{l}{\varepsilon Re_i Sc_i} \frac{\partial \omega_i}{\partial \eta} = -\frac{l}{\varepsilon Re_i Sc_i} \frac{\omega_{i,i}}{\delta_m}$$  \hspace{1cm} (26)$$

where $\delta_m$ is the thickness of the specie boundary layer on the liquid side. Conlisk [1992] showed that value $\delta_m$ is on the order of $1/(\varepsilon Re_i Sc_i)^{1/2}$. In a typical GAX absorber, the value of $\varepsilon Re_i Sc_i$ is on the order of 100, much larger than unity. Therefore the specie boundary layer on the liquid side is very thin. Meanwhile, in most cases, the characteristic length, $L_v$, is of the same order as the mixing distance $L$. The driving potential for diffusion on the vapor side, $\omega_{v,vb} - \omega_{v,i}$, however, can be much larger than the driving potential on the liquid side, $\omega_{i,i} - \omega_{i,lb}$. The computational results in Chapter 5 will show that the driving potential in the vapor flow is about one order of magnitude higher.
than that in the liquid flow. Combining Equations (25) and (26), the ratio of vapor side diffusion to liquid side diffusion can be approximated by:

\[
\frac{\text{Diffusion on Vapor Side}}{\text{Diffusion on Liquid Side}} = 8.6 \times 10^{-7} \left( \frac{\varepsilon \text{Re}_c \text{Sc}_c}{\text{Re}_c \text{Sc}_c} \right)^{1/2} \frac{\omega_v, b - \omega_v, h}{\omega_l, x_i - \omega_l, h} = 8.6 \times 10^{-7} \times 1000^{0.83} \times 100^{0.5} \times 10 = 0.026
\]

(27)

Since this ratio is much less than unity, in the order of magnitude comparison, this term can be neglected from the mass transfer boundary equation (Conlisk and Mao [1996]). Thus, Equation (22) can be approximated by:

\[
- \frac{1}{\varepsilon \text{Re}_c \text{Sc}_c} \frac{\partial \omega_l}{\partial \tilde{y}} = \tilde{m}_c(\tilde{x})
\]

(28)

In boundary conditions (20) and (28) for heat flux and mass flux at the interface, the absorption flux \( \tilde{m}_c \) is an unknown variable needed to be found. Therefore, an additional boundary condition is needed to determine \( \tilde{m}_c \). This additional condition can be the thermodynamic relation defined by Equation (7):

\[
x_{li} = E_i(T_{li}, P)
\]

In general, \( E_i \) is a complex function of \( T_{li} \). Figure 3 shows that, in general, the concentration of ammonia-water solution is a nonlinear function of temperature at a certain pressure. Nevertheless, for temperatures ranging from 260 to 190 °F, which is the typical operating temperature range in a GAX-SCA, the concentration is a fairly linear function of the temperature. This linear function can be approximated by:
\[ x_i = -2.76 \times 10^{-3} T_i + 0.77262 \]. This correlation can be rewritten in the following nondimensional form:

\[ \theta_i = \beta \omega_i \]  

(29)

where \( \beta = -(x_{wi} - x_{li})/(2.76 \times 10^{-3} \Delta T) \).

In boundary conditions (20) and (21), the interface is located at \( y = h \). Since nondimensional film thickness \( h \) is variable of \( \tilde{z} \), not a constant, it is not convenient to apply these boundary conditions. Therefore, an adaptive coordinate system \((\eta, \zeta)\) is introduced, where \( \eta = \tilde{y} / h \), \( \zeta = \tilde{z} \) (Conlisk and Mao [1996]). In this new coordination system, the interface is located at \( \eta = 1 \). The derivative in the coordinate system \((\tilde{y}, \tilde{z})\) can be related to that in the coordinate system \((\eta, \zeta)\) by:

\[
\begin{align*}
\frac{\partial}{\partial \tilde{y}} &= \frac{1}{h} \frac{\partial}{\partial \eta} + \frac{\partial \zeta}{\partial \tilde{y}} \frac{\partial}{\partial \zeta} \\
\frac{\partial}{\partial \tilde{z}} &= -\frac{\eta h_i}{h} \frac{\partial}{\partial \eta} + \frac{\partial \zeta}{\partial \tilde{z}} \frac{\partial}{\partial \zeta}
\end{align*}
\]  

(30)

where \( h_i = dh/d\tilde{z} \). Substituting Equation (30) into Equations (17) and (18), and neglecting terms with \( \varepsilon^2 \), the nondimensional heat and mass transfer equations become:

\[
\frac{\partial^2 \theta_i}{\partial \eta^2} = (\varepsilon Re_i Pr_i) \left[ h \tilde{w}_i \frac{\partial \theta_i}{\partial \zeta} + (\tilde{v}_i - h_i \tilde{w}_i) \frac{\partial \theta_i}{\partial \eta} \right] 
\]  

(31)

\[
\frac{\partial^2 \omega_i}{\partial \eta^2} = (\varepsilon Re_i Sc_i) \left[ h \tilde{w}_i \frac{\partial \omega_i}{\partial \zeta} + (\tilde{v}_i - h_i \tilde{w}_i) \frac{\partial \omega_i}{\partial \eta} \right] 
\]  

(32)
As mentioned before, the absorption rate is low compared to the film flow rate. Thus the film thickness is constant to leading order ($v_i = 0 + \epsilon v_{i,1} + \cdots; h = 1 + \cdots$), one can further neglect the convection terms in the film width direction. From these analyses, the nondimensional energy and mass transfer equations and their corresponding boundary conditions can be simplified as (Conlisk and Mao [1996]):

\[
\frac{l}{\epsilon Re_i Pr_i} \frac{\partial^2 \theta_i}{\partial \eta^2} = \tilde{w}_i(\eta) \frac{\partial \theta_i}{\partial \zeta}
\]

with

\[
\theta_i(\eta,0) = \theta_{iln}
\]

\[-\frac{l}{\epsilon Re_i Pr_i} \frac{\partial}{\partial \eta} \theta_i(0, \zeta) = \tilde{q}_w^-
\]

\[-\frac{l}{\epsilon Re_i Pr_i} \frac{\partial}{\partial \eta} \theta_i(1, \zeta) = \tilde{m}_c^-(\zeta)
\]

\[
\theta_i(1, \zeta) = \beta \omega_i(1, \zeta)
\]

\[
\frac{l}{\epsilon Re_i Sc_i} \frac{\partial^2 \omega_i}{\partial \eta^2} = \tilde{w}_i(\eta) \frac{\partial \omega_i}{\partial \zeta}
\]

with

\[
\omega_i(\eta,0) = 0
\]

\[-\frac{l}{\epsilon Re_i Sc_i} \frac{\partial}{\partial \eta} \omega_i(0, \zeta) = 0
\]

\[-\frac{l}{\epsilon Re_i Sc_i} \frac{\partial}{\partial \eta} \omega_i(1, \zeta) = \tilde{m}_c^-(\zeta)
\]

(33)

3.4 Controlling Parameters for Absorption Process

Examining the Equation set (33), it can be easily found that these equations are the governing equations and boundary conditions for film flow with $\tilde{\rho}_i = 1, \tilde{c}_{p,j} = 1, \tilde{k}_i = l/\epsilon Re_i Pr_i, \tilde{D}_i = l/\epsilon Re_i Sc_i$, and constant film thickness. The boundary conditions show that, for a particular film flow, the mass absorption rate is determined by the
subcooling of the inlet solution, $\theta_w$, and the heat flux through the wall, $q_w$. In order to investigating the their contributions to the mass absorption rate, one can decompose the original problem into two separated problems. Assuming

$$\theta_1(\eta, \zeta) = \theta_{1,1}(\eta, \zeta) + \theta_{1,2}(\eta, \zeta) \tag{34}$$

$$\omega_1(\eta, \zeta) = \omega_{1,1}(\eta, \zeta) + \omega_{1,2}(\eta, \zeta) \tag{35}$$

let $\theta_{1,1}$ and $\omega_{1,1}$ satisfy the governing equations and boundary conditions as shown in equation set (36). The only difference between Equation sets (33) and (36) is the magnitude of heat flux through wall. In Equation set (36), the heat flux through the wall is set to zero. Therefore, $\theta_{1,1}$ and $\omega_{1,1}$ are the temperature and concentration of a film flow which is the same as the original flow except this film flows along an adiabatic wall, instead of a cold wall.

$$\frac{1}{\varepsilon Re_i Pr_i} \frac{\partial^2 \theta_{1,1}}{\partial \eta^2} = \tilde{w}_i(\eta) \frac{\partial \theta_{1,1}}{\partial \zeta}$$

with

$$\theta_{1,1}(\eta, 0) = \theta_{1,in}$$

$$\frac{\partial}{\partial \eta} \theta_{1,1}(0, \zeta) = 0$$

$$-\frac{1}{\varepsilon Re_i Pr_i} \frac{\partial}{\partial \eta} \theta_{1,1}(1, \zeta) = \tilde{m}_{1,1}^-(\zeta)$$

$$\theta_{1,1}(1, \zeta) = \beta \omega_{1,1}(1, \zeta)$$

and

$$\frac{1}{\varepsilon Re_i Sc_i} \frac{\partial^2 \omega_{1,1}}{\partial \eta^2} = \tilde{w}_i(\eta) \frac{\partial \omega_{1,1}}{\partial \zeta}$$

with

$$\omega_{1,1}(\eta, 0) = 0$$

$$\frac{\partial}{\partial \eta} \omega_{1,1}(0, \zeta) = 0$$

$$-\frac{1}{\varepsilon Re_i Sc_i} \frac{\partial}{\partial \eta} \omega_{1,1}(1, \zeta) = \tilde{m}_{1,1}^-(\zeta)$$

$$\omega_{1,1}(1, \zeta) = \tilde{m}_{1,1}^- (\zeta)$$
Subtracting Equation set (36) from Equation set (33), one can obtain the governing

equations and boundary conditions for $\theta_{1,2}$ and $\omega_{1,2}$. They can be expressed as:

\[
\frac{l}{\varepsilon Re_i Pr_i} \frac{\partial^2 \theta_{1,2}}{\partial \eta^2} = \bar{w}_1(\eta) \frac{\partial \theta_{1,2}}{\partial \zeta} \quad \text{with} \quad \theta_{1,2}(\eta,0) = 0
\]

\[
- \frac{l}{\varepsilon Re_i Pr_i} \frac{\partial}{\partial \eta} \theta_{1,2}(0, \zeta) = q_w
\]

\[
\frac{1}{\varepsilon Re_i Sc_i} \frac{\partial^2 \omega_{1,2}}{\partial \eta^2} = \bar{w}_1(\eta) \frac{\partial \omega_{1,2}}{\partial \zeta} \quad \text{with} \quad \omega_{1,2}(\eta,0) = 0
\]

\[
\frac{1}{\varepsilon Re_i Sc_i} \frac{\partial}{\partial \eta} \omega_{1,2}(0, \zeta) = 0
\]

\[
\frac{1}{\varepsilon Re_i Sc_i} \frac{\partial}{\partial \eta} \omega_{1,2}(1, \zeta) = \bar{m}_{c,2}(\zeta)
\]

\[
\theta_{1,2}(1, \zeta) = \beta \omega_{1,2}(1, \zeta)
\]

\[\text{(36)}\]

where

\[
\bar{m}_i(\zeta) = \bar{m}_{c,1}(\zeta) + \bar{m}_{c,2}(\zeta)
\]

\[\text{(37)}\]

Equations set (37) shows that $\theta_{1,2}$ and $\omega_{1,2}$ are the temperature and concentration of a

film flow which is the same as the original flow except the inlet solution is saturated, not

subcooled. Equation (38) also shows that the total mass absorbed in each segment is the

sum of the mass absorbed due to the subcooling at the inlet, $\bar{m}_{c,1}$, and the mass absorbed

due to the cooling by the coolant, $\bar{m}_{c,1}$. These two effects can be directly superimposed.

They independently affect the absorption process.

41
From Equation sets (36) and (37), it is clear that at a certain location, mass absorption flux, \(m_{c1}\), is only affected by \(\theta_{in}, \varepsilon Re_i Pr_i\) and \(\varepsilon Re_i Sc_i\), while \(m_{c2}\) only by \(\bar{q}_w, \varepsilon Re_i Pr_i\) and \(\varepsilon Re_i Sc_i\). Therefore, the average mass absorbed, \(\bar{m}_c\), can be written as:

\[
\bar{m}_c = \bar{m}_{c1} + \bar{m}_{c2} = \theta_{in} \bar{F}_1(\varepsilon Re_i Pr_i, Le_i) + \bar{q}_w \bar{F}_2(\varepsilon Re_i Pr_i, Le_i) \tag{39}
\]

where \(Le\) is the Lewis number and \(\bar{F}_1\) and \(\bar{F}_2\) are functions not yet known. Likewise, the average temperature at the wall, \(\bar{\theta}_w\), and average temperature at the interface, \(\bar{\theta}_{ij}\), can be expressed as:

\[
\bar{\theta}_w = \bar{\theta}_{w1} + \bar{\theta}_{w2} = \theta_{in} \bar{G}_1(\varepsilon Re_i Pr_i, Le_i) + \bar{q}_w \bar{G}_2(\varepsilon Re_i Pr_i, Le_i) \tag{40}
\]

\[
\bar{\theta}_{ij} = \bar{\theta}_{ij1} + \bar{\theta}_{ij2} = \theta_{in} \bar{H}_1(\varepsilon Re_i Pr_i, Le_i) + \bar{q}_w \bar{H}_2(\varepsilon Re_i Pr_i, Le_i) \tag{41}
\]

where \(\bar{G}_1, \bar{G}_2, \bar{H}_1,\) and \(\bar{H}_2\) are unknown functions.

### 3.5 Effects of the Vapor Flow

As mentioned in the literature review, from the papers in open literature, no conclusive results can be drawn about the roles of the mass transfer resistances in the liquid and vapor flows. Nevertheless, from the previous order of magnitude analyses, it is clear that, in a falling film absorption process occurred in a counter flow GAX-SCA, the diffusion effect on the vapor side is much smaller than that on the liquid side. Therefore, the mass transfer resistance on the vapor side is much larger than that on the liquid side and can be neglected. It should be noticed, however, that the conventional analogy between mass
transfer and electrical circuits cannot be directly applied to the absorption process. In this conventional concept, if the mass transfer resistance on side A is much larger than side B, then the mass transfer resistance on side A is the dominant factor. In the absorption problem, however, although the mass transfer resistance on vapor side is much larger than on the liquid side, it is not the dominant factor. The breakdown of the conventional analogy is caused by the phase-change at the interface. The solution concentration is not continuous across the interface. The total ammonia flux to the liquid comprises the diffusion flux and the convection flux from the vapor flow. The mass transfer circuit for the absorption process can be sketched as:

![Mass Transfer Circuit for the Absorption Process across the Flow Direction](image)

*Figure 6 Mass Transfer Circuit for the Absorption Process across the Flow Direction*

The resistance, $R_c$, represents the mass transfer resistance in the "condensation". Its value is mainly controlled by the heat transfer at the interface. This circuit shows that the effective mass resistance between the bulk vapor and bulk liquid is depended on the mass resistances on the liquid and vapor sides, as well as the heat transfer at the interface and the difference of mass fraction across the interface value of $x_{v,i} - x_{l,i}$. Only when the value
of $R_c$ is very large, in other words, the convection flux is very small, will the mass transfer resistance on vapor side directly affect the overall mass transfer. This can occur in a two-phase isothermal mass transfer process.

For comparison purposes, another important process in an absorption cycle, namely the rectification process, will be analyzed and compared to the absorption process. In the rectification process, water vapor is extracted from the ammonia-water vapor mixture. In a solution cooled counterflow rectifier, high concentration vapor flows up along a cold wall and some of the vapor is condensed on the cold wall. Since the liquid mixture contains much more water than the vapor mixture, a significant amount of water leaves the vapor flow. The concentration of vapor flow thus increases. In this process, ammonia is diffused from the interface to the bulk vapor flow. In a counterflow rectifier, coolant flows down from the top of the rectifier. Its temperature increases as it flows down. This causes the temperature of the condensate (reflux) to increase as it flows down. Thus, the interface liquid concentration decreases, and ammonia is diffused out of the liquid flow.

If the magnitude of the condensation flux is $-m_c$ and the diffusion flux on the liquid side is $-D_i \partial c / \partial y$, the diffusion flux on the vapor side should be the sum of $m_c'(x_v - x_i)$ and $-D_v \partial c / \partial y$ (both term are in the same direction, from liquid to the vapor flow). Therefore, in the rectification process, the magnitude of the condensation flux is controlled by the diffusion effect in the vapor flow.
In summary, due to the concentration glide in the ammonia-water solution, the amount of ammonia in the condensation flux in the liquid and vapor flow is not identical; the difference in this amount is $m_c^*(x_n - x_g)$. This amount of ammonia should be either diffused into the bulk liquid or the vapor flow. In either case, the flow to which this amount of ammonia, $m_c^*(x_n - x_g)$, goes will be the controlling factor in the process. In the absorption process, this amount of ammonia goes to the liquid flow, thus the liquid side becomes dominant. In the rectification process, it is just the opposite.
4.1 Introduction

There is no complete analytical solution for Equation (33). Conlisk [1992] obtained the analytical temperature distribution in Laplace transform space for the case with \( \varepsilon Re, Pr_l \ll 1 \), as well as the concentration profile for the case with \( \varepsilon Re, Sc_i \gg 1 \).

These two solutions were coupled together by the thermodynamic relationship between temperature and concentration at equilibrium. Numerical techniques were used to obtain the quantitative results. Note that the values of \( \varepsilon Re, Pr_l \) and \( \varepsilon Re, Sc_i \) are dependent on the film thickness and the physical properties of the liquid solution, as well as the mixing distance, \( L \). The value of \( L \) can range from 0.25 inch to several feet. In practical designs, the value of \( \varepsilon Re, Pr_l \) can range from 0.25 to 50, and the value of \( \varepsilon Re, Sc_i \) from 5 to 1000.

Thus, only numerical methods can solve the differential equations for any practical case. In order to reduce the amount of numerical work in component design, numerical results for different values of \( \varepsilon Re, Pr_l \) and \( \varepsilon Re, Sc_i \) were correlated. Empirical correlations for
the mass absorption rate, wall temperature and interfacial concentration were obtained in this chapter.

The governing equations (33) with their boundary conditions represent the heat and mass transfer for an actual fluid flow with following physical boundary conditions:

\[
\begin{align*}
T &= \theta_{in} \\
c &= 0
\end{align*}
\]

\[
E\frac{dT}{dy} = \bar{q}_w
\]

\[
\frac{dc}{dy} = 0
\]

\[
T = \frac{\beta c}{\rho}
\]

Fig. 7. A Film Flow Represented by Equation (33)

The boundary conditions at the inlet and the wall for this nondimensional film flow are the same as the actual physical film flow, but those at the interface are different. For the nondimensional film flow, the interface solution is at the equilibrium state, but there is no convection flow across the interface. The film thickness and flow length are \( \frac{h_0}{L} \) and unity respectively. Since the film thickness is constant, the velocity component in the \( y \)-
direction is zero. Therefore, the convection terms in the y-direction in this nondimensional film flow are negligible. Although the diffusion terms in the z-direction are still retained, Equations (17) and (18) show their magnitudes are on the order of \( \varepsilon^2 \). Thus, the effect of these terms can be neglected. Therefore, the partial differential Equation set (33) is the approximated governing equation set (neglect the diffusion term in z-direction) for this nondimensional flow. The numerical solutions for the temperature and concentration in this nondimensional film flow will be the solutions for the partial differential Equation set (33).

4.2 Numerical Solution with FIDAP

The nondimensional film flow in Figure 8 was solved with a commercial Fluid Dynamics Application Program FIDAP. FIDAP is a finite element program for analyzing a wide variety of fluid flow and heat and mass transfer problems. The software is capable of analyzing subsonic compressible or viscous incompressible flows in either 2D, axisymmetric or 3D complex geometries. The flow can be either steady or transient, laminar or turbulent, Newtonian or non-Newtonian, flows with chemical reactions and mass transfer etc. FIDAP allows the user to perform all aspects of analysis/simulation using an intuitive graphical pre-processor with interactive model building; advanced automatic mesh generator; data input; solution; and full post-processing capabilities.

The primary procedures to establish a program in FIDAP can be summarized as:

1. Nondimensionalize the governing equations and boundary conditions;
2. Convert the physical space to a logical space; establish the mesh for the calculation domain;

3. Define entities;

4. Define boundary conditions for entities;

5. Define properties for entities;

6. Choose solution scheme and converging criteria;

7. Run the problem.

In FIDAP, the nondimensionalization process is different from what has been shown in Chapter 3. In FIDAP, the characteristic lengths for both y- and z-direction must be identical. Thus, both y and z must be nondimensionalized by \( L \), not \( y \) by \( h_0^* \) and \( z \) by \( L \). Because of this, the definitions of some other nondimensional parameters are different from those in Equations (13) and (19). The definitions of nondimensional parameters in FIDAP are listed at the right column of Table 2. For comparison reason, the definitions of nondimensional parameters in Chapter 3 are listed at the left column. This table is provided to facilitate the interpretation of the results from FIDAP.
Table 2 Definition of Nondimensional Parameters in Current Work And FIDAP

The typical values of these nondimensional parameters, as well as the properties of the liquid solution are listed in Table 3.
In this table, the diffusivity for the ammonia-water liquid mixture is calculated from the correlation provided by Frank etc. [1996]:

\[ D_t = \left( 1.65 + 2.47 x_{\text{NH}_3} \right) \times 10^{-6} \exp(-16600/RT) \]  

(42)

where \( x \) is the mass fraction of ammonia and the unit for \( T \) is K. The diffusivity for ammonia-water vapor mixture is obtained from the following general correlation for binary mixture:

### Table 3 Typical property and parameter values for a GAX absorber

<table>
<thead>
<tr>
<th>Liquid</th>
<th>In British Unit</th>
<th>Nondimensionlized by Eqns (13) and (19)</th>
<th>Nondimensionlized in Fidap</th>
</tr>
</thead>
<tbody>
<tr>
<td>( m_l )</td>
<td>0.873 - 1.182 lbm/min</td>
<td>1/3</td>
<td>0.00286</td>
</tr>
<tr>
<td>( T_l )</td>
<td>251.0 - 167.212 °F</td>
<td>0 - 0.141</td>
<td>0 - 16.75</td>
</tr>
<tr>
<td>( x_l )</td>
<td>0.068 - 0.311</td>
<td>0 - 0.48</td>
<td>0 - 0.48</td>
</tr>
<tr>
<td>( P )</td>
<td>74.8 psi</td>
<td></td>
<td></td>
</tr>
<tr>
<td>( U_0 )</td>
<td>1.626 \times 10^4 - 1.126 \times 10^4 ft/hr</td>
<td>1</td>
<td>1</td>
</tr>
<tr>
<td>( Re )</td>
<td>1004 - 423.90</td>
<td>-4.93 \times 10^{-4}</td>
<td></td>
</tr>
<tr>
<td>( Sc )</td>
<td>22.7 - 62.7</td>
<td>22.7 - 62.7</td>
<td></td>
</tr>
<tr>
<td>( Pr )</td>
<td>1.6123 - 3.30</td>
<td>1.6123 - 3.30</td>
<td></td>
</tr>
<tr>
<td>( l/L_e ) (Sc/Pr)</td>
<td>14.08 - 19.0</td>
<td>14.08 - 19.0</td>
<td></td>
</tr>
<tr>
<td>( h^* ) (thickness)</td>
<td>7.57 \times 10^{-3} - 8.6 \times 10^{-3} inch</td>
<td>7.57 \times 10^{-3} - 8.6 \times 10^{-3}</td>
<td>7.57 \times 10^{-3} - 8.6 \times 10^{-3}</td>
</tr>
<tr>
<td>( L )</td>
<td>1 inch</td>
<td>1</td>
<td>1</td>
</tr>
<tr>
<td>( \varepsilon Re ) Pr</td>
<td>7.57 \times 10^{-3} - 8.6 \times 10^{-3}</td>
<td>12.25 - 12.03</td>
<td></td>
</tr>
<tr>
<td>( \varepsilon Re ) Sc</td>
<td>172.5 - 228.5</td>
<td></td>
<td></td>
</tr>
<tr>
<td>( \rho_l )</td>
<td>54.95 - 52.94 lbm/ft^3</td>
<td>1</td>
<td>1</td>
</tr>
<tr>
<td>( \mu_l )</td>
<td>0.5618 - 1.008 lbm/hr-ft</td>
<td>8.888 \times 10^{-3}</td>
<td>2.028 \times 10^{-5}</td>
</tr>
<tr>
<td>( k_l )</td>
<td>0.3704 - 0.332 Btu/hr-ft-°F</td>
<td>0.08 - 0.083</td>
<td>6.1469 \times 10^{-5}</td>
</tr>
<tr>
<td>( c_{p,l} )</td>
<td>1.063 - 1.089 Btu/lbm °F</td>
<td>1</td>
<td>1</td>
</tr>
<tr>
<td>( D_{AB,l} )</td>
<td>4.495 - 3.03 \times 10^{-4} ft^2/hr</td>
<td>5.68 \times 10^{-3} - 4.37 \times 10^{-3}</td>
<td>-6.40 \times 10^{-7}</td>
</tr>
<tr>
<td>( h_{fg} )</td>
<td>-591 Btu/lbm</td>
<td>1</td>
<td>108.75</td>
</tr>
<tr>
<td>( g )</td>
<td>32.2 ft/s^2</td>
<td>g/(U^2/L) = 0.2743</td>
<td>0.2743</td>
</tr>
</tbody>
</table>
and the film thickness is estimated from Nusselt's correlation

\[ h^* = \left[ \frac{3 \Gamma \mu_i}{g \rho_i (\rho_i - \rho_v)} \right]^{1/3} \]  (44)

In this problem, the energy and the specie equation are coupled through the boundary conditions at the interface, not the governing equations themselves. A special iteration scheme is needed to obtain numerical results. The following scheme was used in this calculation:

1. Solve the momentum equations;
2. Set the maximum and minimum possible values for \( m_a \), \( m_e \) and \( m_b \);
3. Let \( m_a = (m_e + m_b)/2 \);
4. Assume the heat and mass flux at the interface is \( m_a \);
5. Solve the energy and species equations;
6. Check whether the saturated condition is satisfied. If yes, stop the program;
7. If temperature at the surface is larger than \( \beta c \), the values adopted at step 4 are too larger; reset \( m_e = m_b + \text{relax} \times (m_e - m_b) \). Otherwise, \( m_b = m_e - \text{relax} \times (m_e - m_b) \).

Goto 3.

It is vitally important to obtain a converged result before updating the boundary conditions at the interface. For this purpose, the Newton-based solution scheme is used to
solve the equations. It is also critical to have a large relaxation factor at the beginning of
the iteration when the solution is still far away from the true solution. At the beginning of
the iteration, say the first 20 iteration, a very large relaxation factor such as 0.99 may be
used. After that, a smaller value of relaxation factor can be used to accelerate the
converging process.

4.3 Numerical Results from FIDAP
Similar to the decomposition of Equation (33) into Equations (36) and (37), the heat and
mass transfer problem in the nondimensional film flow can also be decomposed into two
separated problems corresponding to Equations (36) and (37). One is a subcooled inlet
solution flowing along an adiabatic wall; the other is a saturated inlet solution flowing
along a cooled wall. Numerical simulations are performed for these two problems
separately, and their results are superimposed to obtain the temperature and concentration
for the nondimensional film flow.

4.3.1 Results for Subcooled Solution along an Adiabatic Wall
In this section, the following problem is investigated: an ammonia-water solution with 5
°F subcooling flows along a vertical adiabatic wall, the film thickness is 0.0086 inch and
the mixing distance in flow direction is one inch. The values of $RePr$ and $Le^{-1}$ for this
flow are 5 and 19, respectively. These values are close to the practical values. In the
numerical calculation, a 31 by 21 (y by z) mesh is generated to represent the continuum
Figure 8 Mesh for the Thin Film Flow
region. In order to capture the phenomena at the entrance and the interface, more nodes are allocated at these places, as shown on Figure 8.

The first step of the computation is to obtain the solutions for velocity components. In *FIDAP*, this is done by setting the flow to be isothermal and a single component and then solving the continuity equation and momentum equations. The solution for the velocity component is then used as an initial velocity in the full scale calculation, in which all the governing equations are solved simultaneously by the Newton-method in each iteration. As mentioned before, an initial range of mass flux at the interface is needed in solving the heat and mass transfer equations. Numerical experiments showed that this range should be chosen very carefully, otherwise, the calculation would not converge. In this calculation, $0 \sim 4.0 \times 10^{-4}$ is the initial range of nondimensional mass flux. For the first 20 iterations, the relaxation factor is set as 0.997. After that, the relaxation can be decrease to 0.9 to accelerate the converging process. The converging criterion is that the sum of the residues is less that $10^{-10}$.

Selected computational results are shown in the Figures 9 to 15. All variables are plotted in their nondimensional form as defined in Chapter 3. In these plots, the positive direction in film width direction is from the wall to the interface. By this definition, the mass absorption flux is always negative.
Figure 9 Nondimensional Mass Absorption Flux at the Interface for Subcooled Inlet Solution

Figure 10 Nondimensional Concentration Profile at the Interface for Subcooled Inlet Solution
Figure 11 Nondimensional Heat Flux at the Interface for Subcooled Inlet Solution

Figure 12 Nondimensional Temperature Distribution at the Interface for Subcooled Inlet Solution
Temperature Profile at Wall ($\varepsilon \text{RePr}=5.0, \text{Le}=1/19.0$)

Figure 13 Nondimensional Temperature Distribution at the Wall for Subcooled Inlet Solution

Concentration Profiles across the Film ($\varepsilon \text{RePr}=5.0, \text{Le}=1/19.0$)

Figure 14 Nondimensional Concentration Distribution across the Film for Subcooled Inlet Solution
Figure 15 Nondimensional Temperature Distribution across the Film for Subcooled Inlet Solution

Figure 9 shows that the mass absorption flux decreases very rapidly at the entrance of the solution. At the entrance, the interface liquid solution becomes saturated, and the concentration increases immediately. Therefore, at the interface, the liquid concentration has a step in the film width direction. As a result, absorption occurs and the magnitude of the absorption flux is infinite at the entrance. Meanwhile, absorption heat in this process is released at the interface. This absorption heat increases the interface liquid temperature and, thus, decreases the interface liquid concentration. Therefore, the interface concentration gradient at the downstream decreases, and the magnitude of the absorption flux drops down.
Absorption heat released on the surface will be conducted into the bulk stream and the wall. This causes a temperature increase in the wall, as shown in Figure 13. This temperature rise at the wall will actually enhance the heat transfer from the coolant side to the wall. Further details will be discussed in the calculation of the heat transfer coefficient.

It is possible to estimate the thickness of the concentration boundary layer, $\delta_c$, by using the classical boundary-layer theory. Let $\tilde{\eta} = (1 - \eta) / \delta_c$; this will stretch the thickness of boundary layer to the order of one. The mass transfer equation given by Equation (33) can be rewritten as:

$$\frac{1}{\delta_c^2 \varepsilon H_i S_{ci}} \frac{\partial^2 \omega_i}{\partial \eta^2} = \tilde{\omega}_i(\eta) \frac{\partial \omega_i}{\partial \zeta}$$

(45)

Since $\tilde{\omega}(\eta)$ is on the order of one, by assuming $\frac{\partial \omega_i}{\partial \zeta}$ and $\frac{\partial^2 \omega_i}{\partial \eta^2}$ are on the same order, one can conclude that $\delta_c$ is on the order of $1 / (\varepsilon H_i S_{ci})^{1/2}$ (Conlisk [1992]). Thus, from the boundary-layer theory, for $\varepsilon H_i S_{ci} \sim 100$, the concentration boundary layer thickness $1 / (\varepsilon H_i S_{ci})^{1/2}$ is on the order of 0.1. Figure 14 shows that the actual concentration boundary layer thickness at the outlet is close to 0.5. Therefore, even when $\varepsilon H_i S_{ci}$ is much larger than unity, say 100, the concentration boundary layer may be not very thin compared to the film thickness. As a result, it may be necessary to consider the variation of velocity inside the concentration boundary layer.
Figure 15 shows that the thermal boundary layer develops very rapidly. It is very clear that the boundary layer has reached the wall at $\zeta=0.2$.

4.3.2 Results for Saturated Inlet Solution along a Cooled Wall

In this section, an absorption problem with a saturated solution flowing along a vertical cold wall is considered. The nondimensional flux through the wall is $\tilde{q}_w = 8.0 \times 10^{-4}$, which corresponds to a dimensional heat flux of about 2500 Btu/hr °F ft². Other parameters are the same as the problem with a subcooled solution. Since the mass absorption is different from the previous problem, the initial range of mass flux is reduced to $-1.0 \times 10^{-6} - 5.0 \times 10^{-5}$. The reason for setting the minimum flux as negative is that, at the entrance, the magnitude of the absorption flux is very close to zero.

![Mass Absorption Rate at Interface](image)

*Figure 16 Nondimensional Mass Absorption Flux at the Interface for Saturated Inlet Solution*
Figure 17 Nondimensional Concentration Distribution at the Interface for Saturated Inlet Solution

Figure 18 Nondimensional Heat Flux at the Interface for Saturated Inlet Solution
Figure 19 Nondimensional Temperature Distribution at the Interface for Saturated Inlet Solution

Figure 20 Nondimensional Temperature Distribution at Wall for Saturated Inlet Solution
Figure 21 Nondimensional Concentration Distribution across the Film for Saturated Inlet Solution

Figure 22 Nondimensional Temperature Distribution across the Film for Saturated Inlet Solution
Unlike the previous case with subcooled inlet solution along an adiabatic wall, for the saturated inlet solution along a cooled wall, the magnitude of the absorption flux increases along the flow direction, as shown in Figure 16. Since the inlet solution is saturated at the entrance, the interface concentration will remain the same as the bulk concentration. At $\zeta=0$, there is no concentration gradient at the interface in the film width direction. Thus, the absorption rate is zero at this point. When the solution flows down along the cooled wall, heat is rejected from the solution to the wall. The temperature at the wall and interface will decrease along the flow direction, as shown in Figure 19 and Figure 20. The decrease in the interface temperature will cause an increase in the interface concentration according to the thermodynamic relationship at the saturated state, as shown in Figure 17. This will initiate a concentration gradient at the interface and begin the absorption process. As the thermal boundary layer at the wall grows along the wall, the interface temperature will further decrease. This results in a larger concentration gradient near the interface at the down stream, as shown in Figure 21, and an increased absorption flux.

Comparing Figure 9 with Figure 16, one can find that the magnitude of the absorption flux in first case is much larger than the second one. It is generally true that the absorption rate is primary determined by the degree of subcooling at the inlet for a short mixing distance. The absorption rate decreases along the flow direction in the first case but increases in the second case. If the mixing distance is kept increasing, the mass absorption rate in the second case will eventually dominate the total absorption rate.
Figure 22 shows that the temperature distribution across the film is not a straight line. Therefore, the heat transfer is not totally dominated by conduction. The value of $\epsilon RePr$ for this film flow is much larger than unity. Thus, heat transfer by convection in the flow direction can not be neglected in this case, especially at the interface.

4.4 Development of Empirical Correlations

In this section, the effects of $\epsilon RePr$ and $Le$ on the mass absorption rate, wall temperature and interface temperatures are investigated. For cases with a subcooled inlet solution flowing along an adiabatic wall, results for $\tilde{m}_c/\theta_{in}$, $\tilde{\theta}_w/\theta_{in}$ and $\omega_{int,v}/\theta_{in}$ are correlated with $\epsilon RePr$ and $Le$. For cases with a saturated inlet solution flowing along a cooled wall, results for $\tilde{m}_c/\tilde{q}_w$, $\tilde{\theta}_w/\tilde{q}_w$ and $\omega_{int,v}/\tilde{q}_w$ are correlated.

The effects of $\epsilon RePr$ and $Le$ can be found by comparing the numerical results for film flows with different values of $\epsilon RePr$ and $Le$. To obtain numerical results for film flow with different values of $Le$, computations for film flows with the same properties and parameters but different diffusivity are performed. In FIDAP, the $Le$ number of the fluid is the ratio of the diffusivity to the conductivity.

The numerical results for film flows with different values of $\epsilon RePr$ can also be obtained another way. The value of $\epsilon RePr$ depends upon the mixing distance of the flow $L$ as well as other parameters. Thus, the effects of $\epsilon RePr$ can be found by comparing the absorption
processes for different mixing lengths $L$. If the absorption process for mixing distance $L$ is known, then the absorption process for a smaller mixing distance $\lambda L$, where $0 < \lambda < 1$, has already been known. Therefore, results for film flow with $\varepsilon RePr = \delta / \lambda$ can be directly obtained from results for film flow with $\varepsilon RePr = \delta$. For example, Function $F_1(\delta / \lambda, Le)$ and $F_2(\delta / \lambda, Le)$ in Equation (39) for $\varepsilon RePr = \delta / \lambda$ can be written as:

$$
F_1(\delta / \lambda, Le) = \frac{\bar{m}_e(\delta / \lambda, Le)}{\theta_{in}}
$$

$$
= \frac{\bar{m}_e(\delta / \lambda, Le) \cdot \lambda L / (\nu_0 \rho U)}{\theta_{in}}
$$

$$
= \frac{\lambda L / (\nu_0 \rho U)}{\theta_{in}} \frac{1}{\lambda L} \int_0^{\mu} \bar{m}_e(\delta / \lambda, Le, z) dz
$$

$$
= \frac{\lambda L / (\nu_0 \rho U)}{\theta_{in}} \frac{1}{\lambda L} \int_0^{\mu} \bar{m}_e(\delta, Le, z) dz
$$

$$
= \frac{1}{L} \int_0^{\mu} \bar{m}_e(\delta, Le, z) \cdot L / (\nu_0 \rho U) dz
$$

$$
= \int_0^{\mu} \frac{\bar{m}_e(\delta, Le, \zeta)}{\theta_{in}} d\zeta = \int_0^{\mu} F_1(\delta, Le, \zeta) d\zeta
$$

In Equation (46), the dimensional mass fluxes for mixing distances $\lambda L$ and $L$ are nondimensionalized by two different variables, $\rho U h^*/\lambda L$ and $\rho U h^*/L$, respectively. The ratio of the nondimensional absorption flux to the heat flux, $F_2$, can be expressed as:
It should be noted that the heat fluxes for mixing distances $\lambda L$ and $L$ are nondimensionalized by two different variables, $\rho U h^* h^* / \lambda L$ and $\rho U h^* h^* / L$, respectively.

Similarly, other functions for $\varepsilon Re Pr = \delta / \lambda$ can be found by:

\[
\overline{G}_1(\delta / \lambda, Le) = \frac{1}{\lambda} \int_0^i G_1(\delta, Le, \zeta) d\zeta
\]  

\[
\overline{G}_2(\delta / \lambda, Le) = \frac{1}{\lambda^2} \int_0^i G_2(\delta, Le, \zeta) d\zeta
\]  

\[
\overline{H}_1(\delta / \lambda, Le) = \frac{1}{\lambda} \int_0^i H_1(\delta, Le, \zeta) d\zeta
\]  

\[
\overline{H}_2(\delta / \lambda, Le) = \frac{1}{\lambda^2} \int_0^i H_2(\delta, Le, \zeta) d\zeta
\]
In this way, after obtaining numerical results for $\varepsilon RePr=\sigma$, one can also determine the results for $\varepsilon RePr$ ranges from $\sigma$ to $+\infty$ by simple integration.

4.4.1 Effects of Parameters $\varepsilon RePr$ and $Le$

Equation (36) and (37) showed that $\frac{m_c}{\theta_{in}}, \frac{\theta_w}{\theta_{in}}, \frac{\omega_{int,v}}{\theta_{in}}, \frac{m_c}{q_c^w}, \frac{\theta_w}{q_w^w}$ and $\omega_{int,v}/q_w^w$ only depend upon $\varepsilon RePr$ and $Le$. These two parameters affect the values of $\frac{m_c}{\theta_{in}}, \frac{\theta_w}{\theta_{in}}$ and $\omega_{int,v}/\theta_{in}$ by quite different mechanisms. Therefore, their effects will be discussed separately in the following paragraph. In each discussion, only one parameter is considered to be variable; all the other parameters are treated as constants.

$\varepsilon RePr$ is a measure of the importance of the convection terms relative to the conduction terms. As mentioned before, the conductivity for the nondimensional film flow is $\tilde{k}_i = 1/\varepsilon RePr$. When $\varepsilon RePr$ increases, the conductivity and diffusivity of the film flow decrease ($Le$ number is fixed). Therefore, the nondimensional mass absorption rate decreases, as shown in Figure 23 and Figure 24.

The effects of $\varepsilon RePr$ on the wall temperature can also be explained in a similar manner.

When the value of $\varepsilon RePr$ increases, the conductivity and the diffusivity of the nondimensional film flow decreases ($Le$ number is fixed). Thus, for the case with a subcooled inlet solution, the absorption flux and heat flux at the interface decrease. As a result, less heat is conducted to the solution near the wall. Therefore, the wall temperature
will be closer to the inlet temperature; and the value of $\theta_\omega / \theta_{in}$ approaches unity asymptotically, as shown in Figure 25. For the case of a saturated inlet solution, when $\varepsilon Re Pr$ increases, the conductivity of the film flow decreases. Since the heat flux through the wall is fixed, the temperature gradient at the wall increases. Thus, the wall temperature will be lower than the bulk temperature. Since the wall temperature and the heat flux through the wall are negative values, the value of $\theta_\omega / q^-$ increases with $\varepsilon Re Pr$, as shown in Figure 26.

The effects of $\varepsilon Re Pr$ on the interface temperature are shown in Figure 27 and Figure 28. For the case with a subcooled inlet solution, when $\varepsilon Re Pr$ increases, the absorption flux and the heat flux at the interface decrease. A smaller temperature change occurs at the interface. The interface temperature becomes closer to the inlet temperature, as shown in Figure 27. For the case with a saturated inlet solution, the heat flux through the wall is fixed. When the conductivity of the film flow $1/\varepsilon Re Pr$ decreases, the interface temperature decreases if the thermal boundary layer of the film flow is well developed at the outlet. Otherwise, the cooling effect of the wall will not significantly affect the interface temperature. The interface temperature begins to increase with $\varepsilon Re Pr$. In this case, the thermal boundary layer near the wall becomes thinner when $\varepsilon Re Pr$ increases. Thus, less temperature change occurs at the interface. The interface temperature approaches the inlet temperature asymptotically. The deflection is shown in Figure 28. The deflection occurs when $\varepsilon Re Pr$ is of the order of one.
If $eRePr$ remains a constant, increasing $Le$ will directly increase the diffusion effect at the interface. Thus, the average mass absorption flux and the heat flux at the interface increase, as shown in Figure 23 and Figure 24. As a result, the wall and interface temperatures also increase. The effect of $Le$ number on the wall temperature, however, is much less significant than the effect of $eRePr$. Figure 25 and Figure 26 show that the wall temperature only slightly depends upon the $Le$ number.

Figure 23 Average Absorption Flux vs. $eRePr$ for Different Values of $Le$ number for a Subcooled Inlet Solution along an Adiabatic Wall
Figure 24 Average Absorption Flux vs. $\varepsilon RePr$ for Different Values of Le number for a Saturated Inlet Solution along a Cooled Wall

Figure 25 Average Wall Temperature vs. $\varepsilon RePr$ for Different Values of Le number for Subcooled Inlet Solution along an Adiabatic Wall
Figure 26 Average Wall Temperature vs. $\varepsilon RePr$ for Different Values of Le number for a Saturated Inlet Solution along a Cooled Wall

Figure 27 Average Interface Temperature vs. $\varepsilon RePr$ for Different Values of Le number for a Subcooled Inlet Solution along an Adiabatic Wall
4.4.2 Empirical Correlations

In a component design program, it is more convenient to calculate variables directly from the analytical correlation than to interpolate from discrete results. Therefore, it is useful to develop empirical correlations from the numerical results obtained in the last section. By curve fitting, the following empirical correlations for mass absorption rate, wall temperature and interface temperature are found:

$$\overline{m_c} = \overline{m_{c,1}} + \overline{m_{c,2}} = \theta_{\text{lin}} \overline{F_1}(e^{5HPr_l,Le_i}) + \overline{q_w} \overline{F_2}(e^{5HPr_l,Le_l})$$

where

$$\overline{F_1}(e^{5HPr_l,Le_i}) = \left(1 + f_{i,7}/(e^{5HPr_l})^{1/2} + f_{i,8}Le_l + f_{i,9}Le_l^2\right)\Phi_i$$

Figure 28 Average Interface Temperature vs. $\varepsilon Re Pr$ for Different Values of $Le$ number for a Saturated Inlet Solution along a Cooled Wall
\[ \Phi_i = \begin{cases} f_{i,1} + f_{i,2} (\varepsilon_5 H_1 Pr_t) + f_{i,3} (\varepsilon_5 H_1 Pr_t)^2 + f_{i,4} (\varepsilon_5 H_1 Pr_t)^3 & \text{if } \varepsilon_5 H_1 Pr_t < 10 \\ f_{i,5} (\varepsilon_5 H_1 Pr_t)^{i,5} & \text{if } \varepsilon_5 H_1 Pr_t > 10 \end{cases} \quad (52) \]

\[
\begin{align*}
f_{1,1} &= 0.047178 & f_{1,2} &= -0.00183 & f_{1,3} &= -0.0002 & f_{1,4} &= 2.150E-05 \\
f_{1,5} &= 0.078251 & f_{1,6} &= -0.4265 & f_{1,7} &= 1.746273 & f_{1,8} &= 52.49933 \\
f_{1,9} &= -284.355 \\
f_{2,1} &= 0.099576 & f_{2,2} &= -0.01911 & f_{2,3} &= 0.001781 & f_{2,4} &= -6.7E-05 \\
f_{2,5} &= 0.794371 & f_{2,6} &= -1.55759 & f_{2,7} &= 1.830013 & f_{2,8} &= 60.36143 \\
f_{2,9} &= -287.859 \\
\end{align*}

\[
\bar{\theta}_{r} = \bar{\theta}_{r,1} + \bar{\theta}_{r,2} = \theta_{r,1} \bar{G}_1 (\varepsilon_5 H_1 Pr_t, Le_t) + \bar{q}_{\theta} \bar{G}_2 (\varepsilon_5 H_1 Pr_t, Le_t)
\]

where

\[
\bar{G}_i (\varepsilon_5 H_1 Pr_t, Le_t) = \left( 1 + g_{i,6} / (\varepsilon_5 H_1 Pr_t)^{y,2} + g_{i,7} Le_t + g_{i,8} Le_t^2 \right) \Gamma_i
\]

\[
\Gamma_i = g_{i,1} + g_{i,2} (\varepsilon_5 H_1 Pr_t)^{i,3} + g_{i,4} (\varepsilon_5 H_1 Pr_t)^{z,3} \quad (53)
\]

\[
\begin{align*}
g_{1,1} &= 0.32344 & g_{1,2} &= 0.9314 & g_{1,3} &= -0.01765 & g_{1,4} &= 0.17937 \\
g_{1,5} &= -2.41768 & g_{1,6} &= -0.4770 & g_{1,7} &= -2.84203 & g_{1,8} &= 13.81213 \\
g_{2,1} &= 0.90498 & g_{2,2} &= 1.78219 & g_{2,3} &= 0.523494 & g_{2,4} &= 0.84504 \\
g_{2,5} &= -1.58903 & g_{2,6} &= -0.49938 & g_{2,7} &= -1.41974 & g_{2,8} &= 6.593848 \\
\end{align*}

\[
\bar{\theta}_{t} = \bar{\theta}_{t,1} + \bar{\theta}_{t,2} = \theta_{t,1} \bar{H}_1 (\varepsilon_5 H_1 Pr_t, Le_t) + \bar{q}_{\theta} \bar{H}_2 (\varepsilon_5 H_1 Pr_t, Le_t)
\]

where

\[
\bar{H}_i (\varepsilon_5 H_1 Pr_t, Le_t) = \varepsilon_5 H_1 Pr_t (1 + h_{i,9} Le_t + h_{i,10} Le_t^2) H_i
\]

75
\[ H_l = \begin{cases} h_{1.1} + h_{1.2} (e^{5H_i Pr_l})^{h_{1.3}} + h_{1.4} (e^{5H_i Pr_l})^{h_{1.5}} & \text{if } e^{5H_i Pr_l} < 10 \\ h_{1.6} + h_{1.7} (e^{5H_i Pr_l})^{h_{1.8}} & \text{if } e^{5H_i Pr_l} > 10 \end{cases} \]  

(54)

\[ \begin{align*}
    h_{1.1} &= 1.43716 & h_{1.2} &= 0.91229 & h_{1.3} &= -0.69873 & h_{1.4} &= -1.623774 \\
    h_{1.5} &= -0.02674 & h_{1.6} &= 0.0011 & h_{1.7} &= 0.84709 & h_{1.8} &= -0.96553 \\
    h_{1.9} &= -7.22182 & h_{1.10} &= 34.28859
\end{align*} \]

\[ \begin{align*}
    h_{2.1} &= 1.32559 & h_{2.2} &= 3.00602 & h_{2.3} &= -0.51915 & h_{2.4} &= -3.241247 \\
    h_{2.5} &= -0.17349 & h_{2.6} &= 0.00011 & h_{2.7} &= 4.85143 & h_{2.8} &= -1.8935 \\
    h_{2.9} &= -6.48403 & h_{2.10} &= 29.29442
\end{align*} \]

In the curve fitting, the target is to find the parameters for a particular equation to the minimum sum of the relative errors at each point, which is

\[ \sum_{i=1}^{n} \left( \frac{\text{actual value} - \text{predicted value from correlation}}{\text{actual value}} \right)^2 \]

The relative errors for each point are shown in the Appendixes. The maximum relative error of these correlations is less than 8%. The average relative errors for these correlations are less than 4%.

### 4.4.3 Heat and Mass Transfer Coefficients

Although one can determine the heat transfer through the wall by using the wall temperature and the flow conditions in the coolant flow, it is helpful to obtain the heat and mass transfer coefficient for the film flow, especially when these coefficients are needed to determine the fin efficiency and other important parameters.
The conventional definition of the heat transfer coefficient, \( h_q \), for thin film is the heat transfer through the wall, \( q_w \), divided by the temperature difference between the wall and the interface, \( T_w - T_{int} \), that is \( h_q = \frac{q_w}{(T_w - T_{int})} \). Based on this definition, if the wall is adiabatic \( (q_w = 0) \), the heat transfer coefficient will be zero. If the heat flux through the wall is a non-zero value, the heat transfer coefficient for the same film flow will also have a nonzero value. This suggests that the heat transfer coefficient should be a function of the heat flux through the wall and the degree of subcooling at the inlet. The average heat transfer coefficient in each segment can be expressed by:

\[
\overline{h}_q = \frac{q_w}{(\theta_w - \theta_{int})} = \frac{\varepsilon \delta H}{h_0} \left( \frac{k_{pl}}{\theta_{lin}/\overline{q}_w} \Delta T \right)
\]

(55)

Equation (55) shows that the heat transfer coefficient is a function of film thickness and thermal conductivity, as well as a function of \( \theta_{lin}/\overline{q}_w \), the ratio of subcooling to the nondimensional heat flux through the wall. Only when the subcooling of the inlet solution is zero, will the heat transfer coefficient become independent of the heat flux through the wall. If the degree of subcooling at the inlet increases, the temperature difference between the interface and wall will increase; therefore, the value of the heat transfer coefficient will decrease.
Whether the subcooling at the inlet increases or decreases the heat transfer to a coolant flow, is depended on the basis of the comparison. If the comparison is based on the same inlet concentration, then the presence of subcooling will decrease the heat transfer from the film flow to the coolant. On the other hand, if the comparison is based on the same inlet temperature, the subcooling will actually enhance the heat transfer to the coolant by raising the wall temperature.

![Graph](image)

*Figure 29 Effect of Nondimensional Parameter $\varepsilon Re_Pr$ on the Average Nondimensional Heat Transfer Coefficient of the Film with $Sc/Pr=20$*

Figure 29 shows that effect of nondimensional parameter $\varepsilon Re_Pr$ on the nondimensional heat transfer coefficient $h_q/(k/h^*)$. Convection effect becomes more significant when $\varepsilon Re_Pr$ increases. Thus, the nondimensional heat transfer coefficient increases with
Figure 29 also shows that the heat transfer coefficient is significantly affected by the subcooling of the inlet solution. When the inlet solution is not severely subcooled, the heat transfer coefficient of a binary mixture in an absorption process is larger than that of a single component fluid in a condensation process.

In the engineering practice, it is more preferable to present the variables in dimensional form. Figure 30 shows that the effect of film flow rate per unit width, $\Gamma$, on the dimensional heat transfer coefficient, $h_q$. The value of $h_q$ first decreases with $\Gamma$. When $\Gamma$ is increased to a certain value, however, the heat transfer coefficient, $h_q$, begins to increase with $\Gamma$. This inflection is quite different from Nusselt’s prediction, which predicts that the heat transfer coefficient is inversely proportional to the film thickness. If the thermal boundary near the wall is still developing at $z=L$, increasing the film thickness will increase the velocity near the wall and further decrease the thermal boundary thickness. As a result of this, the heat transfer increases. This trend is very similar to the heat transfer for the external flow over a flat plate. In that case, the development of the velocity boundary layer may need to be considered for more accuracy.
Figure 30 Effect of Flow Flux on the Average Heat Transfer Coefficient of the Film with Mixing Distance $L=1.0$ inch, $Sc/Pr=20$

Figure 31 shows the effects of mixing distance on the average heat transfer coefficients. For a saturated inlet solution, the average heat transfer coefficient decreases asymptotically with $L$. For a severe subcooled inlet solution, heat transfer coefficient first decreases with $L$ and then rises asymptotically. The inflection is because of the diminishment of the entrance subcooling effect. When $L$ is significantly long, entrance effects can be neglected, and the average heat transfer coefficient begins to approach the value for a saturated inlet solution.
Since the absorption rate is low, the change in the bulk concentration is negligible, and the mass transfer coefficient can be expressed by:

\[
\overline{h}_{m,l} = \frac{\overline{m}_c}{\overline{c}_{l,s} - \overline{c}_{l,bulk}} = \frac{\overline{m}_c}{\overline{c}_{l,s}} = \frac{\beta eU \overline{m}_c}{\partial_{\text{in}}(x_{wi} - x_{li})} = \frac{D}{h_0} \beta eRe_iSc_i \frac{\overline{m}_c}{\partial_{\text{in}}(x_{wi} - x_{li})}
\]  

\[(56)\]
Figure 32 shows the effect of nondimensional parameter $\varepsilon Re_i Pr_i$ on the average nondimensional mass transfer coefficient $h_m / (D_i / h_o^*)$. As $\varepsilon Re_i Pr_i$ increases, the convection effect becomes more significant, the concentration boundary at the interface becomes thinner. Thus, the nondimensional mass transfer coefficient increases. For the purpose of comparison, result from short contact time theory is plotted in Figure 33 and Figure 34. This analytical result is obtained by Pigford [1941], who assumed that the gas-liquid contact time was short enough that the variation of concentration occurred only in a boundary layer near the free interface. Neglecting the heat transfer problem enables him to find a closed-form solution for the mass flux averaged over a column length of $L$. His mass transfer coefficient averaged over a column length of $L$ can be expressed by

$$h_m = \frac{3DvRe_n}{2\pi L h_o^*} \quad (57)$$

where $Re_n$ is the conventional Reynolds number, $4\Gamma / \mu$. This expression can be rewritten in terms of nondimensional variables defined in this work:

$$h_m = \frac{D}{h_0} \left( \frac{2}{\pi} \varepsilon Re_i Sc_i \right)^{1/2} \quad (58)$$

Figure 32 shows that the results from this work have the same trends as the Pigford’s prediction. The difference between them is mainly because the absorption process considered in this work was an exothermal process while the one in Pigford’s work was an isothermal process. The interface concentration changes along the flow direction in this work, but it is a fixed value in the work of Pigford. Figure 32 shows that the mass transfer coefficient in an exothermal process is larger than that in an isothermal process.
Figure 32 Effect of Nondimensional Parameter \( \varepsilon RePr \) on the Average Nondimensional Mass Transfer Coefficient of the Film with \( Sc/Pr=20 \)

For engineering application purpose, the typical magnitudes of the mass transfer coefficient in the absorption process are shown on Figure 33 and Figure 34. Figure 33 shows that the mass transfer coefficient increases with \( \Gamma \). Since the velocity at the interface increases with \( \Gamma \), the concentration boundary layer thickness at the interface decreases with \( \Gamma \). If the concentration difference across the boundary \( \bar{c}_{i,d} - \bar{c}_{i,bulk} \) is fixed, decreasing the boundary layer thickness will increase the concentration gradient at the interface. Therefore, the mass transfer coefficient increases. Both Figure 33 and Figure 34 show that the mass transfer coefficient is not significantly affected by subcooling when subcooling is larger than 2 \(^\circ\)F.
Figure 33 Effect of $\Gamma$ on the Mass Transfer Coefficient of the Film with Mixing Distance with $Sc/Pr=20$

Figure 34 Effect of Mixing Distance on the Mass Transfer Coefficient of the Film with Film Thickness=0.0077 inch, $Sc/Pr=20$
CHAPTER 5

ONE DIMENSIONAL ABSORBER DESIGN MODEL

5.1 Introduction

Currently there are several general component design models available for absorption systems. All of these are based on the one-dimensional control volume method. The simplest model is the equilibrium model. Here, both liquid and vapor flows are assumed to be well-mixed and in thermodynamic equilibrium. Mass transfer effects are completely neglected. Only heat transfer is considered in this model, therefore, this design model is very similar to heat exchanger design models for single component flows. Price and Bell [1973] developed a design model for a binary vapor condenser. In their model, it was assumed that the liquid film is well mixed, and the composition of the condensation flux was determined by the Colburn-Drew equation. Panchal and Arman [1991] considered subcooling in the ammonia-water solution in their design. They applied the Colburn-Drew equation on both the liquid- and vapor-side. The heat and mass transfer coefficients for both the liquid and vapor side were obtained from empirical correlations. Their results show that subcooling on the liquid side is substantial. The empirical mass transfer correlation which they used for liquid flow, however, failed to include the effects of
several of the most important factors, such as subcooling in the solution and the entrance
effect for a short mixing distance.

In order to include these effects, the analyses in Chapter 3 and 4 were applied to develop
a component design model for absorber. A one-dimensional design model based on the
empirical correlations developed in the last chapter was developed. This model then was
applied to the design of a plate type W-fin absorber. The solution flow rate, temperature
and concentration profiles in the entire component were presented. The average
concentration of the absorption flux was given. The effects of mixing distance and other
parameters on the size of the absorber and the subcooling of liquid solution were
introduced. The mass absorption rate due to the subcooling of the solution and cooling of
the coolant were compared. Additionally, simulation results from two widely used
engineering design models were also presented for comparison purposes.

5.2 Control Volume Method

In this method, the geometry between two mixing points is treated as a control volume.
Details of the temperature and concentration distributions inside the control volume will
be not considered. Interest is focused on the flow condition at each mixing point. The
relationship between the flows entering and leaving the control volume will be developed
in the following sections.
The principal of the control volume analysis is that, for steady state conditions, the total mass and energy entering the control volume is equal to the total mass and energy leaving the control volume. Since there are two flows entering and leaving the control volume, the interactions between these two flows need to be considered. In the previous analyses, it has been found that the diffusion term on the vapor side is much smaller than that on the liquid side. Therefore, this term was neglected from the mass transfer boundary conditions given by Equation (21). This simplification is essentially identical to setting the concentration of the absorption flux, denoted as \( \phi \), equal to the local interface vapor concentration, \( x_{vi} \). If only the liquid flow alone is considered, this simplification seems reasonable. However, when the vapor concentration profile along the flow direction is considered, this simplification is obviously questionable, particular for the case where the liquid flow is counter to the vapor flow. In a counter-current absorber, the bulk vapor concentration, \( x_{vb} \), decreases from the bottom to the top of absorber. This can happen only in two ways: 1) The concentration of the absorption flux, \( \phi \), is larger than the bulk vapor concentration, \( x_{vb} \). 2) Water vapor is evaporated from the liquid to the vapor flow. The second case is quite possible if the concentration of vapor is very high, particularly if the vapor is pure ammonia. The mathematical definition of \( \phi \) is:

\[
\phi = \frac{m_{c, NH_3}}{m_{c, H_2O} + m_{c, NH_3}}
\]  

(59)

If the ammonia and the water flux are in different directions and the absolute magnitude of the ammonia flux is larger than that of the water flux, the value of \( \phi \) will be great than 1.0. Thus, in both cases, the value of \( \phi \) is larger than \( x_{vb} \). At the beginning of Chapter 3, it
has been shown that the bulk concentration, $x_{ub}$, is always larger than the interface vapor concentration, $x_{vi}$, at any cross section. Thus, the composition of the absorption flux, $\phi$, should be larger than $x_{vi}$. The approximation that $\phi$ is the same as $x_{vi}$ is not strictly valid. It is necessary to find a more accurate method to determine the value of $\phi$.

Meanwhile, at the bottom of the absorber, the temperature of the inlet vapor flow is much lower than the outlet liquid film. Therefore, even though the heat transfer coefficient of the vapor flow is small, the heat transfer at this portion can be significant. It will be more accurate to include the heat and mass transfer of the vapor flow in the actual component design model. For this purpose, the following assumptions are made in the current design model:

1. The diffusion effects of the vapor flow can be directly superimposed on the results from Chapter 4. Since the heat transfer from the liquid flow to the vapor flow occurs at the interface, it is assumed that this heat transfer directly affects the absorption rate. The absorption rate due to this heat transfer is:

$$m_{senv} = \frac{h_{vb}(T_{li}-T_{vb})}{h_{fk}}$$

(60)

This absorption rate is then directly added to the absorption rate obtained by empirical correlation (52). Thus, the total mass flux absorbed into the liquid is

$$m_i = m_c + m_{senv}$$

(61)
2. In order to determine the actual value of $\phi$, it is assumed that the concentration boundary layer on the vapor side is very thin (Whitman [1923]) and the magnitude of the convection flux, $m^\cdot$, is unchanged across this boundary layer. With this assumption, the value of $\phi$ can be determined by the Colburn-Drew equation:

$$m^\cdot = F_v \cdot \ln\left(\frac{\phi^m - x_{ib}^m}{\phi^m - x_{in}^m}\right) \tag{62}$$

where the superscript $m$ indicates the concentration is the molar fraction instead of weight fraction. This equation can be rewritten in an explicit form as:

$$\phi^m = \frac{x_{ib}^m - x_{in}^m \exp(m^\cdot/F_v)}{1 - \exp(m^\cdot/F_v)} \tag{63}$$

where the mass flux, $m^\cdot$, is defined as positive in the direction of liquid into vapor.

Meanwhile, the dimensional mass transfer boundary condition at interface for the film flow should be changed to:

$$-D_i \frac{\partial c_i}{\partial y} + m^\cdot_x x_i = m^\cdot \phi \tag{64}$$

Its nondimensional form is still the same as Equation (28):

$$-\frac{l}{\varepsilon S h S c_i} \frac{\partial \omega_i}{\partial y} = \tilde{m}^\cdot_c(\hat{z}) + O\left(\frac{\phi - x_{i,l}}{\phi - x_{i,l}} - 1\right),$$

but the concentration $c_i$ is nondimensionlized by $\rho_i (\phi - x_{i,l})_m$, not $\rho_i (x_{v,i} - x_{i,l})_m$. With these assumptions, the governing equations for the control volume can now be summarized.
Mass Balance

For the counter flow arrangement, as shown in Figure 35, the total mass balance and ammonia mass balance equations can be expressed as:

**Total mass balance:**

\[
\dot{m}_{vb,(i)} = \dot{m}_{vb,(i+1)} - \dot{m}_c \Delta A \\
\dot{m}_{t,(i)} = \dot{m}_{t,(i+1)} - \dot{m}_c \Delta A
\]

**Ammonia mass balance:**

\[
\dot{m}_{vb,(i)} x_{vb,(i)} = \dot{m}_{vb,(i+1)} x_{vb,(i+1)} - m_{c,NH_3} \cdot \Delta A \\
\dot{m}_{t,(i)} x_{t,(i)} = \dot{m}_{t,(i+1)} x_{t,(i+1)} - m_{c,NH_3} \cdot \Delta A
\]

*Figure 35 Sketch of Flow Conditions at a Control Volume*
**Energy Balance:**

The total flow enthalpy entering the control volume, along with the heat input, is equal to the flow enthalpy leaving the control volume:

\[ \dot{m}_{t,0}h_{t,0} + \dot{m}_{v,b,0}h_{v,b,0} = \dot{m}_{t,(i+1)}h_{t,(i+1)} + \dot{m}_{v,b,(i+1)}h_{v,b,(i+1)} + q_w \Delta A = 0 \]  

**Energy Transfer between the Liquid and Vapor Flow:**

The change of the sensible heat in the vapor flow can be directly given by:

\[ Q_{\text{sens}} = h_{v,b} (T_{v,b} - T_i) \Delta A \]  

In most practical cases, the heat flux through the wall is not directly available. It needs to be determined by the conditions in the coolant flow and the film flow. In this design, since the empirical correlation for wall temperature has been obtained in Chapter 4, the heat flux can be written by:

\[ q_w = (U \Delta A)_c (T_c - T_w) \]  

where \( (U \Delta A)_c = \frac{\Delta A_c}{1/h_c + t_w/k_w} \). Substituting this equation into Equation (53), one can obtain the explicit expression for the heat flux:

\[ q_w = \frac{\theta_c - \theta_{d,\text{m}} G_1 (eRePr, Le)}{G_2 (eRePr, Le) + \frac{\epsilon \rho U c_p}{(U \Delta A)_c}} \]  

The calculation of the transfer coefficients \( h_c, h_{v,b}, \) and \( F_{v,b} \) are dependent on the geometry of absorber. In most cases, they are calculated from empirical correlations, especially if
there are enhanced surfaces in the absorber. Since this component design model is
developed for general purposes, the calculation of these transfer coefficients will be
postponed until the absorber is specified. The following algorithm is an effective way to
solve the foregoing equations and obtain the flow conditions at the (i+1) node:

1) Assuming a value for \( \phi \);
2) Calculate the nondimensional parameters in Equations (13) and (19) (i.e., \( eRePr, Le \)
etc.);
3) Calculate the heat transfer coefficients on the coolant side \( h_c(i) \);
4) Obtain the heat flux from Equation (72);
5) Calculate the mass absorption rate by Equation (52);
6) Obtain vapor heat and mass transfer coefficients \( h_vb \) and \( F_{vb} \);
7) Calculate the modified mass absorption rate by Equation (61);
8) Calculate \( \phi \) from Equation (63). If this value matches the assumed value at step (1),
   continue to (9). Otherwise, resume a value \( \phi \), goto (1);
9) From the mass and energy balance, calculate \( m_{l(i+1)}, m_{v(i+1)}, x_{l(i+1)}, x_{vb(i+1)}, T_{vb(i+1)} \) and
   \( T_{int(i+1)} \);
10) Calculate the liquid flow enthalpy at the (i+1) node. From this enthalpy, determine
    the liquid temperature, \( T_{l(i+1)} \).
11) Calculate the coolant temperature.
12) Let \( i = i+1 \) and return to step (1)
There are two assumptions implied in the previous algorithm. The first assumption is that variations in temperature and concentration in the liquid and vapor flow are not significant. Instead, the average driving force for heat and mass transfer, the average temperature and concentration differences in each control volume are represented by their corresponding differences at point i. The second assumption is that all the flow parameters at point i are known. In practical situations, these two assumptions are not always valid.

If the mixing distance is quite large, the temperature and concentration in each flow may change significantly from the inlet to the outlet of a control volume. Therefore, temperature and concentration difference may also change quite significantly. If the length of the control volume is still chosen to be the mixing distance, significant error may be introduced in this first order calculation. A smaller length for the control volume is needed to decrease the truncation error. In such cases, there may be several control volumes between two mixing points. The correlations in Chapter 4, however, are developed for the average value between the each mixing point. It is necessary to develop a simple way to obtain the value of a parameter at any location between point i and i+1, as shown in Figure 36. For any variable, since its integral value between i and i+1 is the difference between the integral from j to i+1 and the integral from j to i, the average value between i and i+1 can be expressed by:
\[ \tilde{f}_{i \rightarrow i+1}(z) = \frac{1}{z_{i+1} - z_i} \int_{z_i}^{z_{i+1}} f(z)dz \]

\[ = \frac{1}{z_{i+1} - z_i} \left( \int_{0}^{z_{i+1}} f(z)dz - \int_{0}^{z_i} f(z)dz \right) \]

\[ = \frac{1}{z_{i+1} - z_i} \left( z_{i+1} \tilde{f}_{0 \rightarrow z_{i+1}}(z) - z_i \tilde{f}_{0 \rightarrow z_i}(z) \right) \]

\[ \text{(73)} \]

**Figure 36 Multi Control Volume between Mixing Points**

where \( \tilde{f}_{i \rightarrow i+1}(x) \) is the average value for the mass absorption flux. Wall or interface temperature between \( i \) and \( i+1 \). \( \tilde{f}_{0 \rightarrow z_i}(z) \) and \( \tilde{f}_{0 \rightarrow z_{i+1}}(z) \) can be calculated directly from the Equations (52) to (54) in Chapter 4. In Equation (73), it is assumed that the heat flux through the wall is uniform from mixing point \( k \) to \( k+1 \). Later in this Chapter, it is shown that this assumption is appropriate.

In a counter-flow absorber, the inlet conditions of the liquid and the vapor are completely known, but the outlet conditions for these two flows are not. Only the flow rate for the outlet flows are known. Since the entire inlet vapor is absorbed in GAX-SCA, the outlet liquid flow rate is equal to the sum of the inlet liquid and vapor flow rate, and outlet

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vapor flow rate is zero. Since in an actual situation, the liquid and vapor flows are not in the equilibrium state, the outlet flow temperatures and the concentrations from the cycle modeling cannot be directly applied to the component design. As a result, the flow conditions at each end of the absorber are not completely known. If the calculation proceeded from the top to the bottom of the absorber, one must assume the outlet temperature and concentration for the vapor flow and check whether the resulted vapor inlet conditions match the conditions from cycle modeling. Generally, an iteration scheme is needed to obtain the correct vapor outlet conditions. For a counter-flow absorber, the following scheme, in which iterations alternatively march along the liquid and vapor flow, is proven to be an effective and stable iteration scheme:

1) Assume reasonable flow conditions for the vapor flow at each node;

2) March in the liquid flow direction, and calculate the liquid flow conditions by using the vapor flow conditions obtained in the last step;

3) March in the vapor flow direction, and recalculate the vapor flow conditions by using the liquid flow conditions assumed in step (2);

4) Compare the vapor flow conditions obtained in step (3) with those in previous step. If the differences are small, the iteration is converged. Otherwise go to step (3) and begin another iteration.
5.3 Design of a Falling-Film Type "W" fin Absorber

Figure 38 is a detailed drawing of a "W" fin absorber. The "W" fin is sandwiched between two thin sheets of carbon steel. Absorption occurs in the channel with "W" fin between these two separated sheets, which are attached to the outside of the separator sheets by offset strip fins. A steel sheet on the outside of the offset strip fin will provide a channel for the coolant to flow. In the mechanical design, the GAX absorber/desorber and the solution cooled absorber are combined together. The combined component is called GAX-SCA. In a GAX-SCA, the inlet coolant flow is the high concentration solution out of the solution pump. This solution will be boiled by the heat rejected from the absorption side and desorption occurs in the offset strip fin channel. Figure 37 shows a detailed drawing of the "W" fin.

By using this special type of fin, liquid can be collected in the pockets formed by the fins and the side walls and then be redistributed through each plate as it flows from the top to the bottom. In this collection and redistribution process, the liquid becomes very well mixed. As the result, the heat and mass transfer on the absorption side are significantly enhanced. Meanwhile, the vapor flow through the large vapor passes impinges against the liquid film. This jet flow significantly enhances the interaction between the liquid and vapor flow. This brings the liquid and vapor flows closer to thermodynamic equilibrium. All these features will substantially enhance the absorption. Hence, the size of the absorber is decreased.
As the first phase of the "W" fin absorber design, it is assumed that the GAX_SCA comprises three columns, each column is six inches wide. There are liquid passes and vapor passes on each side of the "W" fin. The diameter of the liquid passes is 3/32 inch and of the vapor passes is one half inch. The distance between liquid passes is 0.24 inch and that for the vapor passes is 0.65 inch. The mixing distance, L, is one half inch. The angle between the side wall and the fin is 30°. The gap between the separator sheets is 0.7 inch. The geometry of the offset strip fin used on the desorption side is specified in Table 4; and the target flow conditions for the GAX-SCA from the cycle modeling are summarized in Table 5.
Figure 38 Detailed drawing of “W” Fin absorber
<table>
<thead>
<tr>
<th>Fin Pitch</th>
<th>Fin Length</th>
<th>Fin Height</th>
<th>Fin Thickness</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.125&quot;</td>
<td>0.25&quot;</td>
<td>0.1&quot;</td>
<td>0.008&quot;</td>
</tr>
</tbody>
</table>

*Table 4 Geometry of the Offset Strip Fins in the GAX-SCA*

<table>
<thead>
<tr>
<th></th>
<th>Mass Flow Rate (lbm/min)</th>
<th>Temperature (°F)</th>
<th>Concentration</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>ABS 74.8 psi</strong></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Liquid Inlet</td>
<td>2.663</td>
<td>251.0</td>
<td>0.082</td>
</tr>
<tr>
<td>Outlet</td>
<td>3.545</td>
<td>167.21</td>
<td>0.311</td>
</tr>
<tr>
<td>Vapor Inlet</td>
<td>0.927</td>
<td>78.6</td>
<td>0.998</td>
</tr>
<tr>
<td>Outlet</td>
<td>0</td>
<td>N/A</td>
<td>N/A</td>
</tr>
<tr>
<td><strong>DES 274.2 psi</strong></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Liquid Inlet</td>
<td>3.86</td>
<td>125.65</td>
<td>0.484</td>
</tr>
<tr>
<td>Outlet</td>
<td>3.17</td>
<td>236.9</td>
<td>0.384</td>
</tr>
<tr>
<td>Vapor Inlet</td>
<td>0</td>
<td>125.65</td>
<td>N/A</td>
</tr>
<tr>
<td>Outlet</td>
<td>0.69</td>
<td>236.9</td>
<td>0.94</td>
</tr>
</tbody>
</table>

*Table 5 Targeted Flow Conditions in GAX-SCA*

In order to check the flooding condition in the absorber, air and water flows were run inside a Plexiglas vessel to simulate the actual flows inside the “W” fin absorber. In the test, the Wallis numbers of the water and air were set to be the same as the Wallis number of the liquid flow and vapor flow in the absorber. The flow visualization by Wilms et al. [1997] confirmed that flooding would not occur in this absorber.
5.3.1 Design Model for "W" Fin Absorber

In addition to the assumptions made in Chapter 3 for the film flow, the following assumptions are made in the "W" fin absorber design:

1. The liquid solution is well mixed when it is redistributed through a "W" fin;

2. On the absorption side, the heat and mass transfer through the fins are neglected. All heat and mass transfer occur at the side walls;

3. The liquid and vapor flows on the desorption side are in thermodynamic equilibrium;

4. All side walls are uniformly wetted;

The heat transfer coefficient on the desorption side is calculated from Chen’s correlation for boiling [1963].

\[ h_{2p} = h_{NB} + h_t F \] (74)

\[ h_{NB} = S (0.00122) \left( \frac{k^{0.79} c_p^{0.45} \rho_f^{0.49}}{\sigma^{0.5} \mu_f^{0.29} h_f^{0.24} \rho_f^{0.24}} \right) (T_w - T_{sat})^{0.24} (\rho(T_w) - \rho(T_{sat}))^{0.75} \] (75)

where

\[ S = \frac{1}{1 + 2.53 \times 10^{-6} (Re_t F^{1.25})^{0.17}} \]

\[ F = 1 \quad \text{for} \quad X_a > 10 \]

\[ F = 2.35((0.213 + 1/X_a)^{0.736} X_a < 10 \]
The original heat transfer correlation was developed for internal pipe flows. In order to apply this correlation to the boiling flow through an offset strip fin, it is assumed that the geometry of the flow channel does not significantly affect the nucleus boiling heat transfer. The convection term can be estimated from the single phase offset strip fin heat transfer correlation by Manglik and Bergles [1990]:

\[
\frac{1}{X_n} = \left( \frac{y}{1-y} \right)^{0.9} \left( \frac{\rho_f}{\rho_g} \right)^{0.5} \left( \frac{\mu_s}{\mu_f} \right)^{0.1}
\]

where the hydraulic diameter is defined by:

\[
D_h = \frac{4sbL_p}{2(sL_p + sL_p + tb) + ts}
\]

It is difficult to estimate the heat and mass transfer coefficients for vapor flow on the absorption side. Impinging jet heat and mass transfer correlations by Martin [1977] were directly applied to estimate the heat and mass transfer coefficient on the vapor side.

\[
\frac{\bar{Sh}_t}{Sc^{0.42}} = \frac{\bar{Nu}}{Pr^{0.42}} = \frac{D}{r} \frac{I - 1.1D/r}{I + 0.1(H/D - 6)D/r} Q(Re)
\]

where

\[
Q(Re) = 2Re^{0.5} \left( 1 + \frac{Re^{0.55}}{200} \right)^{0.5}
\]
In this correlation, the characteristic length in \(Nu\), \(Sh\), and \(Re\) is chosen to be the hydraulic diameter of the nozzles. In our case, this is the diameter of the vapor pass. The vertical distance \(H\) between the nozzle exit and surface and the lateral distance \(r\) from the stagnation point are involved in the problem. Equation (77) is developed for a single round nozzle. If the relative plate distance-to-nozzle \(H/D\) remains below \(0.6/\sqrt{f}\), this correlation is still valid for arrays of round nozzles. The relative nozzle area, \(f\), is the ratio of total nozzle area to the base area. Martin [1977] also claimed that Equation (77) is valid for any angle between the jet axis and surface.

5.3.2 Simulation Results for the “W” Fin Absorber

When a liquid solution flows along the wall through a number of cells formed by a pair of perforated plates and the side walls, subcooling of the inlet liquid solution at each cell will fluctuate along the flow direction and eventually approach a constant value, if the heat flux through the wall is fixed. If the subcooling of the solution at the outlet of cell \(i\) is higher than this constant value, then at cell \(i+1\), more vapor will be absorbed into the film, and the amount of absorption heat correspondingly increases. Since the amount of heat rejected to the coolant still remains the same, subcooling of the outlet solution will decrease. The opposite scenario will occur if subcooling of the solution at the outlet of
cell i is lower than the constant value. Therefore, regardless of the inlet conditions at the inlet of an absorber, subcooling of the inlet solution will vary through the first several cells near the entrance. As a result, the values of mass absorption rate, wall temperature, interface concentration and other parameters averaged over each cell near the entrance will fluctuate.

(Figure 39 Temperature Profiles of Solution Flows)
Figure 39 shows the temperature profiles of the solution flows. Across the flow direction, the highest temperature of the solutions is the liquid saturated temperature. The liquid saturated temperature is slightly higher than the interface temperature because the concentration of the bulk flow is lower than that at the interface. The other temperatures below them are the interface, the bulk liquid, the wall, the coolant flow, and the vapor flow temperature, respectively. At about \( z = 1 \), the strong solution on the desorption side becomes saturated and starts boiling. The heat transfer coefficient of the strong solution flow has a rapid increase. Thus, the wall temperature curve has a rapid change at the corresponding location.

The concentrations of the solution flows are shown in Figure 40. The vapor concentration profile indicates that the vapor concentration does not change substantially in the entire absorption process. The interface vapor concentration, however, changes quite significantly. The maximum concentration difference between the bulk vapor flow and the interface vapor is about 0.4. The concentration difference between the bulk liquid flow and the liquid interface is only about 0.005. Thus, the driving potential for mass transfer on the vapor side is much larger than the liquid side. Therefore, even though the mass transfer coefficient on the vapor side is much smaller than the one on the liquid side, the diffusion effect in the vapor flow still cannot be neglected. This effect can be measured by the value of the absorption flux composition, \( \phi \).
From the inlet of the vapor flow, the value of $\phi$ increases along the vapor flow direction because of the decrease of the total mass absorption flux. As the total flux decreases, the diffusion effect on the vapor side becomes more important. Thus, the composition of absorption flux, $\phi$, increases. At the middle of absorber, the value of $\phi$ becomes greater than 1.0. This means water is absorbed from the liquid to the vapor flow. In this figure, the value of $\phi$ has two rapid changes in the entire process. The first rapid change near $z = 1$ is because of the abruptly change of total mass absorption flux (as shown in Figure 41). The second inflection occurs at about $z = 0.7$, where the vapor flow transits from turbulence to laminar flow.
The total absorption flux through the interface and the diffusion ammonia flux in the vapor flow are shown in Figure 41. The ratio of the diffusion ammonia flux to the total ammonia flux ranges from about 0.2 to 0.01. The ratio of the total amount of ammonia diffused to the interface to the total ammonia absorbed in the absorber is about 2%. The total absorption rate shown on Figure 41 are the values averaged over the films between “W” fins. Figure 42 shows the details of mass absorption flux between the fins at the entrance. The inlet liquid solution of the GAX-SCA is a severely subcooled solution. As a result, at the entrance, a large amount of vapor is absorbed into the liquid and significant absorption heat is released at the surface. Owing to this significant amount of heat, the mixed solution at the outlet of second “W” fin is much less subcooled. Thus, the absorption flux between on the second and third “W” fins is much smaller, as shown on
Figure 42. Hence, less heat is released on this film and the mixed solution become much more subcooled at the outlet of the third fin.

Based on energy conservation, the dimensional bulk temperature change of the solution between two fins is:

\[ \frac{\int_0^L (q_w(z) - m^e_\ell(z)h_{li})dz}{\dot{m}_{i,\in}c_p} \],

while the change of concentration is

\[ \int_0^L m^e_\ell (c_{\in} - c_{\ell})dz/\dot{m}_{i,\in} \].

If the degree of subcooling is constant, then these two changes should satisfy the thermodynamic relation:

\[ \frac{\int_0^L (q_w(z) - m^e_\ell(z)h_{li})dz}{\dot{m}_{i,\in}c_p\Delta T} = \beta \frac{\int_0^L m^e_\ell (c_{\in} - c_{\ell})dz}{\dot{m}_{i,\in} (c_{\in} - c_{\ell})} \]  \( (78) \)

This equation can be rewritten in the following nondimensional form:
\[ \overline{q}_w = (1 + \beta) \overline{m}_c \]  \hspace{1cm} (79)

The "fluctuation" process at the entrance continues until the condition given by Equation (79) is satisfied. Substituting the expression for the nondimensional mass absorption rate into Equation (79), one can express the degree of subcooling as:

\[ \theta_{\infty} = \frac{\overline{q}_w (1 - \gamma F_2 (\varepsilon \text{ Re}_l \text{ Pr}_l \text{ Le}_l))}{\gamma F_1 (\varepsilon \text{ Re}_l \text{ Pr}_l \text{ Le}_l)} \]  \hspace{1cm} (80)

where \( \gamma = 1 + \beta \). Equation (80) shows that the constant value of subcooling is directly proportional to the heat flux through the wall and decreases with the function \( F_1 \).

Figure 43 shows the subcooling of the liquid solution. The inlet weak solution is severely subcooled in the solution heated desorber (SHD) before it enters the GAX-SCA. At the entrance, because of the severe subcooling, a significant amount of vapor is absorbed into the liquid, and a large amount of heat is released into the film flow. As a result, the subcooling of the liquid solution rapidly decreases. Figure 43 also shows that the subcooling has another rapid decrease at about \( z = l \). This occurs at the point where the coolant flow begins its flow regime transition, and the heat transfer to coolant is abruptly reduced. After this rapid decrease, the subcooling in the liquid begins to increase because of the larger temperature difference between the absorption and desorption sides, as shown in Figure 43.
If there is no mass transfer resistance on the liquid film side, the concentration in the liquid film will be uniform across the film. In that case, the average liquid temperature is still lower than the interface temperature, which is also the saturated temperature of the bulk liquid flow. Therefore, subcooling still exists in the bulk liquid flow. If mass resistance exists in the film flow, the liquid film will be more severely subcooled. Assuming that the temperature distribution across the film is linear, then the bulk temperature of the film can be expressed as:

$$T_{\text{ave}} = \frac{\int_0^1 \rho \omega(\eta) T(\eta) d\eta}{\int_0^1 \rho \omega(\eta) d\eta} = T_w + \frac{5}{8} (T_{i,l} - T_w)$$  

(81)
As mentioned before, if there is no mass transfer resistance in the film flow, the interface temperature, $T_{i,f}$, is equal to the saturated temperature of the bulk flow, $T_{sat}$. Therefore, the subcooling of the liquid solution can be expressed by:

$$T_{sc} = T_{sat} - T_{ave} = \frac{3}{8}(T_{i,f} - T_w) \quad (82)$$

This theoretical value of subcooling is also plotted in Figure 43. Figure 43 shows that the actual degree of subcooling is about twice of this value.

The heat transfer coefficients on the absorption and desorption sides are shown in Figure 44. In Figure 44, the effective surface enhance factor is defined as:

$$E_A = \frac{A_{fin} \eta_{fin} + A_{base}}{A_{base}}$$

Figure 44 shows that the heat transfer is limited by the desorption side before the strong solution begins boiling. When the strong solution starts boiling, the heat transfer resistance in absorption becomes dominant. The inception of boiling causes a rapid decrease in the heat flux through the wall along the liquid flow direction. This results in a larger value of $\theta_{in} / \bar{q}_w$. As discussed in the previous chapter, increasing the ratio of $\theta_{in} / \bar{q}_w$ will decrease the heat transfer coefficient of the film flow. Therefore, there is a rapid change in the heat transfer coefficient of the film flow.
Figure 44 shows the absorption flux due to the subcooling at the inlet and the cooling from the wall. From this figure, it is clear that the total absorption flux is controlled by the subcooling of the solution. The absorption due to the cooling from the wall is very small. The actual effect of the cooling is to maintain the subcooling of the solution after each mixing. Therefore, whether the heat flux though the wall is uniform or not is not an important issue. What is important is the total heat rejected from the liquid film. Therefore, the uniform heat flux assumption in the mathematical model developed in Chapter 3 is valid.
5.3.3 Optimal Trends for Geometric Parameters

In order to develop an effective compact "W" fin absorber, the optimal trends in the key geometric parameters need to be identified. Furthermore, in order to employ appropriate heat and mass transfer enhancing techniques to further decrease the size of the absorber, the effects of enhancing heat and mass transfers in the liquid and vapor flows must be analyzed.

As discussed in the previous chapter, the mass transfer coefficient of the film flow increases with the film thickness. For a short developing length, heat transfer coefficient
can either increase or decrease with the film thickness. Therefore, a thinner film is not
necessary better for absorption. In order to investigate the effect of film thickness on the

![Diagram](image)

**Figure 46 Effect of the Width of the Absorption Column**

size of the absorber, the width of each column is adjusted to vary the wetted perimeter of
the film and film thickness. Figure 46 shows the effect of this modification on the height
and the total heat transfer area of the absorber. Changing the width of the absorber will
also affect the heat transfer coefficient on the desorption side, h_coolant. The change of
the heat transfer coefficient on the desorption side may disguise the actual effect of the
film thickness. Therefore, in this investigation, two sets of calculations are performed. In
the first set of calculations, only the effect of film thickness is studied. In order to exclude
the effect of \( h_{\text{coolant}} \), the heat transfer coefficient \( h_{\text{coolant}} \) is always calculated as if
the absorber were six inch wide. In the second set of calculations, the actual effect of the
width of the absorber is investigated. In this study, the value of \( h_{\text{coolant}} \) is calculated
based on the actual width of the column. Figure 46 shows that increasing the film
thickness actually will decrease the heat transfer area of the absorber. The heat transfer
area is defined as the product of the height and the width of the absorber.

Another key geometric parameter on the absorption side is the spacing of "W" fins,
which control the mixing distance of the film flow. Figure 47 shows the effect of the
mixing distance on the size of the absorber. A shorter mixing distance will reduce the
subcooling in the film flow and increase the heat and mass transfer coefficients of the
film flow. Therefore, a shorter mixing distance is better. The smallest spacing distance is
limited by the flooding criteria and the space needed for mixing. A reasonable fin spacing
distance is about 0.5 inch.

Other approaches to enhance absorption are to promote eddies in the vapor flow and
waves in the film by increasing the vapor-liquid interaction or using a corrugated heat
transfer surface. In order to investigate the effects of these techniques on the absorption
process, it is assumed that these techniques enhance the absorption by increasing the
effective transport properties of the flow. It is assumed that, by promoting eddies in the
vapor flow, the viscosity, the conductivity and the diffusivity of the vapor are increased proportionally. On the film side, waves at the interface can enhance the normal velocity in the liquid flow, thus enhancing the convection in this direction. In this work, the effects of waves are modeled as an increase in the diffusivity and the conductivity of the liquid. Figure 48 shows the effects of these enhancing techniques. It is clear that both enhancing techniques substantially decrease the size of the absorber. For this particular case, for the same degree of enhancements in the transport properties, the enhancement in the liquid flow has more effect than the vapor flow.
Effect of Enhancing Heat and Mass Transfer on Liquid and Vapor Flow

Figure 48 Effect of Enhancing Heat and Mass Transfer of Liquid and Vapor Flow on the Size of the Absorber

Wasden and Dukler [1990] claimed that the occurrence of waves on a short film could double the mass transfer coefficient. According to Figure 48, if the conductivity and diffusivity are doubled, the size of the absorber will decrease about 15%. Although the effect of enhancing the heat and mass transfers in the vapor flow is less significant than the liquid flow, its effect is still substantial. Enhancing the mass transfer in the vapor flow will increase the composition of the absorption flux, $\phi$. As a result, more ammonia is absorbed at the bottom of the absorber, and more water is absorbed at the top of the absorber. Thus, the temperature difference between the absorption and desorption sides increases at the top of the absorber. Hence, the size of the absorber decreases.
5.3.4 Proposed "W" Fin Absorber

From the optimal trends found in the previous analyses, the geometries of an effective "W" fin absorber can be identified for a 5RT ammonia-water absorption chiller. From Figure 46, it is clear that decreasing the width of the column can reduce the heat transfer area required for the absorber. Because of the size constraint in commercial transportation, each component in the residential absorption chiller must be smaller than four feet. Deducting the space needed for the header and the collector at the ends of the absorber, the actual available height for absorption is about 42 inches. Figure 46 shows that, with three columns, a three inch-wide absorber will meet this constraint. In order to decrease manufacturing costs and to prevent potential distribution problems, fewer absorption columns is preferred. Considering other constraints in assembly and brazing processes, two 4.5 inches wide columns were selected for the absorber. In short, the proposed "W" fin absorber comprises two columns. In each column, the effective absorption channel is 42 inches tall, 4.5 inches wide and 1 inch deep. The fin spacing, L, is one half inch. Other geometries remain the same as the absorber described at the beginning of the last section. The safety factor for this absorber is 1.15. The sensitivity of the heat load Q on the size of the absorber is showed in Figure 49. According to this figure, if the absorber is 20% undersized or 20% oversized, the heat load will only change about 5%.
5.4 Comparison of Design Models

In this section, results from two other widely used engineering design models were introduced for comparison purposes. The first model is the equilibrium model. In this model, both the liquid and vapor flows are assumed to be well-mixed and in thermodynamic equilibrium state. Thus, the mass transfer problem can be completely neglected. This model is not capable of considering the effects of the subcooling of the liquid solution. Thus, in this model, it is assumed that an adiabatic absorption process occurs very rapidly at the liquid entrance. Through this adiabatic process, the subcooled inlet liquid and the outlet vapor approach the equilibrium state immediately. At the bottom of the absorber, the vapor exiting the precooler bubbles through the liquid
solution pool in the collector. It is assumed that, through this bubbling process, the vapor is in equilibrium with the liquid solution exiting from the SCA.

In a counter-flow absorber, the velocity of the vapor flow is limited by the flooding conditions. Thus, the mass transfer resistance on the vapor side exists. If the liquid film is well mixed, this mass transfer resistance will limit the absorption process. This situation is considered by Kang and Christensen [1993]. In their model, it was assumed that the bulk liquid flow is well-mixed and saturated. The Colburn-Drew equation was applied to determine the composition of the absorption flux. As for the equilibrium model, it is assumed the subcooled inlet liquid and the outlet vapor approach the equilibrium state immediately at the liquid entrance. Unlike the equilibrium model, the inlet vapor flow in this model is not in equilibrium with the exiting liquid solution.

The sizes of the absorber predicted from the equilibrium model, Kang’s model and the current model are different from each other. In order to compare the temperature and concentration distributions inside the absorber, temperatures and concentrations are plotted in a nondimensional coordinate, $z/H_a$, where $H_a$ is the height of the absorber predicted by each model.
Since only the current model considered the subcooling in the liquid flow, the bulk film temperature predicted from the current model is smaller than that from the other two models. Therefore, the temperature difference between the film flow and the coolant flow predicted from the current model is the smallest among the three models. Thus, the size of the absorber predicted from current model is the largest.

Figure 51 shows the values of $\phi$ from the models. All three models predict that the composition of the absorption flux is larger than 1.0 at the lower portion of the absorber and smaller than unity at the upper portion of the absorber. This means that water is
absorbed from the liquid to the vapor at the bottom of the absorber and is condensed back to the liquid flow at the upper portion of the absorber.

Figure 51 Absorption Flux Composition Profiles

Table 6 Comparison of Results from Three Models

<table>
<thead>
<tr>
<th></th>
<th>Current Model</th>
<th>Equilibrium Model</th>
<th>Kang and Christensen's Model</th>
</tr>
</thead>
<tbody>
<tr>
<td>Height (Ft)</td>
<td>3.21</td>
<td>1.84</td>
<td>2.16</td>
</tr>
<tr>
<td>Average $\Delta T$ ($^\circ$F)</td>
<td>15.6</td>
<td>23.2</td>
<td>19.3</td>
</tr>
<tr>
<td>Pinch $\Delta T$ ($^\circ$F)</td>
<td>4.7</td>
<td>12.1</td>
<td>9.2</td>
</tr>
</tbody>
</table>

Table 6 lists the sizes of the absorber, the average and minimum temperature differences between the absorption and the desorption sides predicted from these three models. As
discussed before, the size of the absorber predicted from the current model is much larger than the other two models. In other words, the other two models severely overpredict the temperature difference between the absorption and desorption sides and, thus, underpredict the size of the absorber.
6.1 Conclusions

The objective of this work was to develop a computer design model for falling-film absorbers. In order to determine the heat and mass transfer coefficients for the absorption process, a mathematical model for simultaneous heat and mass transfer in the falling film absorption problem was first developed. The governing equations and their boundary conditions were then nondimensionalized to identify key parameters controlling the absorption process. In general, the heat and mass transfer problems in the liquid and vapor flows must be solved simultaneously. An order of magnitude analysis showed that in a typical GAX absorber, the ratio of the diffusion flux in the vapor flow to the diffusion flux in the liquid flow was less than 5%. Therefore, the contribution from the vapor diffusion effect was neglected. This simplification implied that the concentration of the absorption flux is the same as the concentration of the vapor flow. In addition to other boundary conditions for the liquid flow, the knowledge of the concentration of the absorption flux was sufficient to solve the heat and mass transfer problems in the liquid
flow. Thus the mass transfer problem in the vapor flow can be ignored in this investigation.

The nondimensionalized equations, along with their boundary conditions, showed that the parameters $eRePr$ and $Le$ determine the absorption process. Numerical work was carried out to obtain the solutions for a wide range of $eRePr$ and $Le$. The effects of $eRePr$ and $eReSc$ on the mass absorption flux, species boundary layer thickness and other important parameters were analyzed. In order to apply these numerical results to a computer design model, they were correlated with respect to $eRePr$ and $Le$. Empirical correlations for the absorption flux, the wall and the interface temperatures were achieved. Heat and mass transfer correlations were obtained from these empirical correlations. The trends of these correlations in subcooling and the mixing distance were identified. The resulting heat transfer was compared with Nusselt's prediction and the mass transfer coefficient was compared with Pigford's correlation.

A computer design model was developed using these empirical correlations. This model was applied to the design of a "W" fin absorber. The size of the absorber was determined, and the absorption process in the entire absorber was analyzed. Geometric parameters for this "W" absorber were parametrically varied, and optimal trends in the related key parameters were identified. An effective "W" fin absorber was then found for a 5 RT ammonia-water absorption chiller.
Major contributions and design considerations which were learned from this research are summarized below.

**Contributions:**

1. It has been demonstrate that the overall absorption process can be decomposed to two basic processes: absorption due to the subcooling and absorption due to the cooling effect of the wall. These two processes can be directly superimposed. In the case of subcooled inlet solution, the mass absorption rate decreases rapidly along the liquid flow direction. In the other case, the mass absorption rate increases asymptotically along the liquid flow direction. For short mixing distances, the absorption rate is controlled by the subcooling at the inlet.

2. Empirical correlations for the absorption rate, the wall temperature and the interface temperature were achieved for $eRePr$ ranging from 0.5 to 50, and $eReSc$ from 5 to 3000.

3. Empirical heat and mass transfer correlations for thin film flows in the absorption process have been obtained. These correlations include the entrance and subcooling effects. The correlations indicate that the average heat and mass transfer coefficients in the absorption process are affected by the subcooling of the solution as well as the film thickness and the fluid properties. If the inlet solution is saturated, the heat transfer coefficient for binary mixtures is larger than that for single component fluid, and the mass transfer coefficient for the exothermal processes is larger than that for isothermal processes.
4. A general falling-film absorber design model using the empirical correlations was developed. The effects of the mass transfer resistances in both liquid and vapor flows were considered in this model.

5. Optimal trends in the geometric parameters for a "W" absorber were identified. The geometry of an effective "W" fin absorber for a 5 RT absorption chiller was introduced.

6. The vapor diffusion effect on the absorption process was analyzed. An order of magnitude analysis showed that in a typical GAX absorber, the ratio of diffusion flux in the vapor flow to the diffusion flux in the liquid flow is less than 5%. Nevertheless, the parametric analysis in the present work clearly showed that the diffusion effect in the vapor flow can significantly affect the size of the absorber; and therefore, it is cannot be neglected in the component design.

Design Considerations:

1. In the GAX cycle modeling, the subcooling at the outlet of SCA should be considered. The degree of subcooling is approximately 10 °F.

2. The average temperature difference between the liquid solution on the absorption side and that on the desorption side is about one half of the LMTD value predicted from the inlet and outlet conditions.

3. In an ammonia-water GAX-SCA absorber, decreasing the wetted perimeter and the mixing distance can decrease the heat transfer area of the absorber.
4. Enhancing the diffusion effect in the vapor flow can be as important as doing so in the liquid flow.

The empirical correlations achieved in this work can be directly applied to the development of a computer design model for the GAX-SCA absorber. The resulting computer model can be used to predict the size of the absorber, to investigate the sensitivity of the absorber performance to the key variables, and to provide insights to design more compact and cost-effective absorbers. The focus of this work has been on the ammonia-water absorption process in a falling-film on a flat wall. The analyses and results can be extended to other processes in an ammonia-water system, such as rectification and condensation processes or the absorption process in a water-lithium bromide system.

6.2 Future Work

This work is the first stage in the development of a general design model for a falling-film type absorber. In the mathematical model developed here, effects of waves and ripples on the film flow were neglected. However, as reported in open literature, these effects can enhance the absorption significantly. Therefore, in order to describe the absorption process more accurately, it is necessary to develop a more sophisticated model to take these effects into account.
In developing the empirical correlations, the diffusion effect in the vapor flow was neglected. The design results for a "W" fin absorber, however, show that this effect cannot be neglected. It will be more accurate to consider the heat and mass transfer in the liquid and vapor flows simultaneously.

In order to validate the theoretical model, absorption experiments using a "W" fin absorber should be conducted to quantify the heat transfer and the subcooling. Results for different fin spacing and column width should be obtained to verify the theory and the effects of waves and ripples.
LIST OF REFERENCES


APPENDIX A

FIDAP SOURCE CODES

1. FIDAP Program for Falling Film Flow

TITLE
2-D falling film
FIMESH(2-D, IMAX=3, JMAX=5)
EXPI(LIST)
  1 0 21
EXPJ(LIST)
  1 0 17 0 31
  point
  1  1  1  1  0  0
  2  3  1  1  0.0086  0
  11 1  3  1  0  0.8
  12 3  3  1  0.0086  0.8
  21 1  5  1  0  1.0
  22 3  5  1  0.0086  1.0
  line
  1  2  0.0002  2
  2  12
  12 22  0.005  2
  22 21  0.0002  1
  21 11  0.005  1
  11 1
  surface
  1  22
  ELEM(QUAD, NODE=9, ENTI="liquid1")
  1  22
  ELEM(BOUN, EDGE, FACE, ENTI="wall1")
  1  21
  ELEM(BOUN, EDGE, FACE, ENTI="interface")
  2  22
  ELEM(BOUN, EDGE, FACE, ENTI="linlet1")
  21 22
  ELEM(BOUN, EDGE, FACE, ENTI="loutlet1")
  1  2
end
FIPREP

PROB (2-D, INCO, STEA, LAMI, NONL, NEWT, MOME, ENER, FIXE, SING, SPEC = 1.0)

PRES (MIXE = 0.100000000000E-11, DISC)

EXEC (NEWJ)

SOLU (N.R. = 200, VELC = 0.100000000000E-05, RESC = 0.100000000000E-11,
        ACCF = 0.7, SCHA = 0.100000000000E-02)

OPTI (UPWI)

UPWI (STRE)

  0.00000000000E+00,  0.00000000000E+00,  0.00000000000E+00,
  0.00000000000E+00,  0.00000000000E+00,  0.00000000000E+00,
  0.00000000000E+00,  0.00000000000E+00,  0.00000000000E+00,
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  0.00000000000E+00,  0.00000000000E+00,  0.00000000000E+00,
  0.00000000000E+00,  0.00000000000E+00,  0.00000000000E+00,

ENTI (NAME = "interface", PLOT)
ENTI (NAME = "liquid1", FLUI, MDEN = 1, MVIS = 1, MSPH = 1, MCON = 1)
ENTI (NAME = "linlet1", PLOT)
ENTI (NAME = "loutlet1", PLOT)

ENTI (NAME = "wall1", SURF, DEPT = 11, CONT, MAPP, NORM, X = 1.0,
        Y = 0.0000000000000E+00, Z = 0.0000000000000E+00, ATTA =
        "liquid1")

DENS (SET = 1, CONS = 1.0)

VISC (SET = 1, CONS = 0.202880000000E-04)

SPEC (SET = 1, CONS = 1.0)

COND (SET = 1, CONS = 0.147920000000E-04)

SURF (SET = 1, CONS = 0.5)

DIFF (SET = 1, CONS = 0.778520000000E-06)

BODY (CONS, FX = 0.0000000000000E+00, FY = -0.2743, FZ =
        0.0000000000000E+00)

BCNO (UX, ENTI = "linlet1", CONS = 0.0000000000000E+00)

BCNO (UX, ENTI = "loutlet1", ZERO)

BCNO (VELO, ENTI = "wall1", ZERO)

BCNO (UX, ENTI = "interface", ZERO)

BCNO (UY, ENTI = "linlet1", POLY = 3, SYST = 1, CART)
     0.0000000000000E+00, -0.116200000000E+03, 0.100000000000E+01,
     0.0000000000000E+00, 0.676040000000E+04, 0.200000000000E+01,
     0.0000000000000E+00, 0.0000000000000E+00, 0.0000000000000E+00,
     0.0000000000000E+00, 0.0000000000000E+00, 0.0000000000000E+00,

/ subcooled inlet solution

BCNO (TEMP, ENTI = "linlet1", CONS = -1.0)

BCNO (SPEC = 1.0, ENTI = "linlet1", CONS = 0.0000000000000E+00)
BCNO (COOR, NODE)
0.6510000000E+03, 0.6510000000E+03, 0.2000000000E+01
0.2100000000E+02, 0.2100000000E+02, 0.2000000000E+01
BCNO (TEMP, NODE = 651, FREE)
BCNO (SPEC = 1.0, NODE = 651, FREE)
BCFL (SPEC = 1.0, ENTI = "walll", CONS = 0.000000000000E+00)
BCFL (SPEC = 1.0, ENTI = "interface", FSUB)
BCFL (HEAT, ENTI = "interface", FSUB)
/ Adiabatic Wall
BCFL (HEAT, ENTI = "walll", CONS = 0.000000000000E+00)
ICNO (SPEC = 1.0, CONS = 0.000000000000E+00, ALL)
ICNO (TEMP, CONS = 0.000000000000E+00, ALL)
ICNO (VELO, READ)
BCSY (SET = 2, NORM)
0.1000000000E+01, 0.0000000000E+00, 0.0000000000E+00,
0.0000000000E+00, 0.0000000000E+00, 0.0000000000E+00,
0.0000000000E+00,
0.0000000000E+00
END

2. User Defined Boundary Flux Conditions in FISOLVE

SUBROUTINE USRBCF (VAL, NODE, IDF, TIME, SOL, ID, NDOF, NUMNP, LDOFU,
   1 CONSTR,nodepr,xyz,iflag)
C USER DEFINED FLUX COEFFICIENTS FOR APPLIED FLUX BOUNDARY
C CONDITIONS
C VAL = COMPUTED (SPECIFIED) FLUX COEFFICIENT
C SOL = GLOBAL SOLUTION VECTOR
C ID = GLOBAL ID ARRAY
C NDOF = ACTIVE NUMBER OF DEGREES OF FREEDOM
C NUMNP = NUMBER OF NODAL POINTS
C NODE = NODE NUMBER OF B.C.
C IDF = DEGREE OF FREEDOM FOR NODE
C TIME = TIME
C LDOFU = ACTIVE DEGREE OF FREEDOM ARRAY
C CONSTR = ARRAY OF SPECIFIED NONZERO BOUNDARY CONDITIONS
C XYZ = nodal coordinates
C iflag = flag for user to set (not equal to 0) if coordinates
C are updated
C NODEPR = reverse permutation array
C node(external) = NODEPR(NODE) where NODE = internal node
C
C INCLUDE 'IMPLCT.COM'
INCLUDE 'PARIUS.COM'
DIMENSION SOL(*),ID(NUMNP,NDOF),CONSTR(*),LDOFU(*)
DIMENSION NODEPR(*),xyz(NUMNP,*)
DIMENSION imap(31)
c integer i_inni,itter,i,k,jj

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common/weibo/amass_b(31),amass_e(31),icheck(31)
common/ifirst/i_inni,itter
data imap /39,42,81,84,123,126,165,168,207,210,
$ 249,252,291,294,333,336,375,378,380,382,
$ 422,424,426,428,430,432,434,436,438,440,442/
ZRO = 0.0

write(*,'(a23)')'step1'
if (i_inni.ne.1234) then
itter=0
i_inni=1234
open(unit=11,file='ms.out',status='unknown')
do 10 i=1,31
amass_b(i)=0.0
amass_e(i)=4.e-4
icheck(i)=0
10 continue
end if
relcix=0.95
c1=-72.48*(0.95-0.3)
c2=0.
k=0

20 k=k+1
if (k.gt.31) then
write(*,'(a23)')'could not find NODE,NODE=',NODE
stop
end if
if (imap(k).NE.NODE) goto 20

write(*,'(a23)')'step2'
NADOF=LDOFU(KDT)
IF (NADOF.EQ.0) THEN
write(*,'(a23)')'DEGREE FREEDOM IS NOT ACTIVED_0'
END IF
IEQ=ID(NODE,NADOF)
IF (IEQ.LT.0) THEN
T=CONSTR(-IEQ)
ELSEIF (IEQ.EQ.0) THEN
T=0
ELSE
T=SOL(IEQ)
ENDIF
NADOF=LDOFU(KDS+1)
IF (NADOF.EQ.0) THEN
write(*,'(a23)')'DEGREE FREEDOM IS NOT ACTIVED_1'
END IF
IEQ=ID(NODE,NADOF)
IF (IEQ.LT.0) THEN
omega_s=CONSTR(-IEQ)
ELSEIF (IEQ.EQ.0) THEN
omega_s=0
ELSE
omega_s=SOL(IEQ)
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ENDIF

c write(*,*)'step3'
if ((omega_s.lt.0).or.(omega_s.gt.1.0))
$ write(*,*) 'omega wrong'
Tc=cl*omega_s+c2

c the flux at each point has been updated once
if (Mod(itter,31).eq.0) then
  do 22 jj=1,31
    icheck(jj)=0
  continue
22 end if
val=0.0
if (itter.le.1240) relax=0.997
if (IDF.EQ.(KDS+1)) then
  if (icheck(k).eq.0) then
    icheck(k)=1
    itter=itter+1
  if (T.gt.Tc) then
    amass_e(k)=amass_b(k)+relax*(amass_e(k)-amass_b(k))
  else
    amass_b(k)=amass_e(k)-relax*(amass_e(k)-amass_b(k))
  endif
  if (((k.eq.5).or.(k.eq.6).or.(k.eq.7))
$ write(11,'(I3,4F12.7)')k,T,Tc,amass_e(k),amass_b(k)
  if ((k.eq.5).or.(k.eq.6).or.(k.eq.7))
$ write(*,*)'not conv.'
  end if
  val=0.5*(amass_e(k)+amass_b(k))
end if
if (IDF.EQ.(KDS+2)) then
  val=0.5*(amass_e(k)+amass_b(k))*(1.-omega_s)
c end if
if (IDF.EQ.(KDT)) then
  val=0.5*(amass_e(k)+amass_b(k))*108.75
  if (k.eq.2) write(*,*)'T accessed',amass_e(2),amass_b(2)
end if
if ((IDF.NE.KDT).and.(IDF.NE.(KDS+1)))
$ write(*,*) 'IDF is wrong, IDF=','IDF

  ZRO = 0.0
  CALL ERMSGS (8902, 0, 3,
  1 0,0,0,0,0,ZRO,ZRO,ZRO,' ',' ',' ')
30 RETURN

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3. User Defined Scalar Function In FIDAP

SUBROUTINE USRFN (FUNC, XYZ, UF, T, TRB, SPEC, NSPEC, P, DENS,
  NUMNP, NELEM, NDFCD, NDFVL, IPR, TIME,
  nxyz, mtpar, conmt, mtprp, nlpar, prop,
  mxmpar, mxmcon, mxmlab, mxepar,
  ia, WK, MFIRST, MTOT, IERR)

C
C USER SUPPLIED SUBROUTINE TO CALCULATE FUNCTION FOR USE WITH
C COMMANDS - CONT, LINE, HIST --
C FUNCTION VALUES MUST BE COMPUTED AT ALL NODES
C
C INCLUDE 'IMPLCT.COM'
INCLUDE 'TAPES.COM'
C INCLUDE 'NUMBRS.COM'
DIMENSION FUNC(NUMNP), prop(*), WK(*), ia(*), dens(numnp)
DIMENSION TRB(NUMNP,*), P(NUMNP), UF(NDFVL,NUMNP), T(NUMNP)
DIMENSION SPEC(NUMNP,*), XYZ(NUMNP,ndfcd), nxyz(numnp)
dimension mtpar(mxmpar,*), count(mxmcon,*)
dimension mtprp(mxmlab,*), nlpar(mxepar,*)
DIMENSION Imap(31)
DIMENSION DERIV(NUMNP,ndfcd)
DIMENSION speci(NUMNP)
data imap /I,3,43,45,85,87,127,129,169,171,211,213,253,255,
  295,297,337,339,415,418,476,478,503,505,547,549,551,
  553,555,557,559/

open (unit=12, file='temp_wall.out', status='unknown')
open (unit=13, file='conc_int.out', status='unknown')
open (unit=14, file='mflux.out', status='unknown')
open (unit=15, file='hflux.out', status='unknown')
open (unit=16, file='temp_int.out', status='unknown')
open (unit=17, file='tcross.out', status='unknown')
open (unit=18, file='xcross.out', status='unknown')
sumt=0.0
do 10 i=1, NUMNP
  FUNC(i)=T(i)-(-72.48*(0.95-0.30))*SPEC(i,1)
  continue
10
  sumt=0.
do 20 i=30,1,-1
    jjj=(i-1)*21+1
    jjk=jjj+21
    sumt=sumt+(T(jjj)+T(jjk))/2.*((XYZ(jjk,2)-XYZ(jjj,2))
      &+(1x,4f12.7)'1./(1.-xyz(jjj,2)),sumt/(1.-xyz(jjj,2)),
      & xyz(jjj,2),T(jjj)
  continue
20
write(*,'average T at wall ',sumt
sumt=0.
do 25 i=30,1,-1
  jjj=(i-1)*21+21
  jjk=jjj+21
25

139
sumtl = sumtl + (T(jjj) + T(jjk)) / 2. * (XYZ(jjk, 2) - XYZ(jjj, 2))
write(16, '(1x, 4F12.7)') 1. / (1. - xyz(jjj, 2)), sumtl / (1. - xyz(jjj, 2)), & xyz(jjj, 2), T(jjj)
continue
write(*,*) 'average T at interphase ', sumtl

continue

write(*,*) 'average x at interface ', sumx

continue

write(*,*) 'average absorption flux at interface ', summ

call EXPDVR(IA, SPEC1(1), DERIV, NUMNP, ndfcd, WK, XYZ, NLPAR)

continue

write(*,*) 'average heat flux at interface ', sumh

call EXPDVR(IA, T, 1, DERIV, NUMNP, ndfcd, WK, XYZ, NLPAR)

continue

write(*,*) '(1x, 3F12.7)') xyz(jjj, 2), xyz(jjj, 1), spec(jjj, 1)
write(*,*) '(1x, 3F12.7)') xyz(jjj, 2), xyz(jjj, 1), T(jjj)
jjj = jjj + 1
continue
write(*,*) '(1x, 3F12.7)') xyz(jjj, 2), xyz(jjj, 1), spec(jjj, 1)
write(18,'(lx,3F12.7)')xyz(jjj,2),xyz(jjj,1),T(jjj)

write(17,*)
write(18,*)

55 continue
close(12)
close(13)
close(14)
close(15)
close(16)
close(17)
close(18)

C
C IERR = 1
C CALL ERMSGP (7500,1,2,1,IOUT,BATCH,
C 1 0,0,0,0,ZRO,ZRO,
C 2 'USER FUNCTION (USRFN)',','','')
RETURN
END
APPENDIX B

NUMERICAL RESULTS FOR FUNCTION F1, F2, G1, G2, H1 AND H2
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Table 12 Numerical Value of Function
Relative Errors of Empirical Correlations for Function F1, F2, G1, G2, H1 and H2

Figure 52 Relative Error of Empirical Correlation for F1
Relative Error of Function F2

Figure 53 Relative Error of Empirical Correlation for F2

Relative Error of Function G1

Figure 54 Relative Error of Empirical Correlation for G1
Figure 55 Relative Error of Empirical Correlation for G2

Figure 56 Relative Error of Empirical Correlation for H1
Figure 57 Relative Error of Empirical Correlation for H2